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Topic 1: General and Mathematical Aspects-Posters

Vertex models and foldable origami lattices

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Origami has been finding more and more practical uses in engineering and architecture, and of particular note are regular lattices which can be folded, the Miura-ori origami pattern being the most well known. Using a relationship between origami crease patterns and vertex models, we have related the Miura-ori crease pattern and other regular foldable lattices to vertex models and staggered vertex models on the square and triangular lattices. The free-fermion condition of the vertex models has been employed to determine the unique ground state which corresponds to the wanted origami crease pattern ground state. Folding defects in the lattice correspond to an increase in temperature above the ground state, and with the increase of defects, a critical temperature can be reached beyond which correlations between the crease configurations at different sites decays exponentially with distance in the lattice.

*Poster

Classical and Quantum implications of Non-linear Bath: a Perturbative Approach

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Our work focuses on system-reservoir theory of a generic dissipative system involving non-linear bath modes. At the classical level we study two types of models [1] which extend the standard harmonic bath paradigm: a set of double-wells and a quartic non-linearity. Writing down a suitable Hamiltonian where the system is linearly coupled to the bath, we derive the corresponding Generalised Langevin Equation(GLE). Owing to the non-linearities, the equations need to be solved perturbatively [2] and the initial canonical ensemble for the anharmnic oscillators also acquire a perturbative character. Eventually, we calculate the the first and the second moments of the noise term arising out of the GLEs leading to the Fluctuation-Dissipation Relations (FDR) [3]. The set of double-wells result in a non-zero first moment of noise which is small and bounded (non-equilibrium signature). The quartic non-linearity however, possesses no such bias. More importantly, for both the cases, we show that FDR is modified to 1st order in perturbation theory in higher powers of kBT. Remarkably, the explicit calculation of FDR shows absence of higher harmonics,i.e., any other time-scale other than the lowest harmonic mode. This helps us in redefining the FDR in a form-invariant way and the system-bath coupling acquires a Renormalised form through an explicit dependence on temperature. The Quantum effects of the problem (we take up the quartic case for simplicity) seem more subtle. The non-linearities in the bath modes lead to perturbative expansion of quantum operators [4] via a standard prescription. Only then, the whole programme of canonical averaging can be carried out to achieve the corrected quantum FDR. We observe, that again the higher harmonic modes disappear and corrections in higher powers of hyperbolic cosine emerge and a Renormalised system-reservoir coupling can be defined. We are presently investigating the implications of these quantum corrections on physical observables like the diffusion coefficient, Kramer's rate, etc. References: 1. System-reservoir theory with anharmonic baths: a perturbative approach Chitrak Bhadra,Dhruba Banerjee [accepted for publication in Journal of Statistical Mechanics (IOP) , 2016] 2. Renormalization Group for nonlinear oscillators in the absence of linear restoring force A. Sarkar and J.K. Bhattacharjee Eur. Phys. Lett. 91 60004, 2010 3. The fluctuation-dissipation theorem R.Kubo Rep. Prog. Phys. 29 255, 1966 4. Generalized quantum Fokker-Planck, diffusion, and Smoluchowski equations with true probability distribution functions Suman Kumar Banik, Bidhan Chandra Bag, Deb Shankar Ray Phys. Rev. E 65, 051106, 2002

*Poster

Analytical results for the distribution of shortest path lengths in random networks

Ofer Biham * [1], Eytan Katzav, Reimer Kuhn, Mor Nitzan, Daniel ben-Avraham, Pavel L. Krapivsky and Nathan Ross

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The increasing interest in network research in recent years is motivated by the realization that a large variety of systems and processes which involve interacting objects can be described by network models. In these models, the objects are represented by nodes and the interactions are expressed by edges. The interactions between non-adjacent pairs of nodes are facilitated by paths going through intermediate nodes and edges. The shortest paths between such pairs are of particular importance because they provide the strongest interactions and fastest response. Therefore, the distribution of shortest path lengths is of great relevance to many dynamical processes taking place on networks such as communication, navigation and epidemic spreading. While the average of this distribution has been studied extensively, the analytical calculation of the entire distribution has remained an open problem. In this presentation a novel analytical approach for calculating the distribution of shortest path lengths in random networks will be discussed. This approach is based on the cavity method, and applies to a large family of network types, which includes Erdos-Renyi networks [1], regular graphs and more generally, configuration model networks [2]. The results are found to be in agreement with numerical simulations for a broad range of networks, sizes and connectivities. Being analytical this approach allows shedding light on various phenomena such as an interesting local-global relation between the degree of a specific node and the mean distance of paths originating from it. References: [1] E. Katzav, M. Nitzan, D. ben-Avraham, P. L. Krapivsky, R. Kuhn, N. Ross and O. Biham, Analytical results for the distribution of shortest path lengths in random networks, EPL 111, 26006 (2015). [2] M. Nitzan, E. Katzav, R. Kuhn and O. Biham, Distance distribution in configuration model networks, arXiv:1603.04473.

*Poster

A conjecture on the connection of the second order phase transition and energy fluctuations

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We have analytically explored quantum to classical crossover in energy fluctuations for a number of Bose and Fermi systems, and have given a conjecture that links the existence of a maximum (hump) in the scaled energy fluctuations which exceeds the classical limit to the discontinuity of the specific heat at constant volume [1]. If the specific heat at constant volume can not be directly or precisely measured, then also, it is now possible, from the conjecture, to predict about the occurrence of the second order phase transition of a Bose (or strongly correlated Fermi) system from its energy fluctuation data.

Reference:
[1] S. Biswas, J. Mitra, and S. Bhattacharyya, Energy fluctuation and discontinuity of specific heat, J. Stat. Mech. (2015) P03013

*Poster

MuCa vs WL: A comparison

Elmar Bittner * [1], Wolfhard Janke

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We perform a competitive analysis to study the relative performance of the two best-known generalized-ensemble algorithms: the multi canonical Monte Carlo and the Wang-Landau method. To keep things as simple and clear as possible, we take the exactly solvable two-dimensional Ising model as test case and we show also some results for the three-dimensional Ising model.

*Poster

Noise focusing as a symmetry-breaking phenomenon induced by topological disorder. Understanding nonlinear waves in neuronal cultures.

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Neuronal cultures have been proposed as a model system to understand the physical mechanisms underlying collective behavior in biological neuronal tissues. From the perspective of nonlinear physics, neuronal cultures may be described at the mesoscale as an excitable medium featuring some unusual properties. In a recent paper [Orlandi et al, Nature Physics 9, 582 (2013)] we have shown that the emergence of coherent activity in the form of nearly periodic global pulsation of the neuronal network is due to a new phenomenon that we call noise focusing, which is shown to be generic of networks of excitable elements in metric spaces. The phenomenon consists of a strong localization of the spontaneous noise activity through an amplification of the topological fluctuations associated to the inherent disorder of the network connectivity. As a consequence the pulsation of the system is controlled by excitation waves that appear through an anomalously fast nucleation process. Here we present a continuum stochastic coarse-grained description of a network of excitable elements, that explains the phenomenon of noise focusing as a symmetry-breaking phenomenon induced by disorder, and demonstrates the underlying mechanism that explains the apparent paradox of having (nearly) periodic pulsation and at the same time random selection of the nucleation points of the pulses, in full agreement with experimental evidence and numerical simulation.

*Poster

The critical phases of the Z(5) model

Christophe Chatelain * [1]

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The phase diagram of the Z(5) spin model is studied numerically on the square lattice by means of the Density Matrix Renormalization Group (DMRG). In the regime where the two nearest-neighbor couplings have opposite signs, a critical phase, not observed in earlier Monte Carlo simulations, is identified. The new phase diagram is in agreement with predictions made by M. den Nijs in 1985 but for the Z(7) model rather than the Z(5) one. All critical phases are shown to be compatible with a central charge c=1. The magnetization scaling dimension displays however a different behavior in the different critical phases.

*Poster

Gravitational Riemann Invariants

Philippe Choquard * [1]

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Preambles to the theory of uni-axial meteorological phenomena. One-dimensional, inviscid, compressible, isothermal or isentropic fluids under gravitation. integral representation of Riemann invariants including gravitation. Inverse Jacobian representation of mass densities. Non-linear first order,P.D.E.'s. Exemples of explicit solutions, algebraic and graphical. Comparaison with published results of equivalent nonlinear P.D.E's.

*Poster

A Hierarchical Kinetic Theory of Birth, Death and Fission in Age-Structur ed Interacting Populations

Tom Chou * [1], Chris Greenman

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We study mathematical models describing the evolution of stochastic age-structured populations. After reviewing existing approaches, we develop a complete kinetic framework for age-structured interacting populations undergoing birth, death and fission processes in spatially dependent environments. We define the full probability density for the population-size age chart and find results under specific conditions. Connections with more classical models are also explicitly derived. In particular, we show that factorial moments for non-interacting processes are described by a natural generalization of the McKendrick-von Foerster equation, which describes mean-field deterministic behavior. Our approach utilizes mixed-type, multidimensional probability distributions similar to those employed in the study of gas kinetics and with terms that satisfy BBGKY-like equation hierarchies.

*Poster

Condensation in stochastic continuous mass transport models

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In the last years the phenomenon of condensation have been studied extensively for a series of stochastic particle transport models, such as the zero-range process (ZRP) or processes with pair-factorized steady states (PFSS). Interesting results were produced for these models and it is nowadays known that similar and equally exciting features are revealed for systems in continuous state space. Here we study the dynamics of condensation for a stochastic continuous mass transport process, defined on a one-dimensional lattice. The time evolution of this process is governed by the fraction density, $phi(r)$, which controls the fraction of mass transported at each time-point from each site. The simplest version of this process is the asymmetric random average process (ARAP) [extitJ. Stat. Phys. extbf99 31-55 (2000); extitJ. Stat. Phys. extbf99 943 (2000)], which is defined by an arbitrary state-independent fraction density function, $phi(r) = 1$, with support on the unit interval. Two different variations of state-dependent fraction densities will be presented and the different nature of the corresponding condensates ranging from drifting condensates to explosive condensation will be analyzed. The effects of open boundary conditions and boundary induced drift on condensation phenomena for different variants of the random average process will also be captured. Lastly we use an extreme value approach to investigate phase transition and the occurrence of broken ergodicity in systems truncated mass transfer capability [extitPhys. Rev. Lett. extbf89 090601 (2002)].

*Poster

Understanding the XY model collective behaviours through graph signal analysis

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In various context, high-dimensional data reside on the vertices of networks, so that the network is the "natural space" for such systems. Therefore techniques, as Graph Signal Transform, levering the structure of the network, to grasp the main features of the dynamical process upon it are drawing increasing attention. Graph Signal Transform is, by design, well-suited to treat signals in very irregular domains and it allows applications that span from image compression to uncovering network communities [1]. In a nutshell, this technique is reminiscent of Fourier transform, but at the same time it embeds the inhomogeneities of the underlying graph: the time series on the network nodes, i.e. the graph signal, is decomposed in a sum of components on the Laplacian eigenvectors and this decomposition allows to finger the ones which have an high weight, i.e. that are resonant with the dynamics. In this work, we apply Graph Signal Transform to a classical model for magnetized materials, the XY spin model of which we consider the phenomenology on networks. Remarkably, there is recent evidence that a variety of collective responses can be ignited if a complex network connects the spins [2-3]. In particular, we observe the same collective state on different networks through a fine tuning of the network topological parameters: a magnetized regime, displaying a second order phase transition to a non-magnetized phase and, furthermore, a peculiar oscillating phase has been observed where the order parameter is affected by persistent global oscillations. We thus focus on the Graph Signal Transform to benchmark the time series produced by the model in the three aforementioned macroscopic states at equilibrium[4]. Through this benchmarking phase, we retrieve the 'selected network modes' for each macroscopic state on different topologies and this selection points to the sub-structures of the graph relevant for the dynamics. [1] D. Shuman, S. K. Narang, P. Frossard et al., Signal Processing Magazine, IEEE 30, 83 (2013). [2] S. De Nigris and X. Leoncini, Phys. Rev. E 88, 012131 (2013). [3] S. de Nigris and X. Leoncini, Phys. Rev. E 91, 042809 (2015). [4] S. de Nigris, Paul Expert, R. Lambiotte and T.Takaguchi in preparation.

*Poster

Optimizing exit times to efficiently cool a heated disk

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The problem of choosing an incompressible flow to most efficiently cool a uniformly heated disk held at fixed temperature on the boundary is equivalent to that of selecting the divergence-free drift that minimizes the mean exit time of Brownian particles uniformly distributed over the disk. Asymptotic and numerical methods are employed to investigate the solution of these problems, i.e., the optimally transporting fields.

*Poster

Investigation of finite-size effects in the free energy surfaces of a mean field spin-1 Ising system: A microcanonical formulation using gamma function

Erdem Riza * [1], Orhan Yalcin

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Based on the microcanonical formalism which uses the gamma function [1, 2], we have investigated the size-dependent changes in the free energy surfaces of a spin-1 mean-field Ising system [3] that consist of N particles. We have constructed the contour maps of the free energy surfaces in the phase space of dipolar (M) and quadrupolar (Q) order parameters for various values of N. The general aspects of the mapping for the surfaces strongly depend on the number of magnetic atoms as well as the temperature and the ratio of the exchange energies. In other words, its value at every point of the two-dimensional M-Q phase space for any N may be either real or complex quantity [4] and the number of extremum points (or stable, metastable and unstable states) and their locations in the phase space changes with N for systems smaller than N=100. This result may be useful in the study of phase transitions and critical temperatures of the atomic clusters or nanostructures [5, 6]. However, the differences between the exact free energy values and the approximated ones using the Stirling formula are significant while it is negligible for systems larger than N=10000. [1] D. S. Bertoldi, E. M. Bringa, E. N. Miranda, Eur. J. Phys. 32, 1485 (2011). [2] E. N. Miranda, and D. S. Bertoldi, Eur. J. Phys. 34, 1075 (2013). [3] M. Keskin and Ş. Özgan, Phys. Lett. A 145, 340 (1990). [4] C. M. Newman and L. S. Schulman, J. Stat. Phys. 23, 131 (1980). [5] D. S. Bertoldi, E. M. Bringa, E. N. Miranda, J. Phys.: Condens Matter 24, 226004 (2012) [6] O. Yalçın, R. Erdem, S. Özüm, J. Appl. Phys. 115, 054316 (2014).

*Poster

A universal approach to classical and quantum wave localization in disordered systems

Marcel Filoche * [1], Douglas N. Arnold, Guy David, David Jerison, Svitlana Mayboroda,

[1] Ecole Polytechnique – Switzerland

Localization of Laplacian or bi-Laplacian waves plays a major role in the behavior of numerous physical systems. It can be the result of a complex medium, of the geometry of the vibrating structure, or even due to the presence of disorder. We present here a universal theory of localization applicable to all vibratory systems [1]. The main tool of this theory, the localization landscape, controls the amplitude of the stationary vibrations, and predicts the spatial regions where vibrations will be localized as well as the frequencies above which a delocalization transition occurs. For second order operators such as the Schrödinger operator, this localization landscape is simply the solution of a Dirichlet problem with uniform right-hand side. Moreover, we show that the reciprocal of this landscape plays the role of an effective potential which finely governs the confinement of the quantum states. In this picture, the boundaries of the localization subregions for low energy eigenfunctions correspond to the barriers of this effective potential, and the long range exponential decay characteristic of Anderson localization is explained as the consequence of multiple tunneling in the dense network of barriers created by this effective potential [2]. This effective potential allows us also to derive a remarkably accurate Weyl's formula for the density of states for a large variety of systems, periodic or random, 1D, 2D, or 3D. Finally, we will present ongoing applications of this theory to the understanding of various physical systems. [1] M. Filoche and S. Mayboroda, Proceedings of the National Academy of Sciences of the USA 109, 14761 (2012). [2] D. N. Arnold, G. David, D. Jerison, S. Mayboroda, M. Filoche, Phys. Rev. Lett. 116, 056602 (2016).

*Poster

Derivation of fractional differential equation for modeling mass transport in complex media

Sergei Fomin * [1], Vladimir Chugunov

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Mathematical modeling of mass transport in a complex fractured porous medium is considered. Our main concern is the multi-scale character of the medium, which is constituted by porous domains dissected by the network of fractures. Assuming that porous medium is of fractal geometry and that sizes of pores vary significantly (i.e. have different characteristic scales), the fractional-order differential equations that model the anomalous diffusive mass transport in such type of domains are derived and justified analytically. Analytical solutions of some particular problems of anomalous diffusion in the fractal media of various geometries are obtained. Extending this approach to more complex situation when diffusion is accompanied by advection, solute transport in a fractured porous medium is modeled by the advection–dispersion equation with fractional time derivative. In the case when the conducting fractured porous layer is confined by porous medium of different porosity and accounting for anomalous non-Fickian diffusion in this medium, the adopted approach leads to introduction of an additional fractional time derivative in the equation for mass transport in the conducting layer. The closed-form solutions of the boundary value problems for the obtained equations are obtained.

*Poster

The Winfree model with distributed phase-response curves

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The classical Winfree model describes the dynamical evolution of a heterogeneous ensemble of all-to-all pulse-coupled oscillators. This model aims at explaining the macroscopic synchronization observed in large populations of biological oscillators such as flashing fireflies or spiking neurons. Under certain assumptions, the dynamics of the Winfree model evolves into the so-called Ott-Antonsen manifold in the thermodynamic limit, what eventually allows to describe the dynamics in terms of only two ODEs. In the present contribution we extend the original Winfree model allowing the heterogeneity to be present also in the phase response curves (PRCs) of the oscillators. In spite of the more realistic character of our extended Winfree model, the Ott-Antonsen ansatz can be applied and the influence of different parameters to be investigated analytically.

*Poster

Analytical properties of Quasi-Polynomial systems: stability, permanence and boundedness of trajectories

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In this work we present results concerning analytical properties of a class of general nonlinear systems known as Quasi-Polynomial (QP) systems. We analyze sufficient conditions for the existence of a Lyapunov function, uniformly bounded solutions, permanence of orbits, structure of *omega*-limit sets and a criteria for convergence of the trajectories. We revise results regarding the well known Lotka-Volterra system and generalizations of these results to encompass the class of Quasi-Polynomial systems. We also present a link between evolutionary stable strategies of dynamical games and stability of trajectories in a subclass of QP systems.

*Poster

Nonplanar Ising Model, Graph Theory and the Pfaffian Formula.

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A well known result due to Kasteleyn expresses the partition function of a non planar Ising model as a sum of Pfaffians which number is related to the genus of the oriented surface on which the graph can be embedded. In graph theory, a classical characterization of graph planarity by a property of its cycle space (MacLane, 1937) has been recently extended to nonplanar embeddings on arbitrary surfaces. Here, we show that there is a deep relation between McLane's characterizations and Kasteleyn's results: For instance, in the planar case, it is just what is needed to turn an Ising partition function into a Pfaffian. More generally, we prove here that the Ising partition function on an arbitrary non planar graph can be written as *the real part* of the Pfaffian of a single matrix with coefficients taken in a multicomplex algebra $\mathbb{C}_{\tilde{g}}$, where $\tilde{g}$ is the non-orientable genus, or crosscap number, of the embedding surface. Known representations as sums of Pfaffians can be derived from this result. In contrast to previous geometric derivations, the present approach gives also some hints on why such formulas may appear as optimal.

*Poster

Generalized electrostatics on a lattice - thermodynamics and correlations.

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The Maggs-Rossetto algorithm [1] provides a fast, local method for simulating Coulombic systems on a grid. This is achieved via the introduction of a freely-fluctuating auxiliary field, with dynamics chosen such that the equilibrium distribution gives the required Coulomb physics. We implement this algorithm on a cubic lattice, inspired by the Coulomb phase of spin ice and its characteristic pinch-point scattering pattern [2]. We will present a review of the lattice field theory and consequent thermodynamics associated with the MR algorithm, as well as simulated structure factors in reciprocal space characterising the auxiliary field both in the presence and absence of electric charge. [1] A.C. Maggs and V. Rossetto. extitLocal simulation algorithms for Coulomb interactions. Physical Review Letters 88.19 (2002), p. 196402. [2] T. Fennell et al. extitMagnetic Coulomb Phase in the Spin Ice Ho2Ti2O7. Science 326.5951 (2009), pp. 415–417.

*Poster

Geometric approach to finite size scaling above the upper critical dimension

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[1] Monash University – Australia

Finite size scaling (FSS) is a common method in the field of critical phenomena, which allows the extraction of universal critical exponents. Even though physical systems above the upper critical dimension are described by mean field theory, where all exponent values are known, the theory of FSS in high dimensions is still the subject of considerable debate. Recently, the five dimensional Ising model has been of particular interest, with conflicting views on the correct scaling behavior for free boundary conditions being presented. Moreover, certain aspects of FSS for the percolation model above the upper critical dimensions remain unresolved to date, such as the proliferation of spanning clusters. In this work we investigate FSS above the upper critical dimension, in particular through geometric representations, focussing on both the five dimensional Ising model in the Fortuin-Kasteleyn and loop representations, and the seven dimensional percolation model. Our study utilizes efficient Markov chain Monte Carlo algorithms, including exact sampling methods (coupling from the past), and state of the art (dynamic) graph algorithms.

*Poster

Applications of quantum annealing for data analysis

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[1] Tokyo University of Science – Japan

Quantum annealing is an efficient method to solve such an optimization problem as Traveling salesman problem. Quantum annealing proposed by Kadowaki and Nishimori is based on a basic mechanism of the quantum adiabatic process as follows. To perform the quantum annealing, the time dependent Hamiltonian H(t) is defined in the range of time, 0 ¡ t ¡ T. Here, the initial Hamiltonian H(0) has a trivial ground state, while the final Hamiltonian H(T) corresponds to the target Hamiltonian (or the cost function of the target optimization problem). According to the quantum adiabatic theorem, the state vector initialized to be the ground state of H(0) approaches the ground state of the target Hamiltonian through the adiabatic process. This is the simple outline of the quantum annealing. Recently, we found how to perform the singular value decomposition (SVD) using the quantum annealing. SVD is a general decomposed form of a matrix with respect to the singular values. In some previous studies, the singular values correspond to the scales included in the original matrix. Thus, we can find the important scales shown in the original matrix using the SVD. One of the most important applications of SVD is the principal component analysis which is mathematically the same as SVD form of the data matrix. In the present study, we will show how to perform SVD using quantum annealing for data analysis. To perform SVD by quantum annealing, the target Hamiltonian is assumed as the Gram matrix of the original data matrix. Once we obtain the ground state of the Gram matrix, we can find the first principal component of the original data matrix. The second component can be obtained by the first component and the original data matrix with redefining another proper Gram matrix. This method shows a possible application of quantum annealing for data analysis. For example, using the above method, we will introduce some applications including the image analysis, the experimental data analysis, and so on. Furthermore, we show the present SVD method is an example of quantum speedup by quantum annealing.

*Poster

Scaling functions for vesicle models

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We begin by rigorously analysing the asymptotic behaviour of the generating function of Dyck paths, weighted with respect to their perimeter and area, in the limit of the area generating variable tending towards 1. In particular, we show that there exists a special point in the parameter space, around which the generating function satisfies a simple scaling relation, with the scaling function given by the logarithmic derivative of the Airy function. Mathematically, the Airy function occurs because the phase transition in the model is mirrored by the coalescence of two saddle points in the associated contour integral representation of the involved basic hypergeometric series. This behaviour is also found in other polygon models such as staircase polygons and is conjectured to hold also for unrestricted self-avoiding polygons. The natural question we ask is whether there exist other polygon models where a phase transition originates from the coalescence of more than two saddle points in the associated contour integral representations of the involved basic hypergeometric series. Indeed we find such a model, which we call deformed Dyck paths.

*Poster

Bosonic and Fermionic Constructions of Two-Dimensional Quantum Walks

Yushi Hoshiya * [1], Makoto Katori

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We study two-dimensional quantum walks and, especially in this presentation, we consider them as combinations of two independent one-dimensional quantum walks. Here we construct bosonic and fermionic wave functions of two quantum walkers, and then calculate joint moments of two-component pseudovelocity in the long time limit. Our results show that, although both of the density functions are represented using the product of Konno's limit density functions, there is a large difference between the bosonic and the fermionic constructions.

*Poster

Amplitude Death in a ring of inhomogeneous Stuart-Landau Oscillators

Dong-Uk Hwang * [1], Jung-Wan Ryu, Woo-Sik Son, Jong-Ho Kim

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We study amplitude death phenomena in a ring of inhomogeneous stuart landau oscillators. Oscillators are connected to nearest neighbour through either bidirectional interaction or directed interaction. Amplitude death is a dynamical state where the amplitude of oscillation decays out, and this behaviour can be studied by analyzing Jacobian matrix at origin. Interestingly, the inhonogeneity in eigenvalue spectra disappears when the interaction forming directed ring sturcutre become dominant. To reveal this we perform higher order perturbation correction in two limiting cases. First we get analytic forms of eigenvalus when diagonal inhomogenous diagonal block matrix is dominant. Second we also get analytic form of eigenvalues when ring structure is dominant. By these two cases, we deliver useful insight why the inhomogeneity in eigenvalue spectra disappear in directed ring.

*Poster

Data assimilation for massive autonomous systems based on second-order adjoint method

Shin-ichi Ito * [1], Hiromichi Nagao, Akinori Yamanaka, Yuhki Tsukada, Toshiyuki Koyama, Masayuki Kano, Junya Inoue

[1] Earthquake Research Institute, The University of Tokyo – Japan

Determining the model parameters and initial states of numerical simulation models by using observational data is one of the significant issues in various scientific fields. Data assimilation (DA) is a fundamental computational technique that enables the parameters and initial states to be estimated by integrating the simulation models and data on the basis of Bayesian statistics, and systematically extracting as much information as possible from the given observational/experimental data. One key issue that remains controversial is the implementation of DA in massive simulation models under limited computation time and resources. In this work, we propose an adjoint-based DA method for massive autonomous models that produces optimum estimates and their uncertainties within practical computation time and resource constraints. The uncertainties are given as several diagonal components of an inverse Hessian matrix, which is the covariance matrix of a multivariate normal distribution that approximates the target posterior probability density function in the neighborhood of the optimum. The proposed method using a second-order adjoint method enables us to directly evaluate the diagonal components of the inverse Hessian matrix without computing all of components of the Hessian matrix. The proposed method is validated through estimation tests using synthetic data generated by a massive two-dimensional Kobayashi's phase-field model. We confirm that the proposed method correctly reproduces the parameter and initial state assumed in advance, and successfully evaluates the uncertainty of the parameter. Such information regarding uncertainty is valuable, as it is available for optimizing the design of experiments.

*Poster

Thermodynamics and Inequalities between Means

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Given a finite system and a heat reservoir, which can have one of the two given values of initial temperatures, T_+ and $T_-(< T_+)$, we analyse, in which case the optimal work extraction is higher: when the reservoir is an infinite source at T_+ and the system is a sink at T_-, or, when the reservoir is an infinite sink at T_- and the system is a heat source at T_+? For a reversible process, the inequality between a generalized mean based on the mean value theorem, and arithmetic (geometric) mean of T_+ and T_- decides the relative magnitude of work (efficiency) in the above mentioned two cases. This leads us to consider three regions, in each of which the efficiency at maximum work obeys universal bounds, given only in terms of the ratio of initial temperatures. The conclusions may serve as benchmarks in the design of heat engines, where we can choose the nature of the finite system, so as to tune the extractable work and/or efficiency at maximum work, or for a given system, we may choose between the two scenarios to obtain a higher value of work and efficiency. References: Thermodynamics and inequalities between means, R.S. Johal, arXiv:1601:07035, submitted for publication.

*Poster

Boundary conditions subtleties in plaquette spin models

D. Johnston * [1], M. Mueller, W. Janke

[1] Heriot-Watt University – United Kingdom

We study the use of a product spin transformation in solving various spin models in 3d, 2d and 1d, paying particular attention to the influence of boundary conditions and finite size effects. The transformation may be used to solve plaquette models in 2d and 3d and, amusingly, also provides yet another way of solving the 1d Ising model with periodic boundary conditions.

*Poster

Role of Fourier Modes in Finite-Size Scaling above the Upper Critical Dimension

Ralph Kenna * [1], Emilio Flores-Sola, Bertrand Berche, Martin Weigel

[1] Coventry University – United Kingdom

Renormalization-group theory has stood, for over 40 years, as one of the pillars of modern physics and there should be no remaining doubt regarding its validity. However, finite-size scaling, which derives from it, has long been poorly understood above the upper critical dimension d_c, especially in models with free boundaries. In addition to its fundamental significance for scaling theories, the issue is important at a practical level because finite-size, statistical-physics systems with free boundaries above d_c are experimentally relevant for long-range interactions. Here, we address the roles played by Fourier modes for such systems and show that the current phenomenological picture is not supported for all thermodynamic observables. In particular, the expectation that dangerous irrelevant variables cause Gaussian-fixed-point scaling indices to be replaced by Landau mean-field exponents for all Fourier modes is incorrect. Instead, the Gaussian-fixed-point exponents have a direct physical manifestation for some modes above the upper critical dimension.

*Poster

On a class of Universal Probability Spaces: case of complex fields

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On a class of Universal Probability Spaces: case of complex fields Mahkame Megan Khoshyaran Senior Researcher Economics Traffic Clinic - ETC 34 Avenue des champs Elysées, 75008 Paris, France. Abstract The objective of this paper is to extend the Universal Probability Space (UPS) in [1] to include complex events. The Universal Probability Space consists of Borel sets, elements of which are tensors. It is shown that the UPS has a defined metric and this metric is in fact the probability measure (P). The metric as a probability measure is proven to exist for any tensor event in the space of all tensor fields. In this paper it is shown that for any complex event in the space of all complex tensor fields, a probability measure (P) in the form of a metric exists. To this effect several theorems are introduced and proven, mainly by modifying concepts introduced in [2], [3], [4], [5], to include complex fields. Finally following [6], [7], [8], a case is demonstrated in order to compare probability as a metric for complex events with classical probability. The objective of the case study is to show that metric probability is a more realistic measure than classical probability for complex events. References [1] M.M. Khoshyaran, On a class of universal probability spaces. Advances in Research, Vol. 6, no. 5 (2016), pp. 1-7. [2] A.D. Berenstein, A.V. Zelevinsky, Tensor product multiplicities and convex poly- topes in partition space, Journal of Geometry and Physics 5 (1989),453-472. [3] I.M. Gelfand, A.V. Zelevinsky, Polytopes in the pattern space and canonical basis in irreducible representations of gl3, Funct. Anal and Appl. 2 (1985), 22-31. [4] I.M. Gelfand, A.V. Zelevinsky, Multiplicities and regular bases for gln Group, Theoretical Methods in Physics 19 (1985),72-75. [5] A.D. Berenstein, A.V. Zelevinsky, Involutions on Gelfand-Tsetlin patterns and multiplicities in skew GLn - modules, Doklady Akad. 300 (1988), 1291-1294. [6] J. Weickert, H. Hagen, Visualization and Processing of Tensor Fields, Springer- Verlag, Berlin 2006. [7] I. Hotz, L. Feng, H. Hagen, B. Hamann, K. Joy, Tensor Field Visualization Using a Metric Interpretation, Proceedings of the IEEE Visualization '04 Conference' 1 (2009), 123-130. [8] W. Benger, H-C. Hege, Analyzing curved spacetime with tensor splats, Pro- ceedings of the Tenth Marcel Grossmann Meeting on General Relativity, World Scientific Publishing Co., DC. 2003.

*Poster

Algebraic Test of Material Conservation in Self-Consistent Mean Field Theory of Polymers

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In the standard mean field theory of Gaussian polymer chains, the partition function of a polymer chain is obtained by solving partial differential equations which are essentially modified diffusion equations. Even though this statistical mechanical method is a perfectly accurate theory, the process of numerical solution often has problems in keeping the amount of polymer materials in the system. Recently, for the purpose of tracking material conservation in the self-consistent field theory (SCFT), our research group has developed an algebraic test which uses matrix and bra-ket notation. The test reveals that when Crank-Nicolson method is adopted, finite volume method (FVM) is the only way to conserve material perfectly in the cylindrical and spherical coordinate systems. Alternating direction implicit method combined with FVM cannot conserve material, though it is still a good candidate after considering speed and accuracy simultaneously. We also confirm that the widely used pseudospectral method in the Cartesian coordinate system has the ability to conserve material.

*Poster

Wang-Landau study of first-order and Berezinskii-Kosterlitz-Thouless transitions in classical spin models

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We investigate phase transitions and critical behavior in the two-dimensional Blume-Capel model and the six-state clock model by using the Wang-Landau sampling method including the parallel replica-exchange variant. First, in the Blume-Capel model examined up to the lattice size of 48x48 sites, we construct the first-order transition line with much improved accuracy and resolution, finding out a double-peak structure of specific heat where diverging phase-transition peak and the system-size independent Schottky-like peak appears together. Throughout the phenomenological finite-size-scaling analysis at the tricritical point, we also provide the first Wang-Landau examination on the conjecture of the exact tricritical eigenvalue exponents, $y_t = 9/5$, $y_g = 4/5$, and $y_h = 77/40$. Second, we perform the parallel replica-exchange Wang-Landau calculations on the six-state clock model. We identify the Berezinskii-Kosterlitz-Thouless (BKT) transitions by directly calculating the helicity modulus. The nature of the BKT transitions is further characterized in the map of the Fisher zeros of the partition function. We find that a single leading zero or a discrete impact angle does not exist and the whole line of zeros in the critical area approaches the real axis with the same system-size scaling.

*Poster

Geometrical distance describing the difference between states on phase diagram

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Phase diagram shows a diagram of states which depends on the thermal conditions described by a set of thermodynamic variables on a many-body system. For example, if we chose a set of thermodynamic variables as a thermal condition such as (volume, pressure,...), a state of gas is just defined by them. Thus we can obtain the thermodynamic quantities, namely entropy, internal energy, enthalpy, and so on, at a point of the phase diagram. The important point of the above example is that the state is defined at each point on the phase diagram. Then, the "distance" between states in the phase diagram is meaningless as it is. Clearly, we have to treat a curved manifold describing the difference of states. In the present study, we investigated how to introduce a proper distance between states in the phase diagram from the viewpoint of the differential geometry (Riemann geometry). To achieve this aim, we regard the phase diagram as a manifold, and focus on the distance between states based on Riemann's metric tensor. We defined the metric tensor in order to introduce the Riemann geometry to statistical mechanics similarly to the previous studies on information geometry investigated by Amari et al. Of course, there are some previous studies applying the Riemann geometry to critical phenomena. However, they paid attention to the relation between the scalar curvature and its behaviors on the transition points although we focus on the behaviors of distance between states shown in the phase diagram. As a result, we clarify the distance between states is well expressed by such a geometrical aspects based on the Riemann's metric tensor which is similarly introduced in the previous studies. Furthermore, we apply the present aspects to typical Ising models such as 1D chain and mean-field model whose behaviors are well-known, and clarify the "distance" corresponds to the difference of states. The present results suggest the possibility to study the geometrical structure of statistical physics from the view point of states itself instead of the thermal average.

*Poster

Modelling and analysis of non-stationary observables: the example of wind power production

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*Poster

Entanglement entropy of the $Q \geq 4$ quantum Potts chain

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The entanglement entropy, S, is an indicator of quantum correlations in the ground state of a many body quantum system. At a second-order quantum phase-transition point in one dimension S generally has a logarithmic singularity. Here we investigate the Q-state quantum Potts chain for $Q \geq 4$ and calculate S across the transition point. The density matrix renormalization group (DMRG) method was applied and a logarithmic divergence was found for the $Q = 4$ at the second-order phase transition and finite jump of S for $Q = 6\&8$ at the first-order quantum phase transition. The jump of the entanglement entropy S is analytically calculated in leading order of Q and was found in good agreement with the DMRG results. Furthermore, the DMRG data are considered from several aspects in order to demonstrate that the DMRG method can be an appropriate technique for calculating the entanglement entropy at or around the phase transition.

*Poster

Orientation Effects on the Structural and Mechanical Properties of Graphene on Silicon Heterojunction

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The graphene/substrate heterojunction has been recognized to be the promising candidates for the new-generation diodes, solar cells, logic transistors, and energy-harvesting device. Understanding the topographic characteristic of graphene and its interaction with the supporting substrate is crucial for further development of nanoelectronic devices, because the properties of graphene are strongly affected by the underlying substrate. In this work, we study the orientation effect on the intrinsic stress and the interaction of graphene on the silicon substrates. The results show that the different orientations of graphene on the silicon substrates exhibit the different characteristics of interfacial structure, which would determines the magnitude of the intrinsic stress in the graphene. The armchair orientation of graphene on the silicon substrates has a lower intrinsic stress than the zigzag orientation one. The reasons are attributed to the fitness and interaction between graphene structure and surface characteristic of substrate. With different temperature, the variation of intrinsic stress is strongly affected on the degree of the fitness of the heterojunction structure.

*Poster

A general theory of steady-state copolymerization with applications to DNA replication by DNA polymerase

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Steady-state copolymerization is common either in polymer industry or in biology. The mathematical description of the kinetics based on master equation usually leads to unclosed equations which are hard to solve. Here we report a unified approach to solve the problem for general cases where a monomer at the reactive end (i.e.,the growing end) can either be added or deleted, depent on the identity of neighboring monomer units in proximity. This kinetic theory also leads to a general thermodynamic formula in which the Shannon entropy of the generated copolymer sequence is explicitly introduced as part of the free energy dissipation of the whole copolymerization system (J. Phys.: Condens. Matter 27 (2015) 235105). Based on the kinetic theory, we make a detailed discussion on the fidelity problem of DNA replication which is catalysed by DNA Polymerase (arXiv:1603.02453v2). DNAP is a molecular machine that possesses either a polymerase site for copolymerization or a exonuclease site for proofreading. Our work provides a comprehensive and analytically solvable model for the kinetics of the two-site DNAP.

*Poster

Emergent Long-Range Couplings in Arrays of Fluid Cells

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Recent experimental work by Gasparini and coworkers examined small cubical boxes of about 1 nm edge inscribed in a regular pattern on a silicon wafer and filled with liquid 4He. The boxes are then coupled by addition of more He4 to form a thin supernatant film or via channels. Something most remarkable happens: even though the boxes have a mesoscopic spacing, calorimetric measurements show clear evidence of coupling between different boxes. The authors did not offer any theoretical analysis, but they made the intriguing suggestion that action at a distance effects of this type might be a common feature of critical systems, both quantum (like 4He) and classical. In our work, we have constructed a theoretical model of boxes containing a fluid phase below its critical temperature but at coexistence. The boxes are coupled together by rods (of arbitrary length) also containing the fluid; in this way, we can assemble lattices of coupled boxes like those of Gasparini et al. We have analysed this model using mesoscopic description and by Monte-Carlo simulation, which confirms our phenomenological results. We have shown that, by appropriate tuning of parameters, the lattice of boxes develops long ranged order, even though the rods are very long compared to their lateral dimensions; the simulations produce associated thermodynamic signatures. If we consider two boxes coupled by a single rod, then we have a model system that may have relevance as a potential mechanism for biological control. Our ideas may also be useful for networks in social science. Finally, we suspect that our ideas extend to quantum spin models and maybe even to systems of coupled quantum dots.

*Poster

Energy Probability Distribution Zeros: A New Route to Study Phase Transitions

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In this work we present a novel method to study phase transitions based on the complex zeros of a polynomial with coefficients determined by the energy probability distribution. This is a general method that brings advantages over the conventional Fisher zeros approach since it does not require the knowledge of the full density of states. The method was applied to a variety of classical statistical physics models demonstrating its power in determining the transition temperature and critical behavior. Our strategy can easily be adapted to any model, classical or quantum, once we are able to build the corresponding energy probability distribution.

*Poster

Perturbative calculation of non-equilibrium free energy for mean-field interacting diffusions

Cesare Nardini * [1], Freddy Bouchet, Krysztof Gawedzki

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Large deviations in the low noise limit describe, through Freidlin-Wentzell or Macroscopic Fluctuation Theory, a number of out-of-equilibrium systems. In this context, a meaningful generalisation of non-equilibrium free energy is possible. However, explicit results are available only in very specific cases and there is generically no hope to calculate non-equilibrium free energies exactly for most out-of-equilibrium systems. In this talk we address a very natural and surprisingly still open, question: consider a system depending on a control parameter h and suppose that we are able to calculate the free energy for some value of h, say h=0. The typical situation is the case where h=0 corresponds to an equilibrium dynamics. Can we build a perturbation theory to calculate the quasi-potential for small but finite values of h? We answer to this question proving the existence of a perturbative expansion and giving explicit formulas to iteratively compute each order. These results are very general and can be applied to stochastic differential equations as well as to stochastic PDEs. Explicit results on non-equilibrium model composed of particles interacting via ferromagnetic forces will also be discussed. We will also discuss applications of this approach to fluctuating hydrodynamics relevant for the description of active matter.

*Poster

Population dynamics method with a multi-canonical feedback control

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We discuss the Giardinà-Kurchan-Peliti population dynamics method for evaluating large deviations of time averaged quantities in Markov processes [Phys. Rev. Lett. **96**, 120603 (2006)]. This method exhibits systematic errors which can be large in some circumstances, particularly for systems with weak noise, or close to dynamical phase transitions. We show how these errors can be mitigated by introducing control forces to within the algorithm. These forces are determined by an iteration-and-feedback scheme, inspired by multicanonical methods in equilibrium sampling. We demonstrate substantially improved results in a simple model and we discuss potential applications to more complex systems.

*Poster

Decoherence and Thermalization at Finite Temperature for Quantum Systems

Mark Novotny * [1], Fencing Jin, Shengjun Yuan, Meiji Miyashita, Hans De Raedt, Kristel Michelson

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We consider a quantum system S with Hamiltonian $\mathcal{H}_S$ coupled via a Hamiltonian $\mathcal{H}_{SE}$ to a quantum environment E with Hamiltonian $\mathcal{H}_E$. We assume the entirety $S+E$ is in a canonical-thermal state at an inverse temperature β. The entirety is a closed quantum system which evolves via the time-dependent Schr$\acute{}$odinger equation with Hamiltonian $\mathcal{H} = \mathcal{H}_S+\mathcal{H}_E+\lambda\mathcal{H}_{SE}$ where λ is the overall strength of the system-environment coupling. Using both large-scale simulations and perturbation theory calculations in λ, we have studied a measure $\sigma(t)$ for decoherence and $\delta(t)$ for thermalization of S. We performed large-scale parallel calculations on spin systems with up to $N = 40$ spins in the entirety, with both real-time and imaginary-time quantum calculations. We performed perturbation theory calculations about $\lambda = 0$ and fluctuations about the average for the canonical-thermal ensemble, for both σ and δ. We obtained closed form expressions for both σ and δ, in terms of the free energies of S and E. Our perturbation theory calculations agree very well with our numerical calculations, at least as long as $\beta\lambda$ is small [1]. [1] M.A. Novotny, F. Jin, S. Yuan, S. Miyashita, H. De Raedt, and K. Michielson, Physical Review A, vol. 92, 032110 [46 pages] (2016); arXiv:1601.04209.

*Poster

On the abelianity of the stochastic sandpile model

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We consider a generalized version of the Abelian Sandpile Model (ASM) on a finite graph. Each vertex of the graph can contain up to a certain number of sand grains, except for a sink which can absorb any number of grains. At each step of the Markov chain, a sand grain is added onto the graph, and when a vertex exceeds its maximal number of grains, it becomes unstable and topples, sending sand grains to its neighbors at random, according to any probability law, with some constraints for the chain to be well defined. The case where it always sends exactly one sand grain to each of its neighbors coincides with the ASM. Even though the model becomes much more complicated, some nice properties still hold. We show that on a certain probability space, even if we lose the group structure due to topplings not being deterministic, some operators still commute. More precisely, two stochastic matrices respectively giving the probabilities to go from one state to another by adding a sand grain on two different vertices will commute. As a corollary, we show that the stationary distribution does still not depend on how sand grains are added onto the graph in our model.

*Poster

Dynamical scaling in nonequilibrium relaxation analysis including corrections to scaling

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Dynamical scaling analysis in the nonequilibrium relaxation (NER) method[1] is applied to studies on critical phenomena. The improved dynamical scaling [2] by the use of the kernel method is used, which provides a semi-automatic efficient task for fitting procedure and a reliable result without assuming any parametric model for scaling functions. When corrections to scaling is considered, resulting estimations of transition temperature and critical exponents are much improved. We assume the dynamical scaling form for the NER of order parameter,

$$m(t,T) = \tau^{-\lambda}\Psi(t/\tau), \tag{1}$$

where $m(t,T)$ is a relaxation of magnetization from the all aligned state. One can use relaxation data on larger lattices much close to $T_{\rm c}$. For second order transition cases, $\lambda = \beta/z\nu$ and $\tau(T)$ is the relaxation time, which is expected to diverge as $\tau(T) \sim |T - T_{\rm c}|^{-z\nu}$ both in $T > T_{\rm c}$ and in $T < T_{\rm c}$. To estimate $T_{\rm c}$ and exponents, one may calculate $m(t,T)$ for several values of T, and fit the data to the above formula. We consider corrections to scaling by using the scaling function,

$$\tau^{-\lambda}\ m(t,T) = \Psi(t/\tau, t^{-c}), \tag{2}$$

instead of eq. (1) including the correction term. We apply the present method to some statistical models including fully frustrated XY models in two dimensions.

[1] Y. Ozeki and N. Ito, J. Phys. A: Math. Theor. **40** R149 (2007).
[2] Y. Echinaka and Y. Ozeki in prepartion.

*Poster

Transfer matrix spectrum for cyclic representations of 6-vertex reflection algebra

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We present the study of the transfer matrix spectral problem for the cyclic representations of the 6-vertex reflection algebra associated to the Bazhanov-Stroganov Lax operator. We use the Sklyanin separation of variable method to completely characterize the transfer matrix spectrum in two different ways. The results here derived can apply as well to the lattice sine-Gordon model, with open boundary conditions.

*Poster

Information geometry with parameter dependent correlated data: Bayesian explorations of cosmological predictions for the microwave background radiation

Katherine Quinn * [1], Francesco De Bernardis, Michael Niemack, James Sethna

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We developed a new, generalized fitting algorithm for miltiparameter models which incorporates varying and correlated errors. This was combined with geometrical methods of sampling to explore model prediction space, notably to plot geodesics and determine the size and edges of the model manifold. We illustrate this using the microwave background spectra for all possible universes, as described by the standard Λ-cold dark matter (Λ-CDM) cosmological model. In this case, the predicted data are fluctuations and highly correlated with varying errors, resulting in a manifold with a varying metric (as the natural metric to use is given by the Fisher information matrix). Furthermore, the model manifold shares the hyperribbon structure seen in other models, with the edges forming a strongly distorted image of a hypercube. Practical applications of such an analysis include optimizing experimental instrumentation designed to test more detailed cosmological theories.

*Poster

Using generalized spin distributions to investigate the intermediate temperature RSS phase in the three-state anti-ferromagnetic Potts model

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The intermediate temperature RSS phase in the three-state (q=3) anti-ferromagnetic Potts model on a simple cubic lattice is still not well understood, nor is there agreement on the critical temperatures for the onset and ending of this phase [1]. Utilizing distribution of generalized spin states, we were able, in an earlier paper [2], to successfully resolve the almost one decade-long controversy regarding additional phase transitions in this model. Using a similar approach, we have investigated the critical temperatures for the onset and the termination of the intermediate temperature RSS phase of this system. Sublattice spin distributions were obtained from Monte-Carlo simulation utilizing the Swendsen-Wang cluster-flip algorithm. In this presentation, we describe how distribution of spin states on sublattices can be used to determine the critical temperatures of the various phases in such models, including the intermediate temperature RSS phase. This approach was also used in determining the critical temperatures to a high degree of accuracy for the q=4, 5 and 6 cases. [1] Rotationally symmetric ordered phase in the three-state antiferromagnetic Potts model, R. Heilmann, J-S Wang and R. Swendsen, Phys.Rev. B53, 2210 (1996). [2] Intermediate-temperature ordering in a three-state Antiferromagnetic Potts Model, S. Rahman, E. Rush and R. Swendsen, Phys.Rev. B58, 9125 (1998).

*Poster

Optimal stochastic restart renders fluctuations in first passage times universal

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Stochastic restart may drastically reduce the expected run time of a computer algorithm, expedite the completion of a complex search process, or increase the turnover rate of an enzymatic reaction. These diverse first-passage-time (FPT) processes seem to have very little in common but it is actually quite the other way around. Here we show that the relative standard deviation associated with the FPT of an optimally restarted process, i.e., one that is restarted at a constant (non-zero) rate which brings the mean FPT to a minimum, is always unity. We interpret, further generalize, and discuss this finding and the implications arising from it. Ref: See upcoming letter in PRL

*Poster

Online Compressed Sensing in Absence of Knowledge of the Prior

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In "Online Compressed Sensing" (http://arxiv.org/abs/1509.05108), the authors presented a method for recovering sparse signals in an online fashion. By the use of a mean field approximation to the Bayes recursion formula, the online signal recovery algorithm can be performed with a computational cost that is linearly proportional to the signal length per update and analysis of the resulting algorithm indicates that the online algorithm asymptotically saturates the optimal performance limit achieved by the offline method in the presence of Gaussian measurement noise. Here, we present an extension of this work for the realistic situation where knowledge of the signal generating distribution is unknown. By the addition of a maximization step where the partition function is extremized with relation to the unknown prior parameters, it is possible to learn the correct values of these parameters and achieve a stable learning performance.

*Poster

Driven and undriven uniform states in a granular gas. The role of roughness

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We study a granular gas of inelastic rough spheres for two prototypical homogeneous states: (i) the undriven free cooling state and (ii) the steady state driven by a spatially uniform stochastic white-noise force, the latter acting on the translational particle velocities, by adding them a random impulse. In both cases an analytical solution of the corresponding velocity distribution function is worked out from a Sonine polynomial expansion that displays energy nonequipartition between the translational and rotational modes, translational and rotational kurtoses, and translational-rotational velocity correlations. By comparison with numerical solutions of the Boltzmann kinetic equation (by means of the Direct Simulation Monte Carlo method) we show that our analytical solutions provide good general descriptions that are semiquantitatively and quantitatively accurate in the undriven and driven states, respectively, for wide ranges of inelasticity and roughness. We also find three important features that make the forced granular gas steady state very different from the homogeneous cooling state. First, the marginal velocity distributions are always close to a Maxwellian. Second, there is a continuous transition to the purely smooth limit (where the effects of particle rotations are ignored). And third, the angular translational-rotational velocity correlations show a preference for a quasiperpendicular mutual orientation ("lifted-tennis-ball" behavior).

*Poster

Topological Approach to Microcanonical Thermodynamics and Phase Transition of Interacting Classical Spins

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We propose a topological approach suitable to establish a connection between thermodynamics and topology in the microcanonical ensemble. Indeed, we report on results that point to the possibility of describing *interacting classical spin systems* in the thermodynamic limit, including the occurrence of a phase transition, using topology arguments only. Our approach relies on Morse theory, through the determination of the critical points of the potential energy, which is the proper Morse function. Our main finding is to show that, in the context of the studied classical models, the Euler characteristic $\chi(E)$ embeds the necessary features for a correct description of several magnetic thermodynamic quantities of the systems, such as the magnetization, correlation function, susceptibility, and critical temperature. Despite the classical nature of the studied models, such quantities are those that do not violate the laws of thermodynamics [with the proviso that Van der Waals loop states are mean field (MF) artifacts]. We also discuss the subtle connection between our approach using the Euler entropy, defined by the logarithm of the modulus of $\chi(E)$ per site, and that using the *Boltzmann* microcanonical entropy. The approaches based on entropies associated with the total number of microscopic states, or the total number of critical points of the potential energy, are also considered in our analysis. Moreover, the results suggest that the loss of regularity in the Morse function is associated with the occurrence of unstable and metastable thermodynamic solutions in the MF case. The reliability of our approach is tested in two exactly soluble systems: the infinite-range and the short-range XY models in the presence of a magnetic field. Further studies are very desirable in order to clarify the extension of the validity of our proposal.

*Poster

Stochastic Treatment of Open Systems in Quantum Optics

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Semiconductor microcavities are an outstanding platform for study on non-equilibrium condensation. In the strong coupling regime, new eigenmodes emerge, called exciton-polaritons. Their condensates are now routinely produced in multiple groups over the world with an outstanding control on the system parameters. Moreover, exciton polaritons demonstrate phase coherence and topological defects formation. From the application viewpoint, recent research involves sculpting the polariton landscape down to one and zero dimensions towards realization of all-optical polariton logics embedding low power laser sources. All these developments, however, still rely on collective but classical mean-field effects, most of which can be accurately simulated via a single-particle evolution governed by the driven dissipative Gross-Pitaevskii equations. However, some of the effects require purely quantum modeling which would keep track of quantum correlations. In particular, quantum-mechanical treatment is required on the border between the kinetic and thermodynamic limits. Technically, the exponential growth of the Hilbert space with the increase of the number of modes of the bosonic system forbids any direct master equation treatment. Hence one has to cope with a cumbersome hierarchy of coupled equations for operator averages accompanied by empirical truncation at a certain operator order. We propose a quantum jump approach to exciton-polariton condensation [1], based on a stochastic evolution of the system wave function subject to interaction with the exciton reservoir and coherent/incoherent driving. We compute both the temporal second-order and spatial first-order correlation functions keeping track of the excited state dynamics and inter-state correlations. We discuss the perspectives open up by this model that, as opposed to e.g. DMRG and related algorithms, involves a relatively simple numerical implementation highly parallelizable and easily scalable to clusters. Our model is used to reproduce recent experimental results on the temporal coherence of confined polariton condensates at various pump powers and temperatures [2]. [1] H. Flayac, I. G. Savenko, M. Möttönen, and T. Ala-Nissila, Phys. Rev. B 92, 115117 (2015). [2] M. Amthor, H. Flayac, I. G. Savenko, S. Brodbeck, M. Kamp, T. Ala-Nissila, C. Schneider, and S. Hofling, arXiv:1511.00878 (2015).

*Poster

Markov State Modeling for Water Dynamics

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The unique properties of liquid water are relevant for a broad range of processes throughout many disciplines, e.g. protein folding. A long standing goal has been to relate the macroscopic properties such as the notable anomalies and singularities or transport properties to the microscopic structure, and thus to the hydrogen bonding pattern between individual molecules. We consider a Molecular Dynamics simulation of SPC/E water based on a 10ns long trajectory in bulk water. Pairs of water within a certain separation length R are considered and analyzed. With a Markov state model, we are able to discern different processes which describe switching of hydrogen bonds between different partners of water molecules. The application of transition path theory for discrete Markov chains reveal competitive reaction pathways when a hydrogen bond is broken and a new one is formed with another water molecule.

*Poster

Just one exponent describes diffusion-limited aggregation fractals

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Diffusion limited aggregation (DLA) is one of the models solving Laplace equation. We analyze recent developments in the understanding of DLA in the plane, paying special attention to the universal properties. We discuss phase diagram of DLA grown in the plane under the influence of underlying crystalline field and varying adhesion coefficient. There are two regions in the diagram, with asymptotic values of DLA cluster fractal dimensions 3/2 and 1.710... . Asymptotic values reached approximately for the clusters with at least 10^9 particles. Growing of clusters of this size is still impossible with the current power of computers, and we achieve this asymptotic effectively using estimation of harmonic measure with probe particles of varying size, and taking zero limit. Next, we answer the longstanding problem of multiscaling, which can be deduced from the visible variation of fractal dimension with radius for the cluster of size smaller than 10^9. We present analytical arguments (which are consistent with the numerical data) that visible multiscaling is just the finite size effect, and that DLA fractals do not demonstrate multiscaling asymptotically.

*Poster

Large deviation functions of time-integrated current in stochastic traffic models

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Studying large deviation functions (LDF) in stochastic traffic models typically relies on simulation. Simulation of rare events is a notoriously difficult task however. In the past decade, a number of advanced Monte Carlo techniques have been introduced to investigate the LDF of macroscopic observables in non-equilibrium stochastic models. In this work, we study and compare two of these methods, the cloning method [1], and the iterative measurement-and-feedback method [2]. We adapt the existing methods to the setting of discrete time Markov chains, where necessary, and apply them to a number of variants of TASEP, such as the Nagel-Schreckenberg model, which serves as a minimal discrete model of freeway traffic. [1] Cristian Giardina, Jorge Kurchan, and Luca Peliti. Physical review letters, 96(12):120603, 2006. [2] Takahiro Nemoto and Shin-ichi Sasa. Physical review letters, 112(9):090602, 2014.

*Poster

Geometry of Fubini-Study metric of thermal pure quantum states

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In the foundation of quantum statistical mechanics, every equilibrium state can be represented by almost all pure quantum states in the corresponding energy shell[1-4]. This concept is called typicality. On the other hand, the thermodynamic geometry is gathering much attention in the high energy physics. In condensed matter physics, the Fubini-Study metric of ground states with varying parameters is known to be able to capture the quantum phase transitions and their topological aspects[5,6]. In this talk, we will extend this metric to finite temperature using recently proposed thermal pure quantum (TPQ) state, which is a typical realization of an equilibrium state [7,8]. We will show that the real part of this metric reproduces the thermodynamic geometry when Hamiltonians in different parameters commute with each other. Furthermore, when they do not commute, we will show that Berry phase at finite temperature emerges in the imaginary part of it and an additional quantum correlation emerges in the real part. The quantum metric depends on the holonomy of the TPQ state. We will show that different experimental protocols, e.g., adiabatic time evolution and sudden quench, correspond to different holonomies and geometries. [1] S. Popescu, A.J. Short, and A. Winter, Nature Phys. 2, 754 (2006). [2] S. Goldstein et al, Phys. Rev. Lett. 96, 050403 (2006). [3] A. Sugita, Nonlinear Phenom. Complex Syst. 10, 192 (2007). [4] P. Reimann, Phys. Rev. Lett. 99, 160404 (2007). [5] P. Zanardi, P. Giorda, and M. Cozzini, Phs. Rev. Lett. 99, 100603 (2007). [6] M. Kolodrubetz, V. Gritsev, and A. Polkovnikov, Phys. Rev. B 88, 064304 (2013). [7] SS and A.Shimizu, Physical Review Letters 108, 240401 (2012) [8] SS and A.Shimizu, Physical Review Letters 111, 010401 (2013)

*Poster

Effect of random field disorder on first order transitions

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The effect of quenched disorder on the behavior of a system, whose pure version undergoes a first order transition is well understood by now for d¡=2 [1]. For two dimensions, an infinitesimal amount of disorder is known to change the order of transition to a continuous transition. The situation in higher dimensions is not so clear. In higher dimensions, it was conjectured that there exist a impurity threshold beyond which the transition should change its character [2]. We solve p spin interaction model and Blume Capel model in the presence of random field disorder on fully connected graphs using large deviation theory. For p spin interaction model, we find that for p¿= 3, the first order transition continues to be a first order for all strengths of disorder [3]. While for Blume Capel model with bimodal random crystal field, we find the behavior is modified: for very weak disorder, the phase diagram is similar to the pure model with regions of first and second order transitions separated by a tricritical point. With increasing strength of disorder, the transition soon becomes a continuous transition for all strengths of disorder [4].
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*Poster

Percolation in Segregating Binary Bose-Einstein Condensates

Hiromitsu Takeuchi * [1]

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Percolation theory is applied to phase-separation dynamics of binary Bose-Einstein condensates in quasi-two-dimensional systems [1]. Our finite-size-scaling analysis shows that the percolation threshold of the initial domain pattern emerging from the dynamic instability is close to 0.5 for strongly repulsive condensates. The percolation probability is universally described with a scaling function when the probability is rescaled by the characteristic domain size in the dynamic scaling regime of the phase-ordering kinetics, independent of the intercomponent interaction. It is revealed that an infinite domain wall sandwiched between percolating domains in the two condensates has a noninteger fractal dimension and keeps the scaling behavior during the dynamic scaling regime. In addition, we show that the domain size distribution obeys a scaling law according to the dynamic scaling analysis based on the percolation theory [2]. [1] Hiromitsu Takeuchi, Yumiko Mizuno, and Kentaro Dehara, Phys. Rev. A 92, 043608 (2015). [2] Hiromitsu Takeuchi, J. Low Temp. Phys. 183, 169 (2016).

*Poster

Estimation of spin-spin interactions from magnetization curve based on the Bayesian statistics

Ryo Tamura * [1], Koji Hukushima

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We develop a method for estimating spin-spin interactions in the Hamiltonian from a given magnetization curve by the machine learning based on the Bayesian statistics. In the estimation method, plausible spin-spin interactions that explain the given magnetization curve are determined by maximizing the posterior distribution. It is obtained by statistical physics as the conditional probability of the spin-spin interactions for a given magnetization curve with observation noise. The efficiency of the estimation method is tested for a case of synthetic magnetization curve data obtained by the classical Heisenberg model. Results show that the developed estimation method enables estimation of the spin-spin interactions with high accuracy and, in particular, the relevant terms of the spin-spin interactions are successfully selected from among redundant interaction candidates by using l_1 regularization in the prior distribution. We would like to emphasize that the framework of our estimation method can be used not only for magnetization curves but also for any measured data as the input data. In addition, we strongly believe that our proposed estimation method is expected to form a basis for physics-based machine learning techniques.

*Poster

Thermostat algorithms for generating target ensembles

Diego Tapias * [1], David P. Sandrers Alessandro Bravetti

[1] National Autonomous University of Mexico (UNAM) – Mexico

We present a new algorithm to generate the equations of motion for physical systems in different ensembles. The relevant characteristic of our method is that the dynamics is derived by exploiting the geometric structure of an extended phase space associated with the degrees of freedom of the system and the reservoir, which is assumed to be a contact manifold. Our approach provides both a theoretical framework and a dynamical basis for ensembles different from the microcanonical one and it thus appealing for molecular dynamics simulations. The validity of the method is tested through numerical experiments. In particular we consider the prototypical example of a harmonic oscillator in the canonical ensemble. The results of this talk may be found in: Thermostat algorithm for generating target ensembles, A. Bravetti and D. Tapias, Phys. Rev. E 93, 022139, 24 February 2016. Liouville's theorem and the canonical measure for nonconservative systems from contact geometry, A. Bravetti and D. Tapias, Journal of Physics A: Mathematical and Theoretical 48, 24, 254001, 27 May 2015.

*Poster

Counter-ion condensation around a charged disk: exact results in the intermediate coupling regime

Gabriel Tellez * [1], Juan Pablo Mallarino

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We present an analysis of the condensation of counter-ions around a charged disk. The model under consideration is a two-dimensional (2D) system formed by an impenetrable disk of charge Q1 surrounded by ions of charge q dispersed freely in a larger disk with external charged boundary Q2, at thermal equilibrium at a temperature T. In mean field, it is known that a disk with a dimensionless charge (q Q1/(2 k T)) inferior to unity is unable to bind counter-ions. When the charge is above unity, it attracts an ion cloud in such a way that it neutralizes partially the disk so that the effective dimensionless charge of the disk and the cloud is unity. We explore the faith of this counter-ion condensation beyond the mean field regime for large values of the Coulomb coupling. In particular, for some special values of the coupling, exact analytical results can be obtained for the system, which give an interesting insight on the condensation phenomenon. These exact results can be obtained by recognizing that the Boltzmann factor of the system can be expressed in terms of a Jack polynomial, and expanding it in monomial basis.

*Poster

“Crystallisation pathway of strongly repulsive charged brownian particles”

Efraín Urrutia * [1], Claudio Contreras Aburto, Amir D. Maldonado Arce

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The crystallisation process of a system of charged brownian particles in the metastable melt is described with the help of brownian dynamics computer simulations complemented with an analysis of common neighbours. The results reveal a dominant abundance of icosahedral structures in the metastable melt, which is in agreement with recent static structure measurements. A crystallisation pathway is found that obeys a logistic growth model for the bcc units population, mostly at the expense of the extinction of the icosahedral structures.

*Poster

Novel optimal space partitions

Nicolas Vandewalle * [1], Eric Opsomer

[1] University of Liege – Belgium

Partitioning space into polyhedra with a minimum total surface area is a fundamental question in science and mathematics. In 1887, Lord Kelvin conjectured that the optimal partition of space is obtained with a 14-faced space-filling polyhedron. Kelvin's conjecture resisted a century until Weaire and Phelan proposed in 1994 a new structure obtained from numerical simulations. We report a giant breakthrough in this field. We propose a stochastic method, based on simulated annealing and Voronoi tesselation, for finding efficient polyhedral structures, solving a generalized Kelvin's problem. We show that novel optimal structures emerge. Two particular partitions made of respectively 8 and 24 polyhedra are found to beat the Weaire-Phelan structure. The first partition looks similar but slightly different from the Weaire-Phelan structure, since the polyhedral cells have non-equal volumes. The second structure is new and is composed of 12- and 16-faceted polyhedra. Moreover, our work suggests that more optimal structures are still to be discovered. We give clues for exploring new structures.

*Poster

Lindblad dynamics of a quantum spherical spin

Sascha Wald * [1], Malte Henkel

[1] Université de Lorraine – France

The coherent quantum dynamics of a single bosonic spin variable, subject to a constraint derived from the quantum spherical model of a ferromagnet, and coupled to an external heat bath, is studied through the Lindblad equation for the reduced density matrix. Closed systems of equations of motion for several quantum observables are derived and solved exactly. The relationship to the single-mode Dicke model from quantum optics is discussed. The analysis of the interplay of the quantum fluctuation and the dissipation and their influence on the relaxation of the time-dependent magnetisation leads to the distinction of qualitatively different regimes of weak and strong quantum couplings. Considering the model's behaviour in an external field as a simple mean-field approximation of the dynamics of a quantum spherical ferromagnet, the magnetic phase diagram appears to be re-entrant and presents a quantum analogue of well-established classical examples of fluctuation-induced order.

*Poster

From Nash equilibrium to the Schrödinger equation and a general quantum dynamics

Wolfgang Paul * [1], Jeanette Köppe, Wilfried Grecksch

[1] Martin Luther University – Germany

Complex, non-relativistic quantum systems are analyzed theoretically or by numerical approaches to the Schrödinger equation. Compared to the numerical options available to treat classical mechanical systems, this is limited, both in methods and in scope. However, based on Nelson's stochastic mechanics, a mathematical structure of quantum mechanics has been developped into a form parallel to analytical mechanics. Finding the Nash-equilibrium for the stochastic optimal control problem, which is the quantum equivalent to Hamilton's primciple in classical mechanics, leads to the Schrödinger equation on the one hand and a general set of quantum dynamical equations on the other hand. We show that for the harmonic oscillator these lead to the coherent states and establish a numerical procedure to solve for the ground state process for the stationary problem.

*Poster

Quantum Heat Engine at a Negative Absolute and a Positive Temperature

Jingyi Xi * [1], Haitao Quan

[1] Academy for Advanced Interdisciplinary Studies, Peking University – China

To clarify the ambiguity on negative absolute temperature in literature, we study the Carnot and the Otto cycle with one of the heat reservoirs at the negative absolute temperature. The work extraction, entropy production and the efficiency of these cycles are explored. Conditions for constructing and properties of these thermodynamic cycles are elucidated. We find that the apparent "violation" of the second law of thermodynamics in these cycles are due to the fact that the usual definition of thermodynamic efficiency is inappropriate in this situation. When properly understanding the efficiency and the adiabatic process, in which the system passes through absolute zero, the Carnot cycle with one of the heat reservoirs at a negative absolute temperature can be understood straightforwardly, and it contradicts neither the second nor the third law of thermodynamics. We use a two-level system and a Ising spin system to illustrate our central results.

*Poster

Critical nonequilibrium relaxation in cluster algorithms

Yoshihiko Nonomura * [1], Yusuke Tomita

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Recently we showed that the critical nonequilibrium relaxation in cluster algorithms is widely described by the stretched-exponential relaxation of physical quantities in the Ising [1], XY [2], Heisenberg [3] and Potts [2] models, and that critical phenomena are characterized by the exponent of the stretched-exponential relaxation, σ. That is, $\sigma \approx 1/3$ in the 2D, 3D and 4D Ising models (second-order phase transitions), $\sigma \approx 1/2$ in the 3D and 4D XY and 3D and 4D Heisenberg models (second-order phase transitions in continuous spin models), $\sigma \approx 1$ (i.e. the simple exponential relaxation) in the 2D XY model (BKT phase transition) and $\sigma = 0$ (i.e. the power-law relaxation) in the 2D $q = 5$ Potts model (weak first-order phase transition). Generalization to quantum Monte Carlo calculations will also be discussed.

[1] Y. Nonomura, J. Phys. Soc. Jpn. **83**, 113001 (2014).

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[3] Y. Nonomura and Y. Tomita, Phys. Rev. E **93**, 012101 (2016).

*Poster

Classical many-body theory with retarded interactions: probability-free foundation of irreversibility

A. Yu. Zakharov * [1]

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The exact closed equation of motion for microscopic density of classical many-body system with account of retarded interactions between particles is derived. Qualitative properties of the solutions of this equation are investigated. It is shown that interactions retardation leads to irreversible behaviour of many-body systems.

*Poster

Ground states of a generalized XY model with frustrated magnetic and pseudonematic couplings

Milan Žukovič * [1]

[1] Institute of Physics, P.J. Šafárik University in Košice – Slovakia

Ground state phases of a generalized XY model with magnetic and pseudonematic couplings on a non-bipartite triangular lattice are investigated in the exchange interactions parameter space. We demonstrate that the model displays a number of ordered and quasi-ordered phases as a result of geometrical frustration and/or competition between the magnetic and pseudonematic interactions. The nature and the extent of the respective phases depend on the parameter q, characterizing the higher-order harmonics term of the model Hamiltonian. Motivated by the recent discovery of the experimental realization of the model for $q = 2$ in the seemingly unrelated field of the structural chemistry [1], the present model for $q > 2$ is discussed in the context of the prediction of structural phases of some bimetalic cyanides based on the mapping between the two systems. [1] A.B. Cairns, M.J. Cliffe, J.A.M. Paddison, D. Daisenberger, M.G. Tucker, F.-X. Coudert, A.L. Goodwin, Nature Chemistry (2016) doi:10.1038/nchem.2462.

*Poster

Topic 2: Out-of Equilibrium Aspect-Posters

Fluctuation-dissipation relations far from equilibrium

Bernhard Altaner * [1], Matteo Polettini, Massimiliano Esposito

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Fluctuation dissipation relations (FDRs) connecting the response of a current to a conjugate force with the spontaneous fluctuations of that current are usually considered as the hallmark of an equilibrium system. Here, we show that FDRs also hold for local currents quietly stalling amidst an ocean out of equilibrium, if their response is probed with respect to a control parameter that enters the system only locally. We give several examples and discuss the relation of our result to the notion of local equilibrium in stochastic thermodynamics.

*Poster

Exclusion processes with varying system length

Chikashi Arita * [1]

[1] Saarland University – Germany

The exclusion process is one of fundamental models in non-equilibrium statistical physics. Motivated by queueing and biological applications, we consider variants of the exclusion processes with varying system size. In some cases, exact stationary states can be constructed, and therefore phase diagrams of whether the system converges or diverges are rigorously determined. Various types of density profiles are found, depending on system parameters, by using heuristic argument.

*Poster

Two Dimensional Optical Rocking Ratchet

Alejandro V. Arzola * [1], . *et. al.*

[1]Instituto de FÍsica, Universidad Nacional Autónoma de México – Mexico

Ratcheting mechanism constitute a paradigmatic out-of-equilibrium system which enables transport of matter at the mesoscopic size level. In this work we present a novel experimental realization of a two-dimensional ratchet based on optical micromanipulation techniques. It consists of microscopic dielectric particles immersed in water, which are forced to move periodically on a two-dimensional periodic optical potential with a defined spatial asymmetry. The characteristic behavior of the system is the non-trivial transport given by the dynamic coupling of the spatial asymmetry and the time-dependent non-biased forces. We obtained a two-dimensional current of particles that strongly depends on the shape of the optical potential and on the magnitude, periodicity and direction of the drag force that takes particles out of equilibrium. A thorough theoretical study is also presented. With this system we explored new mechanisms to bias the random motion of microscopic samples. For example, we were able to observe transversal currents previously predicted in theoretical models, and control the motion of a sample of particles in a two-dimensional space by only changing the asymmetry of the pattern of light in real time.
AVA acknowledges financial support from DGAPA-UNAM-PAPIIT grant IA103615.

*Poster

Finding a new job for Maxwell's demon: improving nonequilibrium free energy calculations.

Shahaf S. Asban * [1], Saar Rahav

[1] Technion – Israel

Our understanding of small out-of-equilibrium systems have undergone a revolution in the last two decades, with the development of stochastic thermodynamics and single molecule techniques. Such systems were experimentally verified to satisfy fluctuation theorems, specifically the Jarzynski equality. This equality is widely used to determine free energy differences from repetitions of a non-equilibrium process. However, such experiments or calculations are known to exhibit poor convergence. Under the same framework, the deep connections between information and thermodynamics have also been extensively studied. Information engines driven by measurement and feedback have been studied theoretically and realized in experiments. It is natural to wonder whether measurement and feedback can also be useful in free energy estimation. We argue that they can greatly improve the convergence of such calculations. We demonstrate this argument using a simple two-state model of a DNA hairpin.

*Poster

Condensation of helium in a silica aerogel is described by the athermal Random Field Ising Model

Geoffroy Aubry * [1], Victor Doebele, Edouard Kierlik, Panayotis Spathis, Pierre-Etienne Wolf

[1] Universität Konstanz – Germany

We have experimentally studied the condensation of ^{4}He in light silica aerogels as a model system to probe the influence of dilute disorder on a first order phase transition. In contrast to previous claims, we find that this system is not a realization of the equilibrium Random Field Ising Model (RFIM), but is thermodynamically out-of-equilibrium. More precisely, we show that temperature allows to tune the effective disorder strength, enabling to observe the disorder driven critical point predicted by the athermal RFIM studied by Sethna
textitet al. (PRL 70, 3347, 1993). Using light scattering to measure the fluid state on a local scale, we find that above (below) a critical temperature, the hysteretic transition to the liquid state occurs continuously (abruptly). Our results (Aubry
textitet al., PRL 113, 085301, 2014) are consistent with the extension of the Sethna's model to a lattice gas model developed by Detcheverry
textitet al. (PRE 72, 051506, 2005). The athermal RFIM also predicts the existence of a Return Point Memory (RPM) along minor hysteresis loops. We recently developed a technique based on the sensitivity of the speckle patterns to the fluid spatial distribution to demonstrate RPM at the microscopic level in our experimental system, thus confirming its athermal character. To our knowledge, these measurements are the first demonstration at a microscopic level of RPM for random field disorder.

*Poster

Spontaneous pedestrian laning in a crowded corridor: a non-equilibrium phase separation.

Nicolas Bain * [1], Denis Bartolo

[1] ENS de Lyon – France

Theoretical and numerical studies of pedestrian flows have been the subject of great attention for more that 20 years. Primarily motivated by the prevention of crowd disasters, numerous models were developed to simulate large human crowds in different particular settings: room escape, multi-lane flows, obstructed roads, etc These increasingly complex models are usually based on empirical behavioural or heuristic laws, and the very ingredient responsible for the robust features of large-scale flows remains unknown. With this in mind, our goal is to isolate macroscopic observables making it possible to distinguish between the number of possible repulsive interactions at the 2-body level. Focusing on a prototypical geometry in the context of pedestrian flows, we introduce a minimal yet generic overdamped model for motile individuals propelling on a solid substrate. We demonstrate that unidirectional motile particles generically undergo a transition from a homogenous to a phase separated state (laning) irrespective of the very details of their interactions. However we identify structural and dynamical observables which clearly distinguish between the possible behavioural rules and enables us to discuss the relevance of these predictions to actual human crowd dynamics.

*Poster

Changes in Transport Properties of a Convecting Fluid with Increases in Internal Degrees of Freedom

Stuart Bartlett * [1]

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I present a set of numerical experiments designed to address the following question: How do the thermodynamic transport abilities of a non-equilibrium system change as it is given more internal degrees of freedom? As an archetypal starting point, I use a two-dimensional single phase fluid undergoing buoyancy-driven convection. It was shown already in the mid twentieth century (with other more recent works corroborating those first contributions) that such convecting fluids maximise heat flux under basic hydrodynamic constraints, and fixed temperature boundary conditions. More recently, it has been proposed that such systems exhibit maximum entropy production (MEP). Maximum heat flux under a fixed temperature gradient constraint does indeed seem indicative of MEP, but under other boundary conditions, such as fixed flux or negative feedback, it has been shown that the MEP prediction fails. Some have argued that a system must be 'sufficiently complex', or have 'sufficient degrees of freedom', before it can exhibit MEP. While I do not ascribe to the idea that MEP is a unifying variational principle for non-equilibrium systems, I wished nonetheless to explore how the transport properties of simple driven fluid systems were affected by increases in internal degrees of freedom. Taking the single phase, convecting fluid and adding dissolved passive scalars that can undergo exo/endothermic chemical reactions with one another, what will be the qualitative and quantitative effect on the heat flux and characteristics of the system? In this contribution I present the first set of modelling results that attempt to answer this question.

*Poster

Short-time dynamical behaviour of critical lattice gases

Urna Basu * [1]

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The non-equilibrium short-time behaviours of the driven and undriven lattice gases at the critical point are investigated in two spatial dimensions starting from a fully disordered initial configuration. In particular, we study the time evolution of suitably defined "transverse" order parameters, which account for the anisotropy introduced by the homogeneous driving. We propose that, at short times, the dynamical behaviour of all these models is effectively described by a continuum theory with conserved order parameter in which fluctuations are Gaussian in the transverse direction, irrespective of this being the case at longer times. Strong numerical evidence is provided which agrees very well with the analytical predictions of such a Gaussian theory, both for the driven and undriven systems.

*Poster

Langevin dynamics and a skew probability distribution of nonequilibrium current fluctuations

Roman Belousov * [1], E.G.D. Cohen, C. Wong, J.A. Goree, Y. Feng, L. Rondoni

[1] Rockefeller University – United States

A skewness of the probability for instantaneous fluctuations of a shear flow, in a nonequilibrium steady state, has been discovered in a recent dusty plasma experiment and confirmed by computer simulations. This phenomenon is attributed to the presence of a preferred spatial direction in the system due to the externally applied shear rate. In order to provide a quantitative physical model of the fluctuations in steady-state systems subject to an external force, we extend the Langevin dynamics, suggested by Onsager and Machlup for equilibrium fluctuations in spatially symmetric systems, by adding a new stochastic term. Statistical properties of the fluctuations are then calculated from the solution of the extended Langevin equation, while their probability density function can be approximated by a novel Modulated Gaussian distribution.

*Poster

Integrable dynamics in systems with long-range interactions

Fernanda P. C. Benetti * [1], Ana Carolina Ribeiro-Teixeira, Renato Pakter, Yan Levin

[1] Instituto de Física - Universidade Federal do Rio Grande do Sul – Brazil

Systems whose components interact by unscreened long-range forces?for example, stellar systems and non-neutral plasmas?have characteristics that are anomalous with respect to systems with shielded or short-range forces. Besides presenting unique thermodynamic properties such as negative specific heat and inequivalence of ensembles, their initial dynamics is predominantly collisionless and leads to out-of-equilibrium quasi-stationary states. These states are notoriously difficult to predict given an arbitrary initial condition, and there is still no unified theory to treat them. One thing, however, is clear: unlike thermodynamic equilibrium, the system's initial dynamics plays a fundamental role in determining the profile of the quasi-stationary state. If strong mean-field oscillations occur ? a process known as violent relaxation ? a core-halo configuration is formed, in which ergodicity is broken. In these cases, the core-halo theory of Levin et al successfully characterizes the QSS profiles [1]. If the initial condition is such that there are no strong oscillations ? for example, in a virialized initial state ? the dynamics is close to integrable and there is no core-halo formation, so the core-halo theory does not apply. Here we show the results of a model based on integrable dynamics for describing these QSS profiles. We apply it specifically for a spherically symmetric self-gravitating system with an isotropic velocity distribution [2] and show that it is successful for several different initial conditions. We also compare with Lynden-Bell statistics results, which relies on a fundamentally different assumption, that of ergodicity and violent relaxation. [1] Levin, Y. et al, Phys. Rep. 536 (2014). [2] Benetti, F. P. C. et al, Phys. Rev. Lett. 113 (2014).

*Poster

Time irreversibility of heavy inertial particles in fluid turbulence

Akshay Bhatnagar * [1]

[1] NORDITA, Stockholm – Sweden

For heavy-inertial particles advected by a turbulent flow, time irreversibility arises because of two reasons: (a) turbulent flows are irreversible; and (b) the Stokes drag exerted by the flow on the particle is dissipative. We characterize the time irreversibility of trajectories of heavy inertial particles advected by a turbulent fluid, by carrying out an extensive direct numerical simulation (DNS) obtaining several statistical properties of the non-equilibrium statistically steady state of such particles in a turbulent flow. From our DNS we show that the probability distribution functions (PDFs) of the power input (p) to the particles, by the turbulent flow, are negatively skewed. This shows explicitly the violation of the principle of detailed balance and the lack of time-reversal symmetry, in such a flow. Furthermore, by computing the persistence-time PDFs of the time for which p remains positive or negative, we demonstrate that these PDFs display exponentially decaying tails, from which we obtain characteristic time scales for the acceleration and deceleration of the heavy particles. We find that the time scale over which the particles decelerate is, on average, smaller than the time scale over which it accelerates, i.e., typically, heavy inertial particles in turbulent flows, lose their energy faster than they gain it. We show that, if we replace the turbulent flow by a statistically time-reversal-invariant, white-noise process we find similar statistical properties, because of the dissipation via Stokes drag.

*Poster

Irreversibility and dissipation in multiple-scale systems

Stefano Bo * [1], Antonio Celani, Erik Aurell, Ralf Eichhorn

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Stochastic processes provide an effective modeling tool for a great number of phenomena in physics, chemistry and biology. Systems of relevant interest often involve processes taking place on widely separated timescales. Efficient modeling dictates to restrict the description to the slower processes and it is of great importance to accurately eliminate the fast variables in a controlled fashion, carefully accounting for their net effect on the slower dynamics. Such averaging and homogenization techniques have been extensively studied and reviewed in the mathematical literature. Less is known about the behavior of functionals of the stochastic trajectories such as, counting statistics, entropy production, etc., upon changing the level of resolution. For such functionals, the elimination of the faster degrees of freedom can present additional difficulties and naive procedures can lead to blatantly inconsistent results. I will focus on entropy production and show that, for non-equilibrium systems, under quite general conditions, properties of the fast dynamics still affect thermodynamics on the slower scales therefore compromising a description of the full system in terms of slow variables only. This elucidates the potential pitfalls of defining thermodynamics starting from the effective dynamics. Such feature is due to a symmetry breaking accompanying the change of resolution in the description. In this respect, it is reminiscent of physical anomalies such as the viscous dissipative anomaly and quantum anomalies.

*Poster

Relaxation Dynamics of Interacting Skyrmions in Thin Films

Bart Brown * [1], Michel Pleimling

[1] Virginia Tech – United States

Magnetic skyrmions are topologically protected spin textures which were recently observed in certain chiral magnets such as MnSi. Skyrmions show enormous promise in spintronics due to the very low current density required to move them (five orders of magnitude less than typical magnetic domain walls). A thorough understanding of the relaxation processes for systems of interacting skyrmions far from equilibrium could prove invaluable in real world applications but is currently lacking in the literature. The dynamics are described by the Landau-Lifshitz-Gilbert (LLG) equation, however, simulating many interacting skyrmions by solving the LLG equation is computationally infeasible. In order to explore these relaxation processes, we employ a suitable two-dimensional particle based model derived from Thiele's approach and study the scaling properties of two-time correlation functions.

*Poster

Counting statistics of parity symmetric open interacting spin systems

Berislav Buca * [1], Tomaz Prosen

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We study the full counting statistics for interacting quantum many-body spin systems weakly coupled to the environment. In the leading order in the system-bath coupling we derive exact spin current statistics for a large class of parity symmetric spin-1/2 systems driven by one or more pairs of Markovian baths with local coupling operators. Interestingly, in this class of systems the leading order current statistics are universal and do not depend on details of the Hamiltonian. Furthermore, in the specific cases of symmetrically boundary driven anisotropic Heisenberg (XXZ) spin 1/2 chain and the Hubbard model we derive explicitly the next-to-leading order non-linear corrections to the current statistics. Reference: B. Buca and T. Prosen. Phys. Rev. Lett. 112, 067201 (2014)

*Poster

Numerically Solving the Fractional Fokker-Planck Equation through Unbiased Density Estimation of Anomalous Diffusion Processes

Sean Carnaffan * [1], Reiichiro Kawai

[1] The University of Sydney – Australia

Anomalous diffusion is a ubiquitous physical phenomenon that is differentiated from classical diffusion by its power law scaling of variance with time [1]. The probability density function of a random walker undergoing an anomalous diffusion is given by the fractional Fokker-Planck equation (FFPE). In its most general form, this equation does not admit an analytic solution, and deterministic numerical methods for computing its solution are significantly more complex than their non-fractional counterparts. In this talk, we describe nondeterministic methods of solving this equation numerically by estimating empirical density functions of anomalous diffusion processes. We introduce, by means of the Malliavin calculus, an unbiased expression for the solution which overcomes the inherent bias in typical kernel density estimation methods [2, 3]. It will be seen that this expression may be computed simply and efficiently using the Monte Carlo method and has the flexibility to model many different cases of anomalous diffusion. We also discuss practical concerns involved in implementing this numerical solution, including stochastic representations of anomalous diffusion processes and simulation algorithms thereof. [1] R. Metzler and J. Klafter. The random walk's guide to anomalous diffusion: a fractional dynamics approach. Physics Reports, 339(1):1–77, 2000. [2] A. Kohatsu-Higa and K. Yasuda. Estimating multidimensional density functions using the Malliavin-Thalmaier Formula. SIAM Journal on Numerical Analysis, 47(2):1546–1575, 2009. [3] R. Kawai and A. Kohatsu-Higa. Computation of greeks and multidimensional density estimation for asset price models with time-changed Brownian motion. Applied Mathematical Finance, 17(4):301– 321, 2010.

*Poster

A unified framework for the direct evaluation of large deviations in both Markovian and non-Markovian processes

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We propose a general framework to simulate stochastic trajectories with arbitrarily long memory dependence and efficiently evaluate large deviation functions associated to time-extensive observables. This extends the "cloning" procedure of Giardiná et al. [Phys. Rev. Lett. 96, 120603 (2006)] to non-Markovian systems. We demonstrate the validity of this method by testing non-Markovian variants of an ion-channel model and the Totally Asymmetric Exclusion Process, recovering results obtainable by other means.

*Poster

Additivity and mass fluctuations in conserved-mass transport processes

Sayani Chatterjee * [1], Arghya Das, Punyabrata Pradhan, Pradeep Kumar Mohanty

[1] S. N. Bose National Centre for Basic Sciences – India

Understanding fluctuations is fundamental to the formulation of statistical mechanics. Unlike in equilibrium, where fluctuations are obtained from the Boltzmann distribution, there is no unified principle to characterize fluctuations in nonequilibrium. We aim to provide a statistical mechanics framework to characterize steady-state mass fluctuations in conserved-mass transport processes. We demonstrate that mass distributions in a broad class of nonequilibrium mass-transport processes can be obtained from an additivity property, the tenet of equilibrium thermodynamics. References: 1. Phys. Rev. Lett. 112, 030601 (2014) 2. arxiv 1602:03345

*Poster

Motion of self-propelled particles in heterogeneous media

Oleksandr Chepizhko * [1]

[1] Department of Applied Physics, Aalto University – Finland

We study the effect of randomly placed obstacles on the transport properties and collective properties of self-propelled particles. In [1] it is shown that the diffusion coefficient depends on the density of obstacles and displays a minimum at an intermediate density of obstacles. For high density of obstacles, trapping of self-propelled particles is observed. If a velocity-alignment acts among the self-propelled particles [2,3], it is shown that in the presence of obstacles the order parameter for collective motion depends on the noise strength in a non-trivial way. Furthermore, it is found that there exists an optimal noise value that maximizes collective motion. It is shown that for large densities of obstacles, long-range order disappears. Other effects of active particles in heterogeneous media, such as giant number fluctuations, traveling bands, and clustering properties are discussed. 1. O. Chepizhko, F. Peruani, PRL 111, 160604 (2013) 2. O. Chepizhko, E.G. Altmann, F. Peruani, PRL 110, 238101 (2013) 3. O. Chepizhko, F. Peruani, Eur. Phys. J. Special Topics 224, 1287–1302 (2015)

*Poster

Irreversibility of trajectories along dissipative processes

Kuan-Hsun Chiang * [1], Chi-Lun Lee, Pik-Yin Lai, Yung-Fu Chen

[1] Department of Physics, National Central University – Taiwan

We experimentally identify the equivalence between physical dissipation and the irreversibility of a phase space trajectory of a dissipative process in electric RC circuits. In our experiments, a trajectory is a measured time series of voltage fluctuations of a circuit. We study two different types of non-equilibrium steady states: the circuit is driven out of equilibrium either by constant current source or temperature gradient. The results strongly imply the momentary dissipation in certain time interval is equivalent to the trajectory irreversibility in phase spaces.

*Poster

Entropy production and Fluctuation Relation in turbulent convection

Sergio Chibbaro * [1], Francesco Zonta

[1] UPMC Paris 6 – France

We report on a numerical experiment performed to analyze fluctuations of the entropy production in turbulent thermal convection, a physical configuration that represents here a prototypical case of an out-of-equilibrium dissipative system. We estimate the entropy production from instantaneous measurements of the local temperature and velocity fields sampled along the trajectory of a large number of point-wise Lagrangian tracers. The entropy production is characterized by large fluctuations and becomes often negative. This represents a sort of "finite-time" violation of the second principle of thermodynamics, since the direction of the energy flux is opposite to that prescribed by the external gradient. We provide a physical-sound definition of energy-scale characterizing the sytem, based upon Kolmogorov theory. Then, we show that the fluctuations of entropy production observed in the present system verify neatly the Fluctuation Relation (FR), even though the system is time-irreversible.

*Poster

Exact results for the random average process with a driven tracer

Julien Cividini * [1], Anupam Kundu, Satya N. Majumdar, David Mukamel

[1] Weizmann Institue of Science – Israel

In this talk I will present recent results concerning the statistics of the random average process (RAP) with a driven tracer (DT) in two one-dimensional geometries: the ring and the infinite line. The RAP is an instance of single-file system in which each particle hops of a random fraction of the distance towards its nearest neighbor in the direction of the hop. The DT is a particle hopping preferentially towards, say, right while all the other particles hop symmetrically towards right and left. For this particular dynamics the equations for the correlations of the particles' positions close at each order, which enables exact out of equilibrium calculations. The system can also conveniently be mapped on a mass transfer model, where the masses are the gaps between successive particles. In the presence of a DT, the average displacements of the particles are easily obtained at finite time t on a ring of finite size N, as they just obey a very simple recursion. The two- particle correlations are then obtained in the thermodynamic limit by solving an electrostatic problem. As the correlations between the gaps between gaps become negligible for large N, we also have access to their marginal distributions. The infinite line corresponds to the infinite N limit of the ring case, which does not commute with the infinite time limit that we took to obtain the stationary state. The crossover function betweeen the two geometries is obtained exactly, in the scaling regime where t/N^2 is kept constant. The average displacement of the tracer is shown to grow like sqrt(t) at large times and the density profile can be obtained in parametric form. The two-particle correlations have a scaling form at large times, where space is rescaled by sqrt(t) and the correlations themselves grow like sqrt(t). In the case of a totally asymmetric DT, the variance of the position of the DT can be obtained exactly from microscopic calculations.

*Poster

Efficiency of thermal machines at maximum power.

Bart Cleuren * [1], Bob Rutten - Christian Van den Broeck

[1] Hasselt University – Belgium

Universal properties of efficiency at maximum power are investigated in a general setting. In particular, it is demonstrated how successive symmetries placed upon the dynamics manifest themselves at the macroscopic level. A general condition is derived under which thermodynamic devices are able to attain a reversible operation.

*Poster

First passage fluctuation relations rules by cycle affinities

F. Cornu * [1], Michel Bauer

[1] CNRS – France

For a non-equilibrium stationary state described by a Markovian process it is well known that the entropy production rate can be expressed in terms of the affinity associated with every transition in the graph representation of the master equation. We exhibit the invariance of cycle affinities in finite state Markov processes under various natural probabilistic constructions : for instance under conditioning and under a new combinatorial construction that we call "drag and drop". For semi-markovian processes whose corresponding graph is made of a single cycle, we establish that the cycle current obeys a fluctuation relation for first passage times at integer winding numbers, which is dual to the fluctuation relation for the cycle current at fixed time : contrarily to seminal fluctuation relations about the probabilities for measuring a random cumulative exchange quantity or its opposite value during a given time, the latter fluctuation relations deal with the probabilities for the random time needed for one cycle to be performed in one sense or in the opposite one with a given winding number. Reference : M. Bauer and F. Cornu, J. Stat. Phys. **155** (2014) 703-736.

*Poster

Motility-induced bacterial pattern formation

Agnese Curatolo * [1], Martin Evans, Yariv Kafri, Julien Tailleur

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Driven diffusive systems define a broad class of non-equilibrium systems whose stochastic dynamics is not simply diffusive. It is instead biased in one direction, due to an intrinsic drift in the bulk. The Totally Asymmetric Simple Exclusion Process (TASEP) is a minimal model of driven diffusive systems which captures many of their interesting properties, such as the existence of non-equilibrium steady states and of phase transitions in one spatial dimension. In this lattice-based model, particles hop on empty neighboring sites at constant rates, with a left-right bias that drives the system out of equilibrium. This model has been largely used to describe a range of systems, from molecular motors to traffic jams. When connected at its ends to particle reservoirs, the TASEP exhibits a prototypical example of one-dimensional boundary driven phase transitions. Realistic examples, however, seldom involve only one lane; microtubules are made of several tubulin tracks while cars and pedestrians seldom move along a single line. In our work, we analytically construct the phase diagram of more general multilane systems, in which particles can also hop between parallel lanes. In particular, we show that the "one-dimensional" phase transition seen in the TASEP survives this additional complexity but involves new features such as non-zero steady transverse currents and shear localization.

*Poster

Surprises in two-species annihilation with exclusion

Rahul Dandekar * [1]

[1] International Centre for Theoretical Physics – Italy

We explore the effect of initial conditions on the decay of the reaction $A + B \to \phi$ in one dimension, with exclusion interaction between particles. It is well-known that the late-time density of surviving particles goes as $t^{-1/4}$ with random initial conditions, and as $t^{-1/2}$ with alternating initial conditions (ABABAB...). However, recent simulations (Lee, 2014) a nontrivial exponent for periodic i.c.s with longer periods. By means of extensive first-passage Monte Carlo simulations, and a mapping to a q-state coarsening model which can be solved in the Independent Interval Approximation (IIA), we show that the late-time decay of the density of surviving particles goes as $t^{-1/2}(\log(t))^{-1}$ starting from initial conditions made of even-length blocks (AABBAABB...), but as $t^{-1/2}$ for odd-length blocks (AAABBBAAABBB...). We relate this to what has been called kinetic symmetry breaking in case of the Glauber Ising model. We also explain the slowly varying decay exponents, seen in previous studies, for i.c.s which made of random mixtures of odd- and even-length blocks.

*Poster

Kinetics of Vapor-Solid Phase Transition

Subir K. Das * [1], Jiarul Midya

[1] Jawaharlal Nehru Centre for Advanced Scientific Research – India

In this talk I will present results for kinetics of vapor-solid transition (the solid phase having only quasi-long-range order) from molecular dynamics simulations of a single component Lennard-Jones system in space dimension d=2. Having been quenched from high temperature to the vapor-solid coexistence region, the system evolves via formation and growth of fractal domains of the solid phase, in the vapor background. For very low overall density, these fractal objects exhibit ballistic motion and grow via coalescence mechanism, the average mass following a power-law behavior with time. The computationally estimated value of the exponent is understood via appropriate theoretical argument.

*Poster

Driving-induced stability with long-range effects

Pierre De Buyl * [1], Urna Basu, Christian Maes, Karel Netoný

[1] KU Leuven – Belgium

Stabilizing an otherwise unstable configuration or phase by external action is an important challenge for a range of applications but also for the physical understanding of spatio-temporal patterns induced by nonequilibrium effects. Many examples exist for dynamical systems where by using feedback mechanisms one achieves the necessary control or steering. Other examples such as the Kapitza (inverted) pendulum which is stabilized by a time-dependent external force do not require feedback. A further step would be to eliminate the time-dependence and to use the steady nonequilibrium character of a medium to achieve such a stabilization, possibly leading to robust time-independent control strategies. We give a sufficient condition under which an applied rotation on medium particles stabilizes a slow probe in the rotation center. The nonequilibrium character of the system originates in the rotational driving. We characterize the motion of the probe close to the origin by the stiffness matrix, the symmetric part of which gets a positive Lamb shift with respect to equilibrium. For illustration we take diffusive medium particles with a self-potential in the shape of a Mexican hat, high around the origin. There is a short-range attraction between the medium particles and the heavier probe, all immersed in an equilibrium thermal bath. For no or small rotation force on the medium particles, the origin is an unstable fixed point for the probe and the precise shape of the self-potential at large distances from the origin is irrelevant for the statistical force there. Above a certain threshold of the rotation strength, while the medium particles are still repelled from the origin, the probe stabilizes there and more details of the medium density at large distance start to matter. The effect is robust around the quasi-static limit with rotation threshold only weakly depending on the temperature but the stabilization is strongest at lower temperatures. We use an expansion in distance with respect to the origin and not in nonequilibrium strength. Approaches via an effective temperature or radial density-profile changes in the driven medium do not appear to work.

*Poster

What does virialization mean?

T.O. Zolacir jr. * [1], Jose Roberto Steiner de Moura

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The virial theorem was first demonstrated by R. Clausius in 1870 and it establishes that $2langleKangle - langlesummathbfF.mathbfrangle = 0$, where $langleKangle$ is the average kinectic energy and $langlesummathbfF.mathbfrangle$ the average Clausius virial. But to achieve this result, it is needed to take a time average in a time interval that runs from the initial to a final time t [0,t] for instance. The question is: what would be the value of t to get as a result the virial theorem? In order to answer this question we considered the route to equilibrium in a long range interacting system. It is well known that in those systems the equilibrium is only achieved after a long time evolution. The convergence to equilibrium is very slow and it usually is said to be a sluggish one. But how is the virialization of this kind of system? We performed simulations in a Hamiltoniam mean field model (HMF) for large times to seek for equilibrium and virialization. Despite the fact that equilibrium and virialization could be different concepts, once equilibrium is related to thermodynamics and the virial has a mechanical origin, our results show that these two notions are imbricated. We show that the route to equilibrium occurs in the same way as virialization. In astrophysics, is said that a virialized system is the one that the fractions of the energies are established: $2langleKangle - langleUangle = 0$; where $langleUangle$ is the average gravitational potential energy. Astrophysicists use to say that an observed cluster nowadays is virialized, in the sense that the mean kinetic energy a related to the mean potential energy (those fractions) is as showed above, even if the system may not be in the thermodynamic equilibrium. What we show is that the virialization comes with the thermodynamic equilibrium or the thermodynamic equilibrium comes with virialization. These two concepts come together and they are achieved in a sluggish way.

*Poster

Extended local equilibrium approach to stochastic thermodynamics

Jean-François Derivaux * [1], Yannick De Decker

[1] Université libre de Bruxelles – Belgium

Over recent years, a new field of statistical physics called stochastic thermodynamics has emerged, which aims at describing small systems subjected to fluctuations [1]. In this description, the temporal evolution of thermodynamic quantities (e.g. work, entropy, ...) follows a fluctuating trajectory. Recently a new approach in the definition of stochastic thermodynamic variables was proposed by De Decker et al. [2] based on an extension of the local equilibrium hypothesis. The essence of this method is to make the state variables stochastic by adding a noise term to their deterministic (i.e. macroscopic) evolution equation. This method allows us to extend quite naturally the macroscopic non-equilibrium thermodynamics to small scale systems. Furthermore we can easily compute the probability distribution of stochastic thermodynamic quantities or relate them to macroscopic parameters. This new formulation seems promising to describe mesoscopic systems. Using this new framework we investigated in particular the entropy production associated with chemical reactions and heat transfer in steady states. Entropy production is knew to play a central role in the stability criterion and is a measure of efficiency for small systems. We will present how the fluctuations can induce novelties in its behavior. For instance it can be showed that the mean of entropy production (i.e. the experimentally accessible measurement) can slightly differ from the deterministic prediction in the case of non-linear chemical reactions. We can go a step further and also obtain the probability distribution of entropy production in and out equilibrium, which allows us to derive fluctuation theorems[3]. Deviations of the mean behavior can be so completely characterized. Current efforts are made to complete this formalism and apply it to more sophisticated problems (thermodiffusion, complex chemical reactions). [1] Seifert, U. Stochastic Thermodynamics, Fluctuation Theorems and Molecular Machines. Rep. Prog. Phys. 2012, 75 (12), 126001. [2] De Decker, Y. ; Cantú Ros, A. G. ; Nicolis, G. Extended Local Equilibrium Approach to Stochastic Thermodynamics. Eur. Phys. J. Spec. Top. 2015, 224 (5), 947–968. [3] De Decker, Y.; Derivaux, J.-F.; Nicolis, G. Stochastic Thermodynamics of Reactive Systems: An Extended Local Equilibrium Approach. Phys. Rev. E 2016, 93 (4), 42127.

*Poster

Steady-state properties of an inhomogeneous two-channel exclusion process

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In protein synthesis, the genetic information is deciphered into proteins by molecular machines called ribosomes, which attach themselves at the start end of mRNA, move along the chain in a unidirectional manner and finally detach at the stop end [1]. Each translation step requires the binding of a freely diffusing transfer-RNA (tRNA) molecule, carrying the amino acid specific to each codon. The important factor affecting the ribosome translation rate is relative concentrations of tRNA, which may vary from codon to codon. The codons with lower concentrations of tRNA reduce the protein synthesis rate and thus play the role of an inhomogeneity (or bottleneck) in a homogeneous system [2]. Apart from this, inhomogeneities also occur naturally in many other transport systems such as vehicular traffic [3] and data flow in Von Neumann architecture [4]. In traffic flow, the ongoing construction on roads, a slow moving vehicle or an accident can lead to slow down the flow rate on highways and produces congestion. Further, the separation of the CPU and the memory in computers creates Von Neumann bottleneck, which limits the performance of the computer via limited bandwidth between the CPU and the memory [4]. This work is devoted to the study of effects of a localized bottleneck in a two-channel totally asymmetric simple exclusion process (TASEP) with Langmuir kinetics (LK), which is a non-equilibrium system. The hybrid mean-field approach, combined with singular perturbation technique, is used to get steady-state phase diagrams and density profiles. We have thoroughly examined the role played by the strength of bottleneck, binding constant and lane-changing rate in the system dynamics. The origin and dynamics of a bottleneck-induced shock, the bottleneck phase and bottleneck-induced phase transitions are also investigated. Further, the critical values of bottleneck rate are identified, which signify the changes in the topology of phase diagram. It is also found that an increase in lane-changing rate as well as unequal attachment, detachment rates can weaken or enhance the bottleneck's effect under different coupling conditions. Our theoretical arguments are in good agreement with extensively performed Monte Carlo simulations. References: 1. Chou, T. and Lakatos, G., Clustered bottlenecks in mRNA translation and protein synthesis, Phys. Rev. Lett., 93 (19), 198101, 2004. 2. Sørensen, M. A., Kurland, C. G., and Pedersen, S., Codon usage determines translation rate in escherichia coli, J. mol. biol. 207(2), 365–377, 1989. 3. Gupta, A. K., and Dhiman, I., Phase diagram of a continuum traffic flow model with a static bottleneck, Nonlinear Dynamics, 79 (1), 663–671, 2014. 4. Lin, Y., Wang, F., Zheng, X., Gao, H. and Zhang, L., Monte Carlo simulation of the Ising model on FPGA, J. Comput. Phys., 237, 224–234, 2013.

*Poster

Critical behavior of a vector-mediated epidemic model

Adriana Gomes Dickman * [1], Ronald Dickman

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We study a lattice model for vector-mediated transmission of a disease in a population consisting of two species, A and B, which contract the disease from one another. Individuals of species A are sedentary, while those of species B (the vector) diffuse in space. Examples of such diseases are malaria, dengue fever, and Pierce's disease in vineyards. There are several ways of interpreting the model: A contact process (CP) on the A population, mediated by B; a diffusive epidemic process (DEP) on the B population, mediated by A; or a multicomponent epidemic process in which B and A are equally essential. The model exhibits a phase transition between an absorbing (infection free) phase and an active one as parameters such as infection rates and vector density are varied. We study the static and dynamic critical behavior of the model using spreading, initial decay, and quasistationary simulations. Although phase transitions to an absorbing state fall generically in the directed percolation (DP) universality class, this appears not to be the case for the present model. Our results clearly exclude DP scaling and strongly suggest DEP universality. They also raise the possibility of two phase transitions in spreading: At the critical point for survival, the number $n(t)$ of infected individuals grows more slowly than a power law, while, for parameters such that $n(t)$ grows as a power law, the survival probability decays more slowly than a power law.

*Poster

Arcetri models

Xavier Durang * [1], Malte Henkel

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Building on an analogy between the ageing behaviour of magnetic systems and growing interfaces, the Arcetri models, three new exactly solvable models for growing interfaces are introduced. The long-time behaviour of the interface width and of the two-time correlators and responses is analysed. The first of these models shares many properties with the kinetic spherical model and with the Edwards-Wilkinson model, but for d
$le2$ the non-equilibrium exponents are different. For the second and third model, the long-time behaviour of the correlation and response shows respectively multiscaling and logarithmic scaling behaviour. We also discuss the relation of these models with the $p = 2$ spherical spin glass and with the $O(n)$ model in the large-n limit.

*Poster

Uniform derivation of Coulomb collisional transport thanks to Debye shielding

Yves Elskens * [1], Dominique Escande, Fabrice Doveil

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The effective potential acting on particles in plasmas being essentially the Debye-shielded Coulomb potential, the particles collisional transport in thermal equilibrium is calculated for all impact parameters b, with a convergent expression reducing to Rutherford scattering for small b. No cutoff at the Debye length scale is needed, and the Coulomb logarithm is only slightly modified.
J. Plas. Phys. 81 (2015) 305810101 (9 pages) http://dx.doi.org/10.1017/S0022377814000415

*Poster

Evidence of an absorbing phase transition in a bi-stable system with delay feedback

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It is well known that complex dynamical evolution may originate from simple low dimensional dynamical systems when a time-delayed feedback mechanism is considered. These may typically happen in systems where the propagation time of a signal is not negligible with respect to the typical timescale of the local dynamics. Examples include many biological systems and laser physics, where a long delayed feedback may be easily obtained by optical or electronic device. A deep analogy exists between delayed feedback and spatially extended dynamical systems. In particular, it is well known that deterministic systems with long time-delay au may be interpreted in terms of a suitable spatiotemporal dynamics citeuno of spatial size au. In this work we extend this interpretation to stochastic differential equations, considering a simple bistable system with long delayed feedback and multiplicative noise, introduced in a way to preserve the lowest energy state. This dynamics can be described with the following prototype equation:

$$dx_t = -U'_a(x_t) + g, x_{t-au} + x_t, dW_t \tag{3}$$

where dW is a Wiener process, $U'_a(x_t) = x_t(x_t - 1)(x_t + 1 + a)$, a is the asymmetry coefficient of the potential $U(x_t)$ and $g > 0$ is the feedback coefficient. Our numerical analysis shows that – as the asymmetry in the bi-stable potential is carefully changed – our system undergoes a transition into an absorbing state of the effective spatio-temporal dynamics , i.e. the lowest energy state, with critical exponents compatible with the celebrated Directed Percolation class. This simple model is believed to qualitatively capture the behavior of a class of laser systems such as a bistable semiconductor laser with long delayed feedback [2-3]. While extending the validity of the space-time analogy and verifying several features of front dynamics, we expect our results to possibly trigger new directions of theoretical and experimental research. The possibility to independently generate and erase localized states in our setup as in spatially-extended systems, enable their use as otpical information bits in a fast, all-optical setup. beginthebibliography9 bibitemunoG. Giacomelli and A. Politi, Phys. Rev. Lett. 76, 2686 (1996). bibitemdueG. Giacomelli, F. Marino, M.A. Zaks and S. Yanchuk, Europ. Phys. Lett. 99 58005 (2012). bibitemtreGiacomelli, F. Marino, M.A. Zaks and S. Yanchuk, Phys. Rev. E 88 062920 (2013). endthebibliography enddocument

*Poster

Exact symmetries in the velocity fluctuations of a hot Brownian swimmer

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Symmetries constrain dynamics. We test this fundamental physical principle, experimentally and by molecular dynamics simulations, for a hot Janus swimmer operating far from thermal equilibrium. Our results establish scalar and vectorial steady-state fluctuation theorems and a thermodynamic uncertainty relation that link the fluctuating particle current to its entropy production at an effective temperature. A Markovian minimal model elucidates the underlying non-equilbrium physics

*Poster

Emergence of Brownian Motor

Alexander Feigel * [1]

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Emergence of motion out of thermal equilibrium will be discussed. Significant effort was dedicated to the research of mechanisms of motion out of thermal equilibrium. Mechanical system, such as Brownian ratchet, generates motion out of thermal fluctuations if spatial symmetry is broken and if the ratchet is coupled to several thermal bathes. Brownian ratchet is a leading physical model for molecular motors. To the best of my knowledge, the question of emergence and thermodynamic stability of Brownian Ratchets remains open. One can ask a question: if Brownian ratchet can be either in symmetric or asymmetric states whether thermodynamic forces favor transition to asymmetric state and, therefore, favor emergence of motion? Answering this question will help estimating required conditions and universality of directed motion out of thermal equilibrium. These conditions and universality may be an important link between non-equilibrium thermodynamics and Origin of Life as well as a guide to micro-fabrication of the novel nano motors. Here, I'll present detailed analysis of emergence Brownian Motor using Triangula model[1] of Brownian ratchet. The results are general to any system with multiple degrees of freedom, for instance molecules. [1] Van den Broeck, R. Kawai, and P. Meurs, Phys. Rev. Lett. 93 , 090601 (2004)

*Poster

Modeling the Earth: Climate on an Icosphere

Stephanie Fouts * [1], L. Jonathan Cook

[1] Washington and Lee University – United States

The totally asymmetric simple exclusion process with Langmuir kinetics is a one-dimensional transport model used to study the motion of particles through a lattice. Its applications include systems in the fields of biology, climatology, mathematics, civil engineering, and physics. In our research, we examine the temporal dynamics through the power spectra, as well as the time-averaged particle distribution on the lattice via Monte Carlo simulations. We have applied our particle transport model to an icosahedron in an attempt to model Earth's changing climate. In our research, we examine the temporal dynamics of the particle distribution on the lattice, as they correspond to seasonal heat fluctuations in the polar and equatorial regions of the globe. Using Monte Carlos simulations, we alter the input parameters of the system to explore the resultant actions of the Earth-system model. Our findings include seasonal oscillations consistent with those seen in reality. We also built a mathematical framework for our model which, when solved numerically, matches the oscillations seen in our physical system.

*Poster

Between universality subclasses: numerical and experimental results for KPZ interfaces with curved initial conditions

Yosuke Fukai * [1], Kazumasa A. Takeuchi

[1] the University of Tokyo – Japan

The concept of universality class is important to understand scale-invariant phenomena such as critical phenomena, which has been successfully applied to non-equilibrium systems as well. Particularly, the Kadar-Parisi-Zhang (KPZ) universality class[1,2] is thought to be one of the most fundamental universality classes for non-equilibrium growing interfaces. Recently, it has been shown both theoretically and experimentally that the 1+1D KPZ class splits into "subclasses", which are characterized by the same scaling exponents yet different statistical properties, depending on initial condition. For example, height fluctuations of interfaces with flat initial condition (flat subclass) show the Gaussian orthogonal ensemble Tracy-Widom distribution, while those with point initial condition (circular subclass) agree with the Gaussian unitary ensemble Tracy-Widom distribution. Spatial and temporal correlation functions are also shown to be dependent on the initial condition[2,3,4]. Here, I would like to present our numerical and experimental results about KPZ-class interfaces with finite-curvature initial conditions, which can be considered as "intermediate" initial conditions interpolating the flat and point initial conditions. These results were obtained by simulations of a cluster-growing model (Eden D model) and experiments using liquid crystal electroconvection. When the curvature is positive, it is shown that the height distribution, spatial correlation function and temporal correlation function change from those for flat inter- faces to circular interfaces, indicating a crossover between subclasses. In contrast, for negative initial curvatures, the statistical properties always shows those for flat interfaces in our time window. The characteristic time of the crossover in the positive-curvature case and the reason for the difference between the positive and negative cases are also discussed. [1] M. Kardar, G. Parisi, and Y.-C. Zhang, Phys. Rev. Lett. 56, 889 (1986). [2] I. Corwin, Rand. Mat. Th. Appl. 1, 1130001 (2012). [3] K. A. Takeuchi and M. Sano, J. Stat. Phys. 147, 853 (2012). [4] P. L. Ferrari and H. Spohn, arXiv:1602.00486 [cond-mat, physics:math-ph] (2016).

*Poster

Large deviation theory as a measure of the entropy reduction in systems under feedback

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The idea of developing a thermodynamic theory of systems under an external feedback dates back to the origin of statistical physics when Maxwell made his famous gedanken experiment concerning the effect of a Demon with some information about the system and the effect on the thermodynamics of the system itself. Recently this branch of thermodynamics has got a rapid boost thank to fluctuation theorems [1, 2]. An interesting complementary perspective comes from a branch of information theory named Large deviation theory (LDT). LDT is the mathematical framework which copes with the probability of large fluctuations departing from the average ensemble values of statistical quantities. In particular LDT demonstrates that for a large class of probability density functions (PDF), defined on the phase space, the probability of having a fluctuation respect to the average value drops exponentially. The exponent is related to the Legendre-Fenchel transform of the scaled cumulant generating function [3]. It has been demonstrated that the LDT provides a very elegant way to derive the thermodynamic principles of maximum entropy and minimal free energy for the microcanonical and canonical ensemble respectively in thermodynamic equilibrium [4]. Extension to non equilibrium conditions have been investigated [5]. We present here an extension of the formalism that allows to use LDT also for systems under an external feedback, in particular we show how it is possible to define a direct connection between the measurement performed by the feedback and its accuracy and the maximum entropy reduction that can be achieved with that feedback. [1] T. Sagawa and M. Ueda, Phys. Rev. E, 85, 021104 (2012). [2] T. Sagawa and M. Ueda, Phys. Rev. Lett., 109, 180602 (2012). [3] R.S. Ellis, Entropy, Large Deviations, and Statistical Mechanics, Springer, New York, 1985. [4] H. Touchette, Physics Reports, 478, 169 (2009). [5] H. Touchette, (Chapter 11), Non equilibrium Statistical Physics of small systems, Edited by R. Klages, W. Just and C. Jarzinsky; Wyley, 2013.

*Poster

Nonequilibrium dynamics of a dry friction model subjected to coloured noise

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We investigate a model with pure dry friction and coloured (exponentially correlated) noise

$$\dot{v} = -\Delta\sigma(v) + n.$$

Δ is the friction coefficient, $\sigma(v)$ is the sign function, representing the dry friction and n denotes the coloured noise $\langle n(t)n(s)\rangle = (D/\tau)\exp(-|t-s|/\tau)$.
By using the unified coloured noise approximation, developed by P. Jung and P. Hänggi, an approximate expression for the stationary probability density $P(v)$ can be obtained, which becomes delta-peaked for an increasing correlation time of the noise, signalling a nonequilibrium localisation phenomenon, related to stick-slip transitions in systems with dry friction. These results show good agreement with the numerical simulations.
To gain deeper insight to the model, we studied the equivalent two-dimensional system (v, n), computing the stationary distribution as well as the direct computation of the probability current. The latter is a clear signature of the nonequilibrium properties of the underlying dynamics. By computing the power spectral density S_{vv} and increasing the correlation time of the noise τ, we observe a decrease of the full width at half maximum, starting around a "critical" value of τ, which indicates the above mentioned stick-slip transition.

*Poster

Relativistic hydrodynamic theories versus numerical experiments: molecular dynamics simulation of an imperfect relativistic gas

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Relativistic generalization of hydrodynamic equations has gained much attention in high energy physics as well as statistical physics community ever since it has been formulated. Despite its long history and wide usage the fundamental postulates and basic variables of the theory are still under debate especially in the presence of dissipative effects. A unique formulation of relativistic hydrodynamics is thus not available neither in the context of first-order theories nor the so called causal extended theories. In this work we propose to numerically test the validity of four different types of first-order theories (and consequently the validity of their basic assumptions) in the hydrodynamic limit where causality effects are less important and thus such theories are supposed to give a fairly good description of the system. In this regard, we study the propagation of fluctuations in a dissipative relativistic gas in static background and compare the analytical prediction of these theories to numerical data obtained from our fully relativistic molecular dynamics simulation of hard-sphere gas [1]. The results indicate that the predictions of the recent formulation due to Tsumura-Kunihiro-Ohnishi [2] are more consistent with our results than the traditional theories due to Meixner [3,4], modified Eckart [3,5] and modified Marle-Stewart [2,6]. [1] A. Montakhab, M. Ghodrat, M. Barati, Phys. Rev. E 79 (2009) 031124, L. Shahsavar, M. Ghodrat, A. Montakhab, Unpublished. [2] K. Tsumura, T. Kunihiro, K. Ohnishi, Phys. Lett. B. 646 (2007) 134. [3] A. L. Garcia-Perciante, L. S. Garcia-Colin, A. Sandoval-Villalbazo, Phys. Rev. E 79 (2009) 066310. [4] J. Meixner, Ann. Phys. 43 (1943) 244 . [5] C. Eckart, Phys. Rev. 58 (1940) 919. [6] J. M. Stewart, Non-Equilibrium Relativistic Kinetic Theory, volume 10 of Lecture Notes in Physics, Springer, Berlin, 1971.

*Poster

Transport resistance of the surface of nanoporous materials

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Nanoporous materials are important in industrial separation, but their application is subject to strong interfacial barriers to the entry and transport of fluids. At certain conditions the fluid inside and outside the nanoporous material can be viewed as a two phase system, with an interface between them, which poses an excess resistance to matter flow. We show that there exist two kinds of phenomena which influence the interfacial resistance: hydrodynamic effects and thermodynamic effects, which are independent of each other. Here, we investigate the role of the thermodynamic effects in carbon nanotubes (CNTs) and slit pores, and compare the associated thermodynmic resistance with that due to hydroynamic effects traditionally modelled by the established Sampson expression. Using CH4 and CO2 as model fluids we show that the thermodynamic resistance is especially important for moderate to high pressures, at which the fluid within the CNT or slit pore is in the condensed state. Further, we show that at such pressures the thermodynamic resistance becomes comparable with the internal resistance to fluid transport at length scales typical of membranes used in fuel cells, and of importance in membrane-based separation, and nanofuidics in general.

*Poster

Effective thermodynamics for a driven athermal system with dry friction

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Which are the situations where an effective thermodynamic theory works even in the lack of thermal equilibrium? Which is the meaning of "temperature" for an out-of-equilibrium system? I present here the study of a driven athermal system, which is a one-dimensional chain of masses connected by harmonic springs and subject to Coulomb dry friction, where answers to the above questions can be provided. The main result of this investigation is the evidence that, even in presence of a driven dissipative dynamics, the probability to visit the mechanically stable configurations of this system fulfills the Edwards conjecture[1]: an effective equilibrium description for frictional systems is possible. Such an evidence is obtained by comparing the exact calculation of the partition function of our system, done by means of transfer matrix approach, to the numerical simulations of the driven dissipative dynamics. Interestingly enough, the existence of a critical point at infinite effective temperature is pointed out[1]. Finally, I will show how the prescription of the Edwards thermodynamics can be generalized to the situation where the viscous friction is added on the top of dry friction[2]. [1] G. Gradenigo, E. E. Ferrero, E. Bertin, J.-L. Barrat, Phys. Rev. Lett. 115, 140601 (2015). [2] G. Gradenigo, E. Bertin, J.-L. Barrat, in preparation.

*Poster

Computation of maximum likelihood transition pathways in nonequilibrium statistical mechanics

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We describe the long time behavior of meta-stable nonequilibrium systems subject to random noise by computing the minimizer of the associated large deviation rate function. This allows us to quantify transition rates, probabilities and transition pathways precisely in the limit of a vanishing control parameter. The computation is exemplified with several "non-standard" transitions, that each exhibit a different complication: First, transitions for nucleation and phase separation, where competing gradient flows break detailed balance. The appearance of a slow manifold leads to a maximum likelihood transition pathway that approaches the separatrix far from any saddle point. Second, a bi-stable spatially extended chemical reaction-diffusion equation, where transitions occur via traveling waves, and the relative stability of the fixed points is determined by the spatial extend of the system. Third, a bi-stable slow-fast system in the limit of large time-scale separation, where the Hamiltonian associated with the large deviation principle is non-quadratic in the conjugate momentum variable. In this case the large deviation principle for the slow variable is different from that of any stochastic differential equation one would write for the slow variable alone.

*Poster

Large Deviations and Discreteness Effects in Population Dynamics

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We analyse numerically the effects of small population size in the initial transient regime of a simple example population dynamics. These effects play an important role for the numerical determination of large deviation functions of additive observables for stochastic processes. A method commonly used in order to determine such functions is the so-called cloning algorithm which in its non-constant population version essentially reduces to the determination of the growth rate of a population, averaged over many realizations of the dynamics. However, the averaging of populations is highly dependent not only on the number of realizations of the population dynamics, and on the initial population size but also on the cut-off time (or cut-off population) considered to stop their numerical evolution. This may result in an over-influence of discreteness effects at initial times, caused by small population size. We overcome these effects by introducing a (realization-dependent) time delay in the evolution of populations, additional to the discarding of the initial transient regime of the population growth where these discreteness effects are strong. We show that the resulting improvement in the estimation of the large deviation function comes precisely from these two main contributions.

*Poster

Steady State Thermodynamics : exploring contact between out-of-equilibirium systems

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Although equilibrium thermodynamics is well established and universal, an equivalent theoretical framework remains to be built for non-equilibrium systems, at least for simple ones which are in a steady state. Oono and Paniconi (1998) and some years after, Sasa and Tasaki (2006) have developed a "Steady State Thermodynamics" (SST) which is exploring the general thermodynamic structure that steady state systems should obey. On the other hand, an analytic approach based on simple statistical systems has led to the definition of Intensive Thermodynamic Parameters (ITP) with respect to conserved quantities (Bertin, Martens, Dauchot and Droz (2007)). They play an analogous role as temperature or chemical potential at equilibrium. More recently, Pradhan, Seifert et.al. (2011) and Dickman et.al. (2014, 2015) have revived these studies with numerical simulations of driven lattice gas models. They have tested in particular the consistency of Sasa and Tasaki's SST by exploring the zeroth law that must be satisfied by intensive parameters. They have found that a thermodynamic structure is at best approximately verified. The aim of this project is to pursue this latter work by investigating in more details the contact between steady state systems and to make the link between statistical approaches on one side, and Sasa and Tasaki's thermodynamical approach on the other side. In particular, one would like to understand why Sasa and Tasaki's SST may fail and, if it does so, to discuss a potential extension of it. In this poster, we will present theoretical results on mass transport models, emphasizing the important role of contact dynamics in determining the steady state reached by two systems in contact. More precisely, we show explicitly on a mass transport model that imposing a null net flux at contact does not lead in general to an equalization of the chemical potentials defined for each single systems. The latter have to be modified in general to describe the steady state repartition of mass between two systems. Hence, the central issue we address is to find the relevant definition of the chemical potential, if any.

*Poster

Stochastic quantum Zeno by large deviation theory

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Quantum measurements are crucial for observing the properties of a quantum system, which, however, unavoidably perturb its state and dynamics in an irreversible way. Here we study the dynamics of a quantum system being subjected to a sequence of projective measurements applied at random times. In the case of independent and identically distributed intervals of time between consecutive measurements, we analytically demonstrate that the survival probability of the system to remain in the projected state assumes a large deviation (exponentially decaying) form in the limit of an infinite number of measurements. This allows us to estimate the typical value of the survival probability, which can therefore be tuned by controlling the probability distribution of the random time intervals. Our analytical results are numerically tested for Zeno-protected entangled states, which also demonstrate that the presence of disorder in the measurement sequence further enhances the survival probability when the Zeno limit is not reached (as it happens in experiments). Our studies provide a new tool for protecting and controlling the amount of quantum coherence in open complex quantum systems by means of tunable stochastic measurements.

*Poster

Effect of Mutually Interactive Langmuir Kinetics on the Collective Dynamics in a Two-Lane Asymmetrically Coupled TASEP

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The present work concentrates on analyzing the role played by the mutual interaction (MI) in two-channel biological transport processes. The problem is modeled using a two-channel totally asymmetric simple exclusion process (TASEP) coupled with Langmuir kinetics (LK). Motivated by the recent in-vitro experimental observations on clustering of motor proteins on microtubules filament, the attachment and detachment rates are assumed to be dependent on the configuration of the neighboring sites.
The model is analyzed within the framework of continuum mean-field theory and the phase diagrams along with density profiles are obtained using boundary layer analysis. The effect of mutual interactions on the phase diagram for two different situations of attachment and detachment (LK) rates is discussed. For symmetric MILK, the topological structure of the phase diagram remains similar to the one in without MI; while for the antisymmetric MILK, after a certain critical value of attractive/repulsive MI, significant changes are found in the qualitative nature of phase diagram. Moreover, it is shown that the type of MI affects the dynamic properties of motor proteins. The theoretical findings are supported by extensive Monte-Carlo simulations.

*Poster

Experimental discovery that the Green-Kubo theory fails for viscosity in a 2D dusty plasma

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The Green-Kubo relation provides a way to obtain a transport coefficient using data for equilibrium conditions. It is widely used with simulation data; however, experimental tests are lacking to confirm whether the Green-Kubo relation yields the same result as a hydrodynamic measurement. This problem exists because few experimental systems are available where the individual particles are underdamped and an imaging diagnostic allows the recording of data needed an input to a Green-Kubo relation. The required data are positions, velocities, and potentials for individual particles. A dusty plasma is a physical system in which these measurements are possible [1]. A dusty plasma is a mixture of micron-size polymer spheres along with the usual electrons, ions and neutral gas atoms of a weakly ionized plasma. The microspheres can be levitated in a single horizontal layer and tracked individually by video microscopy. This single layer of particles, if unmodified, takes the form of a 2D Wigner lattice, which can be heated using laser manipulation [2] to maintain a 2D liquid for the purpose of studying its transport properties. Recently a dusty plasma was used to demonstrate, for the first time, that experimental data can be used as an input to the Green-Kubo relation for viscosity [3]. Since then, we have improved the instrumentation so that we can perform an accurate test of the validity of the Green-Kubo relation for viscosity. In this test, we compare experimental runs with and without shear. The runs with shear are analyzed using the usual constitutive relation for viscosity,

$$\eta = P_{xy}/\gamma \quad (1)$$

where P_{xy} is the local time-averaged shear stress and *gamma* is the local time-averaged shear rate. The runs without shear are analyzed using the Green-Kubo relation,

$$\eta = \frac{1}{Ak_BT}\int_0^\infty C_\eta(t)dt \quad (2)$$

which also makes use of P_{xy} through its autocorrelation function C_η. Testing the Green-Kubo relation by comparing an experiment to a simulation, for example using water or liquid argon, poses the difficulty that there are two assumptions in the simulation: the validity of Green-Kubo and the validity of the potential model. The model for interparticle interactions for many systems is uncertain, so that any discrepancy between the experiment and simulation is usually attributed to errors the potential model rather than the Green-Kubo relation. Our experiment avoids this difficulty since we compare two results from the same experiment, both using the same assumption for the interparticle potential, so that any discrepancy can be attributed to the Green-Kubo relation. For our 2D dusty plasma, we find a discrepancy of a factor of two in the experimental values of viscosity obtained from the two methods. The one obtained using the Green-Kubo relation, Eq. (2), is twice as large as the one obtained using the reliable constitutive relation, Eq. (1). Work supported by the US Department of Energy, National Science

*Poster

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Sensory capacity: an information theoretical measure of the performance of a sensor

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For a general sensory system following an external stochastic signal, we introduce the sensory capacity [1]. This quantity characterizes the performance of a sensor: sensory capacity is maximal if the instantaneous state of the sensor has as much information about a signal as the whole time-series of the sensor. We show that adding a memory to the sensor increases the sensory capacity. This increase quantifies the improvement of the sensor with the addition of the memory. Our results are obtained with the framework of stochastic thermodynamics of bipartite systems, which allows for the definition of an efficiency that relates the rate with which the sensor learns about the signal with the energy dissipated by the sensor, which is given by the thermodynamic entropy production. We demonstrate a general tradeoff between sensory capacity and efficiency: if the sensory capacity is equal to its maximum 1, then the efficiency must be less than 1/2. As a physical realization of a sensor we consider a two component cellular network estimating a fluctuating external ligand concentration as signal. This model leads to coupled linear Langevin equations that allow us to obtain explicit analytical results. [1] D. Hartich, A. C. Barato, and U. Seifert (2015) arXiv:1509.02111

*Poster

Temperature-driven and chemical-potential-driven adiabatic pumping in coherent electron transport

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Adiabatic pumping is a process by which a finite charge(heat) current is induced under periodic slow modulation of external control parameters. This phenomenon has been studied for long time as an important issue in time-dependent quantum transport. Adiabatic pumping has also gained attentions as a method for discussing the thermodynamics properties of mesoscopic systems. Temperature pumping has been examined only in incoherent transport(whereby a system and reservoirs are strongly coupled) so far, rather than in coherent transport(whereby a system and reservoirs are strongly coupled)[1,2]. To capture nonequilibrium thermodynamic features in coherent transport, a theoretical framework for pumping induced by thermodynamic variables of the reservoirs(i.e., temperatures and chemical potentials), is strongly required. We discuss adiabatic charge pumping in a single-level quantum dot (QD) system strongly connected with two reservoirs whose temperature and chemical potential are periodically driven[3]. We consider the Coulomb interaction within the QD, because the interaction is necessary for adiabatic pumping through the QD driven by reservoirs' parameter. We derive an expression of pumping current by the Keldysh formalism and estimate it for appropriate parameters. The present adiabatic pumping is induced by delayed response of the system to changing of the reservoir parameters. We also compare temperature-driven pumping with chemical-potential-driven one and show their different properties in low temperature region. References: [1] J. Ren, P. Hanggi and B. Li, Phys. Rev. Lett. **104**, 170601 (2010). [2] T. Yuge, T. Sagawa, A. Sugita and H. Hayakawa, J. Stat. Phys. **153**, 412 (2013). [3] M. Hasegawa and T. Kato, arXiv:1601.05812 (2016).

*Poster

Predicting nonlinear response from equilibrium measurements

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We investigate a small statistical mechanical system trapped in a non-harmonic potential subjected to external driving. This is realised by a single spherical colloidal particle dispersed in water, which is trapped and potentially driven in an optical tweezers. The non-linear potential is realized by interactions with a neraby flat wall. Monitoring the particles trajectory in equilibrium we use a recently developed theory [Basu et al. PCCP 17, 6653 (2015)] to predict its non-equilibrium behaviour up to second order, from dynamical details and dissipation of the system. Predictions are veryfied by comparison with non-equilibrium trajectories measured for the same parameters showing good agreement for various driving amplitudes and frequencies.

*Poster

Local stationarity for out-of-equilibrium phenomena

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This presentation discusses local stationarity in time explaining rigorously how stationary solutions can remain slowly time dependent after a long time limit. A mathematical definition of almost invariant and nearly indistinguishable states on C*-algebras is introduced using functions of bounded mean oscillation. Rescaling of time yields generalized time flows of almost invariant and macroscopically indistinguishable states, that are mathematically related to stable convolution semigroups and fractional calculus. The infinitesimal generator is a fractional derivative of order less than or equal to unity. Applications of the analysis are given to irreversibility and to a physical experiment.

*Poster

Statistical physics of memory driven systems

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For classical systems, statistical description is usually required when the dimension of the system phase space is important. This description is used when considering many body problems such as the thermodynamical description of fluids, granular media or the diffusion of Brownian particles in the presence of a thermal reservoir. Can this limit be reached at the single particle level? We address this question by considering a single particle coupled to its own past, via a wave-mediated size-controllable memory, which stores the past trajectory of the particle. Such an object has been turn into reality by Couder et al [1,2] by using liquid bouncing droplets that interact with the waves they generate by impacting a liquid surface. In those experiments, the memory is made by stationary waves with a tunable damping time. The wave memory triggers various regime from individual self-propelled particle motion to structured chaos [3] or self-organization processes between a particle and its waves [4]. In the limit of a large amount of "souvenirs" stored in the wave field, we will show that the dynamics can be well described by the tools of non-equilibrium statistical mechanics. Both the dynamics of the particle and the wave-mediated memory are investigated. We show that, from the particle-point of view, the memory acts as a random force. The particle dynamics is adequately described by a Langevin equation for self-propelled systems. The corresponding Fokker-Planck equation shows that the memory can be seen as a thermal reservoir whose temperature is tuned via the amount of "souvenirs" in the dynamics. The features of this unusual wave-like thermal reservoir are investigated from an energetic and entropic perspective. We show that the global wave field is on average weaker that one would expect from superposition of random wave fields. This depletion originates from destructive interferences that the particle generates along its trajectory, corresponding to a kind-of minimization principle.

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*Poster

Anomalous yet Brownian Diffusion of a Colloidal Particle close to a Flat Surface: A Monte Carlo Investigation

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Anomalous yet Brownian diffusion refers to a process where a linear mean-square displacement coexists with a non-Gaussian Displacement Distribution (DispD) [1]. Recently, Bechhoefer's group has reported experimental evidence that the diffusion of a colloidal particle close to a flat surface exhibits non-Gaussian displacement distributions with exponential tails. Due to hydrodynamic interactions, the diffusivity D(r) of the particle is space-dependent near the surface, which makes it explore a diffusivity landscape in time as it moves in space. This space-dependent diffusivity implies the possibility of different interpretations of the stochastic term in the overdamped Langevin equation (i.e. the Ito-Stratonovich dilemma). Furthermore, in the presence of properly chosen external potentials (e.g., gravity and electrostatic repulsion), the colloid is confined to diffuse in a high gradient diffusivity region in the vicinity of the wall. Using Lattice Monte Carlo simulations and a novel algorithm, we explore the role of these effects on the diffusion properties of the particle. Finally, we discuss the possibility for this system to test the "diffusing diffusivity" model propose by Chubynsky and Slater [2]. [1] B. Wang et al., PNAS 106, 15160 (2009), [2] M. V. Chubynsky and G. W. Slater, PRL 113, 098302 (2014)

*Poster

Heating in integrable periodically driven systems

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We discuss the relaxation process of quantum many-body systems under periodic driving fields (e.g., ac optical fields). In such systems, even if the instantaneous Hamiltonian may be simple, the non-equilibrium steady state can have highly non-trivial structures. One of the key features to understand the relaxation process is the energy absorption from the periodic driving fields [1]. We suppose that the system heats up owing to the periodic driving and ends up in a steady state with infinite temperature, which is indeed believed to be the universal scenario for steady states of non-integrable periodically driven systems [2]. On the other hand, the situation can be rather different for integrable periodically driven systems. Such systems have many conserved quantities, and hence may reach the steady state with the generalized Gibbs ensemble dependent on the initial state [3]. This has led to the prevalent belief that the periodic driving cannot heat up integrable systems to the steady state at infinite temperature. We here reveal that it is not always the case; we give a prototype integrable model which heats up to infinite temperature and show that local properties of the steady states are described by the infinite-temperature states in the thermodynamic limit. [1] T. Mori, T. Kuwahara, and K. Saito, Phys. Rev. Lett., 116, 120401 (2016). [2] L. D'Alessio and M. Rigol, Phys. Rev. X 4, 041048 (2014). [3] A. Lazarides, A. Das, and R. Moessner, Phys. Rev. Lett. 112, 150401 (2014).

*Poster

Derivation of Stokes' law without the hydrodynamic equations

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In this presentation, we study the friction coefficient of a Brownian particle in a viscous incompressible fluid at low Reynolds number. According to Kirkwood's formula, the friction coefficient is expressed in terms of the stress correlation on the surface of the Brownian particle. Then, with the aid of large deviation theory, we phenomenologically relate the surface stress correlation to the stress correlation in the bulk of the fluid, where the bulk stress correlation is characterized by the viscosity from the Green–Kubo formula. By combining Kirkwood's formula and the Green–Kubo formula in large deviation theory, we derive Stokes' law without explicitly employing the hydrodynamic equations.

*Poster

Backward transfer entropy: Informational measure of non hidden-Markov property

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The transfer entropy is a well-established measure of the information flow, which has been shown useful not only in time series analysis but also in nonequilibrium physics. Here, we introduce the transfer entropy of the backward path, called the backward transfer entropy, which quantifies non hidden-Markov property. Thermodynamically, the backward transfer entropy can be interpreted as a thermodynamic loss, where the transfer entropy gives a possible thermodynamic benefit. Moreover, in the context of the gambling with side information, the backward transfer entropy quantifies the loss of the gambler's wealth, where the transfer entropy gives a possible benefit of the gambler's wealth.

*Poster

The second law of thermodynamics and the fluctuation theorem for pure quantum states

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The origin of macroscopic irreversibility under microscopic reversible dynamics is a fundamental problem in nonequilibrium statistical mechanics. The fluctuation theorem [1] and thermodynamics of information [2] shed modern light on this problem, which lead to the second law of thermodynamics and its generalizations. A crucial assumption in this research direction is that the initial state of the heat bath is, at least in the initial time, in the canonical distribution, which effectively breaks the time-reversal symmetry. On the other hand, it has been shown that even a pure quantum state, described by a single wave function, can relax to macroscopic thermal equilibrium by reversible unitary dynamics [3]. The second law and the fluctuation theorem in pure quantum states have been elusive, and the gap between the microscopic reversible and macroscopic irreversible dynamics has not yet been bridged. We here show that the second law of thermodynamics and the fluctuation theorem hold true for isolated genuine quantum systems, where pure quantum states obey unitary reversible dynamics, by a rigorous proof based on the Lieb-Robinson bound, and by numerical simulation of hard-core bosons [4]. The entanglement entropy of a subsystem is shown connected to thermodynamic heat, highlighting the foundation of the information-thermodynamics link. Our results imply that thermal fluctuations emerge from purely quantum fluctuations in nonequilibrium dynamics, which is a novel scenario of the emergence of thermodynamics from quantum mechanics. Our results can experimentally be tested by ultracold atoms. [1] M. Esposito, U. Harbola, and S. Mukamel, Rev. Mod. Phys. 81, 1665-1702 (2009); T. Campisi, P. Hanggi, P. Talkner, Rev. Mod. Phys. 83, 771 (2011). [2] J. M. R. Parrondo, J. M. Horowitz, and T. Sagawa, Nature physics 11, 131 (2015). [3] J. von Neumann, Euro. Phys. J. H 35, 201 (1929); M. Rigol, V. Dunjko, and M. Olshanii, Nature 452, 854 (2008); S. Trotzsky et al., Nature physics 8, 325 (2012). [4] E. Iyoda, K. Kaneko, and T. Sagawa, arXiv:1603.07857 (2016).

*Poster

Microstructural evolution of semicrystalline polymers during tensile deformation

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Semicrystalline polymers are composed of ordered and amorphous regions and exhibit a particular mechanical response that combines the strength of purely crystalline materials with the flexibility of amorphous polymers. The underlying mechanisms of deformation in semicrystalline polymers, especially in their non-linear regime of response, are poorly understood. We examine the microstructural evolution during tensile response of semicrystalline sates of a crystallisable bead-spring model [1] by means of molecular dynamics simulations. To understand the link between the underlying structure and the resulting response, we perform a statistical analysis of polymers conformations and configurations during the deformation [2,3]. Especially, we employ the local nematic order parameter of bond vectors to identify the ordered and disordered regions. We perform a cluster analysis based on the local nematic director to determine the volume distribution of crystalline domains and density of tie-chains that connect the ordered and disordered regions. We measure the tensile response of semicrystalline polymers of various chain lengths prepared with identical protocol of continuous cooling. We find that the plastic deformation mechanism is universal for all the chains lengths longer than the entanglement length [4]. The plastic flow beyond the elastic limit is initiated by reorientation of crystalline blocks that leads to a partial loss of crystallinity at moderate deformations. Further increase of deformation triggers unfolding of chain-folded structures and extension and alignment of all the chains along the tensile direction. At large deformations, there exists a chain length dependent critical strain for which the melting-recrystallization occurs. This transition is concomitant with development of a percolating crystalline domain as a result of alignment of chains majority with the tensile axis [4].

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*Poster

Transitional Steady States of Exchange Dynamics between Finite Quantum System

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We examine particle and heat currents between finite quantum systems and find a unique form of nonequlibrium states unveiled so far. The currents undergo stepwise evolution in time, and their magnitude and direction dramatically change according to system size differences. Despite those characteristics different from the traditional concept of steady state, Onsager's reciprocal relation remains universally valid. We present an analytic formula and physical picture to explain such behaviors.

*Poster

Steady-state fluctuation relations for a non-chaotic system

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A cornerstone of Gallavotti and Cohen's proof of their celebrated steady-state Fluctuation Relation (FR) was the almost-everywhere-hyperbolic nature of the underlying dynamical system. However, we demonstrate that chaotic dynamics, in the sense of positive largest Lyapunov exponent, is not a necessary condition to observe a steady-state FR. To achieve this, we investigate a modified non-equilibrium Ehrenfest wind-tree model, where scatterers are removed from the standard model with probability f. We find that the Lyapunov exponent of the Poincaré map can be tuned by varying f – in particular, the dynamics can be made chaotic or non-chaotic through suitable choices of f. Over a range of f that produces non-chaotic dynamics, we observe a FR. We also observe a strong decay in flux auto-correlation, suggesting that this dynamical system has mixing properties, despite not being chaotic. The presence of auto-correlation decay is consistent with the more recent proposal of T-mixing, rather than chaos, as the relevant sufficient condition for a steady-state FR to hold. We discuss these results in the context of practical considerations for observing FRs in nanoscale systems, as well as our recent work on the connection between T-mixing and relaxation from out-of-equilibrium states.

*Poster

Simulations for testing the validity of the Jarzynski relation for non-Gibbsian initial states in isolated quantum spin systems

Fengping Jin * [1], R. Steinigeweg, H. De Raedt, K. Michielsen, M. Campisi, J. Gemmer

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Quantum spin systems provide rich opportunities to study properties of collective quantum behavior. There exist various numerical algorithms to simulate the real- and imaginary-time evolution of quantum spin systems, such as the second-order product formula [1] and Chebyshev polynomial algorithms [2]. These algorithms can easily simulate systems with up to 36 spins on current supercomputers. The system size is much larger than the size one can simulate with the exact diagonalization approach. We present large-scale simulation results for a spin ladder system to test the validity of the Jarzynski relation for non-Gibbsian initial states [3]. Since the introduction of the Jarzynski equality many derivations of this equality have been presented in both, the classical and the quantum context. While the approaches and settings greatly differ from one to another, they all appear to rely on the initial state being a thermal Gibbs state. Here, we present an investigation of work distributions in driven isolated quantum systems, starting off from pure states that are close to energy eigenstates of the initial Hamiltonian. We find that, for the nonintegrable system in quest, the Jarzynski equality is fulfilled to good accuracy. References: [1] H. De Raedt, Comp. Phys. Rep. 7, 1 (1987). [2] V. V. Dobrovitski and H. De Raedt, Phys. Rev. E 67, 056702 (2003). [3] F. Jin, R. Steinigeweg, H. De Raedt, K. Michielsen, M. Campisi, J. Gemmer, arXiv: 1603.02833.

*Poster

New interpretation of pre-thermalization in the Tomonaga-Luttinger model

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A well-isolated system often shows relaxation to a quasi-stationary state before reaching thermal equilibrium. Such a pre-thermalization has attracted considerable interest recently in association with closely related fundamental problems of relaxation and thermalization of isolated quantum systems. Motivated by the recent experiment in ultracold atoms, we study the dynamics of a one-dimensional Bose gas which is split into two subsystems, and find that individual subsystems relax to Gibbs states, yet the entire system does not due to quantum entanglement. In the Lieb-Liniger model, it is made clear that the pre-thermalization can be understood as a phenomenon due to an influence of the initial entanglement between subsystems [1]. We call it the entanglement pre-thermaliation. On the other hand, in the Tomonaga-Luttinger model, it has been argued that the pre-thermalization occurs due to the presence of many conserved quantities in the literatures. However, in this talk, I will give a new interpretation of the pre-thermalization in the Tomonaga-Luttinger model; I will show you that this pre-thermalization can be also understood in terms of the initial entanglement between the subsystems. Therefore, the pre-thermalization in the Tomonaga-Luttinger model, which was observed in experiment, is also a kind of entanglement pre-thermalization. I will also show you that the spin-charge separation explains the reason why there are two interpretations. [1] E. Kaminishi, T. Mori, T. N. Ikeda and M. Ueda, Nature Physics, 11, 1050 (2015)

*Poster

Heat transport via a local two-state system coupled to non-ohmic baths

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The recent progress of micro-fabrication technology has enabled us to study quantum transport phenomena of phonons and photons experimentally. It is remarkable that there are several similarities between heat transport and electron transport. For example, quantization of heat conductance, which is an analogue of quantization of conductance in electron transport, has been observed experimentally. Recently, it has been shown that a phenomenon similar to the Kondo effect occurs in heat transport via a local two-state system[1]. In this study, the heat conductance has been calculated based on the spin-Boson model with the spectral function $I(omega)(proptoomega^s)$ for the ohmic case ($s = 1$). However, the sub-ohmic case ($s < 1$) and the super-ohmic case ($s > 1$) have not been studied in detail. In this study [2], we study heat transport via a local two-state system coupled to non-ohmic heat baths by using a quantum Monte Carlo method. We show that the heat conductance is proportional to T^{2s+1} at low temperatures whenever the system has a delocalized(singlet) ground state. This result is consistent with the general Shiba's relation. For the sub-ohmic case ($s < 1$), if the coupling strength was larger than a critical value, the behavior of heat conductance at low temperatures changes drastically, because of a quantum phase transition. References [1] K. Saito and T. Kato, Phys. Rev. Lett. ref 111, 214301 (2013) [2] M. Kato, T. Kato, and K. Saito, in preparation.

*Poster

Study on Interacting Particle Systems Motivated by Microbial Division of Labor

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Division of labor is believed to underlie many important evolutionary transitions including the evolution and proliferation of multicellularity. In this study, we formulate interacting particle system model for the emergence of multicellular organisms from unicellular cells cooperating through division of labor. First, we present the mean-field analysis of the model to explain the basic effect of division of labor. From the linear stability analysis, we construct the phase diagram showing the conditions that co-existence of species doing division of labor is predominant and maintained. Further, we perform the extensive stochastic simulation of the lattice version of the model in 1D to examine the effect of dimensionality and stochasticity. Depending on the effective cooperation rate, the model exhibits two different "phases." When the cooperation effect is weak, the system is dominated by the segregated single-species domains, in each of which each species is living separated from the other by a well-defined boundary. On the other hand, when the cooperation effect is strong enough, the mixed-species domain emerges, within which both species live and mingle together. Within such domain, different species cells tend to locate adjacent to each other and effectively behave like bi-cellular organisms. We characterize this "phase transition" and critical phenomena from the perspective of nonequilibrium phase transition.

*Poster

Phase transitions and dynamic entropy in out-of-equilibrium small systems of interacting particles in complex plasmas: numerical simulation and experiment

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Small systems of interacting particles are widely used in various fields of science and technology: in vacuum heat insulation systems, as hydrocarbons in porous materials, as nanocluster structures (and the properties of these structures, e.g. the melting temperature, may differ greatly from the properties of large systems). To study these structures on a "kinetic" level, we can use the special object, namely, the dusty plasma. The dusty plasma is an ionized gas containing macroscopic grains, which become charged via the electron and ion flows. The electric force acting on these grains balances the gravitational one, and the macroparticles can levitate. When the kinetic temperature of the grains rises, they act like atoms or molecules of a solid body: their motion becomes more chaotic, and they explore larger and larger areas of a phase space. The experiments were carried out in the quasi-two-dimensional system of dust grains in gas discharge plasma. Thanks to their high electrical charge ($10^3 - 10^4 e$), the system of 7 grains levitated above the lower electrode, forming a cluster confined by an external electrical field. This system was simulated with the help of Langevin molecular dynamics method. The interparticle interaction potential was taken to be of Yukawa type; for the details see [Complex and Dusty Plasmas, ed. by V. E. Fortov and G. E. Morfill, CRC Press, (2010)]. We use the concept of the "dynamic entropy" introduced by Shannon, Kolmogorov and Sinai in its simple approach called "mean first-passage time" (MFPT) dynamic entropy [Pierre Gaspard and Xiao-Jing Wang, Physics Reports 235, No. 6 (1993) 291—343; P. Allegrini, J. F. Douglas, and S. C. Glotzer, PRE 60, 5714 (1999)] to study numerically and experimentally obtained small systems of interacting particles. We have obtained the MFPT entropy functions for the systems under study and analyzed them to find out their phase states. Three phase states of the considered small systems are registered: crystal, liquid and transitional. The character of motion for different states was examined using the functions of dependence of mean-square displacement of particles on time. The suggested technique of the analysis of the system dynamics can be applied to the structures as small as desired, independent on the degree of the thermal isolation of the system. This work was supported by the Russian Science Foundation (project No 14-12-01440).

*Poster

The role of mutual information change in information thermodynamic processes

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The paradox of Maxwell's demon states that the thermodynamic second law is violated in feedback process in response to the demon's measurement. We explain measurement, feedback, post-measurement by standard thermodynamics from a recent view point that the system and the memory (demon) is considered as a joint system with correlation between subsystems. Mutual information as measure of correlation is an entropic interpretation of information gain during measurement by demon. Post-measurement process, where demon's paradox was claimed, is set in motion by feedback to reenter measurement outcome as protocol of dynamics. The generalized total entropy change of the system and the heat reservoir is defined in addition of mutual information change and is shown not to decrease, which resolves the demon's paradox. Such total entropy could be accepted as the most legitimate if it stops increasing for quasi-static process. We consider two examples having quasi-static motions and confirm rigorously that the total entropy does not change in quasi-static limit for each case, for which the rigorous treatment of mutual information change during time period is crucial. We also investigate the optimal protocol for the maximum extraction of work limited by mutual information change.

*Poster

Torque-Induced Rotational Dynamics in Polymers: Torsional Blobs and Thinning

Laleman Michiel * [1], Marco Baiesi, Boris P. Belotserkovskii, Takahiro Sakaue, Jean-Charles Walter, Enrico Carlon

[1] KU Leuven, Institute for Theoretical Physics – Belgium

By using the blob theory and computer simulations, we investigate the properties of a linear polymer performing a stationary rotational motion around a long impenetrable rod. This rotation is induced by a constant torque applied at one end of the polymer. We try to find relations between relevant observables as torque and angular velocity and to describe the shape of this truly non-equilibrium system. Analytically the rotating polymer can be described using the concept of - in this case rotational - blobs. We find three distinct regimes: a quasi equilibrium one, one where the polymer is fully and tightly wrapped around the rod and an intermediate regime. In this intermediate regime the polymer assumes a trumpet shape and shows "thinning" behaviour. This means that a small change in the applied torque changes the configuration dramatically. The predictions from the blob theory nicely agree with the simulations performed in LAMMPS.

*Poster

Generic dynamical phase transition in driven exclusion processes

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The asymmetric simple exclusion process, or ASEP, is a continuous time Markov process where particles jump stochastically on a 1D lattice, preferentially to one side, and with hard-core interactions. It is possibly the most studied model in non-equilibrium statistical mechanics, for a number of reasons: it is relatively simple and elegant in its definition and has a complex and physically insightful behaviour, it is connected to many other models or mathematical objects, and it is integrable and therefore exactly solvable, at least in principle. It has been shown that the large deviations of that model exhibit a dynamical phase transition between a hydrodynamic regime, where the fluctuations of the system only depend on the local density of particles, and a correlated regime where that is no longer the case. We will go over those results, and show that this phase transition can be identified in a broad class of models with arbitrary extra physical interactions and spatial inhomogeneities.

*Poster

A protocol for reaching equilibrium very fast

Anne Le Cunuder * [1], Ignacio A Martinez, Artyom Petrosyan, David Guéry-Odelin, Emmanuel Trizac, Sergio Ciliberto

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When a control parameter of a system is suddenly changed, the accessible phase space changes too and the system needs its characteristic relaxation time to reach the final equilibrium distribution. An important and relevant question is whether it is possible to travel from an equilibrium state to another in an arbitrary time, much shorter than the natural relaxation time. This reduction of the relaxation time, which is frequently desired and necessary, is often obtained by complex feedback processes. In this talk, we present a protocol, named Engineered Swift Equilibration (ESE),that shortcuts time-consuming relaxations. We tested experimentally this protocol on a Brownian particle trapped in an optical potential first and then an AFM cantilever. We show that applying a specific driving, one can reach equilibrium in an arbitrary short time. We also estimate the energetic cost to get such a time reduction.Beyond its fundamental interest, the ESE method paves the way for applications in micro and nano devices, in high speed AFM, or in monitoring mesoscopic chemical or biological process. References: (1) Engineered Swift Equilibration, Ignacio A Martinez; Artyom Petrosyan; David Guéry-Odelin; Emmanuel Trizac; Sergio Ciliberto, to be published in Nature Physics (2) Arbitrary fast modulation of an atomic force microscope, Anne Le Cunuder; Ignacio A Martinez; Artyom Petrosyan; David Guéry-Odelin; Emmanuel Trizac; Sergio Ciliberto. Submitted to Applied Letters.

*Poster

Efficiency at the maximum power output for simple two-level heat engine

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We introduce a simple two-level heat engine to study the efficiency in the condition of the maximum power output, depending on the energy levels from which the net work is extracted. In contrast to the quasi-statically operated Carnot engine whose efficiency reaches the theoretical maximum, recent research on more realistic engines operated in finite time has revealed other classes of efficiency such as the Curzon-Ahlborn efficiency maximizing the power output. We investigate yet another side with our heat engine model, which involves the population difference caused by different transition rates. Due to the nature of our model, the explicitly time-dependent part is completely decoupled from the other terms in the generated work and the efficiency is independent of the operating time, which allows us to analyze the dependence on other system variables that are the transition rates, or implicit time dependence in this case. We provide the optimal combination of transition rates maximizing the generated power output and discuss its implication on general premise of realistic heat engines. In particular, we prove that the engine efficiency of our model for maximum power output is clearly different from the Curzon-Ahlborn efficiency in spite of its endoreversibility, although they share the universal linear and quadratic coefficients at the near-equilibrium limit with similar values of transition rates.

*Poster

Fluctuations of entropy production in partially masked electric circuits

Chi-Lun Lee * [1], Kuan-Hsun Chiang, Chia-Wei Chou, Pik-Yin Lai, Yung-Fu Chen

[1] National Central University – Taiwan

We investigate experimentally and theoretically the validity of fluctuation theorem (FT) of a coupled-RC circuit. In particular, we intentionally neglect part of the circuit and consider the remaining as an effective single-RC circuit. We observe the violation of fluctuation theorem in the effective entropy production of this reduced circuit in the strong coupling regime. The violation indicates the non-Markovian signature in the coarse-grained system. Analysis is performed via the examination of the symmetry function. We find that in the case where FT fails, the symmetry function still exhibits a linear behavior.

*Poster

Fluctuation-Dissipation Theorem and Detailed Balance in Langevin Systems

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We study the relation between the fluctuation-dissipation theorem and the detailed balance in Langevin systems. It is shown that the two properties are equivalent/exclusive to each other in the absence/prsence of a velocity-dependent force. We discuss that the existing near-equilibrium theories are based on the equivalence, as simultaneously requires the two properties. The exclusivity indicates that any of the two properties, alone, cannot be an identifier of equilibrium, in general.

*Poster

First-passage times of random walkers with memory

Nicolas Levernier * [1], Thomas Guérin, Olivier Bénichou, Raphaël Voituriez

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The first-passage time (FPT), defined as the average time a random walker takes to reach a target point in a confining domain, is a key quantity in the theory of stochastic processes. Its importance comes from its crucial role to quantify the efficiency of processes as varied as diffusion-limited reactions, target search processes or spreading of disease. Most methods to determine the FPT properties in confined domains have been limited to Markovian (memoryless) processes. However, as soon as the random walker interacts with its environment, memory effects can not be neglected. Examples of non Markovian dynamics include single-file diffusion in narrow channels or the motion of a tracer particle either attached to a polymeric chain
cite or diffusing in simple or complex fluids such as nematic, dense soft colloids or viscoelastic solution. Here, we introduce an analytical approach to calculate, in the limit of a large confining volume, the mean FPT of a Gaussian random walker to a target point that encompasses the non-Markovian features of the dynamics. We determine the statistical properties of the trajectory of the random walker in the future of the first-passage event and show that they govern the FPT kinetics. This analysis is applicable to a broad range of stochastic processes, possibly correlated at long-times. Our theoretical predictions are confirmed by numerical simulations for several examples of non-Markovian processes including the emblematic case of the Fractional Brownian Motion in one or higher dimensions. These results show, on the basis of Gaussian processes, the importance of memory effects in first-passage statistics of non-Markovian random walkers in confinement. T. Guérin, N. Levernier, O. Bénichou, R. voituriez, First-passage times of non-markovian random walkers in confinement, Nature (2016) (to be published)

*Poster

On asymptotic behavior of work distributions for driven Brownian motion

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We propose a simple conjecture for the functional form of the asymptotic behavior of work distributions for driven overdamped Brownian motion of a particle in confining potentials [1]. This conjecture is motivated by the fact that these functional forms are independent of the velocity of the driving for all potentials and protocols, where explicit analytical solutions for the work distributions have been derived in the literature. To test the conjecture, we use Brownian dynamics simulations and a recent theory developed by Engel and Nickelsen (EN theory) [2], which is based on the contraction principle of large deviation theory. Our tests suggest that the conjecture is valid for potentials with a confinement equal to or weaker than the parabolic one, both for equilibrium and for nonequilibrium distributions of the initial particle position. For potentials with stronger confinement, the conjecture fails and gives a good approximate description only for fast driving. In addition we obtain a new analytical solution for the asymptotic behavior of the work distribution for the V-potential by application of the EN theory, and we extend this theory to nonequilibrated initial particle positions. [1] V. Holubec, D.Lips, A. Ryabov, P. Chvosta, P. Maass, Eur. Phys. J. B (2015) 88: 340 [2] D. Nickelsen, A. Engel, Eur. Phys. J. B 82, 207 (2011)

*Poster

Calculating work in quantum Markovian master equations

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*Poster

Harmonic chain with velocity flips: thermalization and kinetic theory

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We consider position-momentum correlations in harmonic chains with pinning and a bulk velocity flip noise during the heat relaxation phase which occurs on diffusive time scales, for $t = O(L^2)$ where L is the chain length. It has been shown earlier that for non-degenerate harmonic interactions these systems thermalize and the dominant part of the correlations is given by local thermal equilibrium determined by a temperature profile which satisfies a linear heat equation. In the present contribution we explicitly compute the first order corrections in $1/L$ to the local equilibrium correlations and we investigate the applicability of kinetic theory to study the relaxation process. In particular, by suitably revising the definition of the Wigner transform we derive a phonon Boltzmann equation whose predictions agree with the explicit computation. Comparing the two results, the corrections can be understood as arising from a current-related term and from a spatial changes in the phonon eigenbasis.

*Poster

Non-Equilibrium interface dynamics with correlated noise: Emergent symmetries and non-universal observables

Steven Mathey * [1], Léonie Canet, Elisabeth Agoritsas, Vivien Lecomte

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The Kardar-Parisi-Zhang (KPZ) equation provides one of the simplest non trivial examples of a Non-Equilibrium Steady State. Its universal features capture a very wide range of physical phenomena ranging from varied types of interfaces to turbulent hydrodynamic flows or thermodynamics of polymers in noisy environments. Enormous progress has been made in the last 10 years thanks to an exact derivation of the statistics of the KPZ dynamics in the case of one-dimensional systems driven by a stochastic white noise. The cases of higher dimensions and/or correlated noise remain however unsolved. In this contribution we investigate the physics of a one-dimensional interface that is subjected to a noise with smooth spatio-temporal correlations. This problem was previously studied numerically as well as with the Replica Trick in a Gaussian variational approach[1-4]. It was found that the small scale features depend on the details of the microscopic noise while (up to the overall amplitude factors) the exact solution with white noise governs the large scales. In the present work, Functional Renormalisation Group (FRG) methods are employed in order to resolve the non-perturbative features of KPZ dynamics. The FRG makes it possible to follow the renormalisation group flow from its initial conditions all the way down to its fixed point, that is from microscopic dynamics to the large distance properties. We show that the exact solution emerges on large scales independently of the details of the noise correlations. Moreover the small scale features (and their dependence on the particular choice of the noise correlations) are resolved and compared to direct numerical simulations[5].
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*Poster

Planar Poiseuille flow of highly confined polymer solutions

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When polymer solutions are confined to small channels of the order of nanometers in width, they exhibit unexpected behaviour. These systems can be difficult to investigate experimentally, but molecular dynamics simulations now have the power and flexibility to allow us to investigate them. In this work, we simulate coarse-grained model polymer solutions in highly confined channels both in equilibrium and undergoing Poiseuille flow, using molecular dynamics. We find that the temperature, velocity, and concentration profiles across the channel vary with flow rate. In particular, increasing the flow rate leads to an increase in the wall-mediated polymer depletion region. We show that for sufficiently large channel-widths a bulk-like flow can be achieved that behaves according to classical continuum equations for velocity and temperature. For narrower channels, we find that the classical Navier-Stokes-Fourier description of fluid flow breaks down. Finally, we have also implemented an algorithm to calculate the local pressure tensor across the channel, and have studied the variation of the first normal stresses with position and compared the results with predictions of the first normal stress coefficients from equilibrium molecular dynamics simulations.

*Poster

Typical pure states and nonequilibrium processes for quantum many-body systems

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Analysis of the work distribution for time dependent processes is an important subject. We address this issue on the basis of the typicality: Each single typical pure state in an energy shell of isolated quantum many-body systems well represents the microcanonical state. First, we apply such an intrinsic thermal nature of a pure state to the analysis of the work distribution [1], and also explore the energy current of nonequilibrium steady states [2,3]. The subtlety is that the typicality holds only for the calculation of small number of linearly independent operators such that we cannot discriminate a pure state and the microcanonical ensemble, while the calculation of the work distribution certainly requires continuously many data. We rationalize this issue theoretically and numerically, and explain that we can calculate almost the entire distribution including the rare events only from a single pure state.

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*Poster

Quantum Jarzynski equality of measurement-based work extraction

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Recent developments of experimental technology are realizing small-size heat engines which are out of the scope of the standard thermodynamics [1, 2]. To understand these heat engines, many researchers often use statistical mechanics and micro-dynamics. However, this analysis has a problem as to how we represent the thermodynamic work to in terms of microscopic quantities. When the internal system is quantum mechanical, it is difficult to define the thermodynamics work, because the system is affected by an external agent. Many studies of such engines adopt an approach in which the effect of the external agent is represented as the time-dependence of the Hamiltonian of the internal quantum system [3, 4]. In this approach, the dynamics of the internal quantum system is unitary and the work is defined as the energy loss of the internal system. It is based on the model of a microscopic internal quantum system connected to a macroscopic external agent. However, there are two concerns about the validity of this approach: one is about the assumption of the unitary time evolution and the other is about the definition of the work. In spite of these concerns, many studies rely on the approach because there have been results out of this approach which seem to be consistent with thermodynamics [4, 5]. We here employ another approach [6] in which the dynamics of the internal system is described by a measurement process and the work is given as a measurement outcome, because the effect from the quantum system to the microscopic system is formulated as measurement processes in quantum mechanics. This approach is called the measurement-based work extraction, recently introduced by Hayashi and Tajima [6]. We here show the variance of the energy gain of an external system diverges when the dynamics of the internal system is approximated to the unitary time evolution. This result demands us to change the derivation of the quantum Jarzynski equality from the pervious one [4] based on the conventional approach. We second derive the Jarzynski equality using the measurement-based work extraction. The resulting equality has a constant different from the original Jarzynski equality. [1] S. Toyabe, T. Sagawa, M. Ueda, E. Muneyuki and M. Sano, Nat. Phys. **6**, 988 (2010). [2] A. Shuoming et al., Nat. Phys. **11**, 193 (2014). [3] Y. Morikuni and H. Tasaki, J. Stat. Phys. **43**, 1 (2011). [4] M. Campisi, P. H′anggi and P. Talkner, Rev. Mod. Phys. **83**, 771 (2011). [5] H. Tasaki, arXiv:cond-mat/0009206 (2000). [6] M. Hayashi and H. Tajima, arXiv:1504.06150 (2015).

*Poster

Resolving the Gibbs paradox in small thermodynamic systems

Yuto Murashita * [1], Masahito Ueda

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The Gibbs paradox involves three distinct issues on the foundations of thermodynamics and classical statistical mechanics. Among them, we consider the interrelation between thermodynamic and classical statistical-mechanical entropies. In the thermodynamic limit, this problem was resolved by Pauli and Jaynes by requiring extensivity for the thermodynamic entropy. However, this resolution cannot apply to small thermodynamic systems because extensivity breaks down. In this talk, we offer a resolution applicable to interacting small thermodynamic systems based on the fluctuation theorem in the presence of absolute irreversibility. Absolute irreversibility is singularly strong irreversibility and leads the conventional integral fluctuation theorems inapplicable. It is remarkable that the flaw of the fluctuation theorem plays the vital role in resolving the Gibbs paradox in small thermodynamic systems.

*Poster

Diffusion in presence of stochastic resetting at power-law times

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What happens when simple diffusion is interrupted with resetting to the starting position at random times τ distributed with fat tails $\sim \tau^{(1+\alpha)}$; $\alpha > 0$? We show by exact analytical results that depending on α, the dynamics exhibits a spectrum of rich long-time behavior, from a time-dependent spatial distribution for $\alpha < 1$, to a time-independent and non-equilibrium spatial distribution characterized by power-law tails for $\alpha > 1$. The dynamics has strong consequences on the first-passage time to reach an absorbing fixed target, which we characterize analytically; in particular, there exists an optimal $\alpha_{\min}$

*Poster

Flux quench in a system of interacting spinless fermions in one dimension

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We study a quantum quench in a one-dimensional spinless fermion model (equivalent to the XXZ spin chain), where a magnetic flux is suddenly switched off. This quench is equivalent to imposing a pulse of electric field and therefore generates an initial particle current. This current is not a conserved quantity in presence of a lattice and interactions and we investigate numerically its time-evolution after the quench, using the infinite time-evolving block decimation method. For repulsive interactions or large initial flux, we find oscillations that are governed by excitations deep inside the Fermi sea. At long times we observe that the current remains non-vanishing in the gapless cases, whereas it decays to zero in the gapped cases. Although the linear response theory (valid for a weak flux) predicts the same long-time limit of the current for repulsive and attractive interactions (relation with the zero-temperature Drude weight), larger nonlinearities are observed in the case of repulsive interactions compared with that of the attractive case.

*Poster

Internal structures and packing in dynamical clustering

Martial Noirhomme * [1], Eric Opsomer, François Ludwig, Nicolas Vandewalle

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We numerically and theoretically investigate the internal structures of a driven granular gas in cuboidal cell geometries. Clustering is reported and particles can be classified as gaseous or clustered via a local density criterion based on a Voronoi tesselation. We observe that small clusters arise in the corners of the box. These aggregates have a condensation-like surface growth until a critical size is reached. At this point, a structural transition occurs and all clusters merge together, leaving a hole in the center of the cell. This hole becomes then the new center of nucleation. Taking into accoun all structural modifications, we propose an empirical law for the cluster's growth and deduce packing properties such as the random loose packing of granular aggregates in microgravity environment.

*Poster

A simple method to calculate first?passage time densities with arbitrary initial conditions

Markus Nyberg * [1], Tobias Ambjörnsson, Ludvig Lizana

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Numerous applications all the way from biology and physics to economics depend on the density of first crossings over a boundary. Motivated by the lack of general purpose analytical tools for computing first–passage time densities (FPTDs) for complex problems, we propose a new simple method based on the Independent Interval Approximation (IIA). We generalise previous formulations of the IIA to include arbitrary initial conditions as well as to deal with discrete time and non–smooth continuous time processes. We derive a closed form expression for the FPTD in z and Laplace–transform space to a boundary in one dimension. Two classes of problems are analysed in detail: discrete time symmetric random walks (Markovian) and continuous time Gaussian stationary processes (Markovian and non–Markovian). Our results are in good agreement with Langevin dynamics simulations.

*Poster

Collective dynamics of fully packed classical dimers from a large deviation perspective

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The classical dimer model on the square lattice is a paradigmatic example of a system subject to strong local constraints. We study its behaviour under local stochastic dynamics, by means of Monte Carlo simulations and theoretical arguments. We observe clear signatures of correlated dynamics in both global and local observables and over a broad range of time scales, indicating a breakdown of the simple continuum description that approximates well the statics. We show that this collective dynamics can be understood in terms of one-dimensional "strings" of high mobility, which govern both local and long-wavelength dynamical properties [1]. We also explore the statistical properties of the space of dynamical trajectories, by means of large deviation methods, with the aim of identifying transitions between active and inactive dynamical phases. [1] T. Oakes, J. P. Garrahan, and S. Powell. Emergence of cooperative dynamics in fully packed classical dimers. Phys. Rev. E, 93:032129, Mar 2016.

*Poster

Space-time cluster-variational approach to stochastic dynamics on networks

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In the last few years there have been considerable efforts to devise approximate methods to deal with stochastic-dynamic processes taking place on large graphs.
Such processes are involved in a number of different (natural or artificial) systems: classical spin-glass models, boolean networks, neural networks, and other technological, biological, and social networks.
A number of studies have attempted to generalize the so-called cavity method, which has proved so successful in the analysis of equilibrium phenomena on (specially sparse) networks. Nevertheless, this approach is in principle still of exponential complexity with respect to time, and it needs some extra approximation to make it computationally tractable.
Here we propose and develop an alternative approach [1], whose main original feature is that the time dimension is incorporated into a unique free-energy-like functional, which can be subsequently approximated (with a tunable accuracy) according to the cluster-variation method.
We evaluate the resulting algorithms, in terms of numerical accuracy and computational effort required, on simple model systems such as the SIS epidemic model or the kinetic Ising model. We compare the results with both Monte Carlo simulations and state-of-the-art approximate methods.
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*Poster

Universal bounds on current fluctuations

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For current fluctuations in non-equilibrium steady states of Markovian processes, we derive four different universal bounds valid beyond the Gaussian regime. Different variants of these bounds apply to either the entropy change or any individual current, e.g., the rate of substrate consumption in a chemical reaction or the electron current in an electronic device. The bounds vary with respect to their degree of universality and tightness. A universal parabolic bound on the generating function of an arbitrary current depends solely on the average entropy production. A second, stronger bound requires knowledge both of the thermodynamic forces that drive the system and of the topology of the network of states. These two bounds are conjectures based on extensive numerics. An exponential bound that depends only on the average entropy production and the average number of transitions per time is rigorously proved. This bound has no obvious relation to the parabolic bound but it is typically tighter further away from equilibrium. An asymptotic bound that depends on the specific transition rates and becomes tight for large fluctuations is also derived. Our bounds generalize a recently derived relation for the relative uncertainty in current fluctuations and provide a new general class of constraints for nonequilibrium systems.

*Poster

Topology and stochastic thermodynamics of chemical networks

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Large and intricate Chemical Networks (CN) comprising thousands of species, some of which at low particle numbers, regulate cellular physiology and metabolism. Interestingly, while some reaction pathways are detailed balanced, others are constantly held very far from equilibrium. We discuss the interplay between the deficiency of a CN, a crucial topological property that, in a way, quantifies its degree of auto-catalysis, and a CN's stochastic non-equilibrium thermodynamics. In particular, we discuss the excess entropy production due to non-deterministic behaviour, we provide a statement of the zeroth law of thermodynamics and discuss its irreversible character, and finally we discuss the fluctuation-dissipation relations when only some currents are locally stalling at equilibrium, while the rest of the network is far from equilibrium.

*Poster

Linear thermodynamics for periodically driven systems

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We show how to formulate thermodynamics for periodic driving including small scale systems. As an application we discuss the efficiency of a small scale engine.

*Poster

Non-equilibrium critical dynamics of low-dimensional magnetics

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A significant interest has been recently focused on non-equilibrium processes in magnetic low-dimensional materials. The reduction of the dimension of magnets is accompa nied by an increase in fluctuations of the spin density and the manifestation of the effects of critical slowing down and "memory" in the non-equilibrium behavior of low dimensional magnetic systems. Thin films and low-dimensional demonstrates the slow critical evolution from a nonequilibrium initial state. Aging, coarsening and memory effects are nontrivial features in the non-equi librium behavior of such systems with slow dynamics [1]. Here the Monte Carlo study of non-equilibrium critical evolution from different initial states of low-dimensional systems will be reported. The low-dimensional systems are described by two-dimensional XY-model, and anisotropic Heisenberg model. The influence of structural disorder on aging and coarsening effects will be discussed. The reported study was supported by Grant No. MD-6024.2016.2 of Russian Federation President and Project No. 1627 of the Ministry of Education and Science of the Russian Federation. The simulations were supported by the Supercomputing Center of Lomonosov Moscow State University, Moscow and St. Petersburg Joint Supercomputer Center of the Russian Academy of Sciences. [1] P.V. Prudnikov, V.V. Prudnikov, I.S. Popov (2015) JETP Letters 101 539 http://dx.doi.org/10.1134/S0021364015080135.

*Poster

Non-equilibrium critical dynamics in 3D pure and diluted Ising-model

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We study the non-equilibrium critical evolution of three-dimensional pure and site-diluted spin systems described by Ising model from different initial states specified by values of initial magnetization m_0 with displaying such features as aging and violation of the fluctuation-dissipation theorem [1]. We investigate an influence of initial states with different m_0 and nonmagnetic impurities on relaxation of system magnetization $M(t)$ and two-time dependence of correlation and response functions on characteristic time variables as waiting time t_w and time of observation t. The Monte Carlo simulation results for systems with the spin concentration p varying in a wide range are given. The obtained curves for autocorrelation $C(t, t_w)$ and response $R(t, t_w)$ functions demonstrate that the aging effects are increased with growth of defect concentrations. We found for magnetization $M(t)$, autocorrelation $C(t, t_w)$ and response $R(t, t_w)$ functions their universal scaling functions which are independent on the initial values of magnetization m_0 in frame of universal classes of critical behavior for pure, weakly and strongly diluted Ising systems. The reported study was supported by the Russian Science Foundation through project No. 14-12-00562. [1] Prudnikov P.V., Prudnikov V.V., Pospelov E.A., Malyarenko P.N. and Vakilov A.N. (2015) Prog. Theor. Exp. Phys. 053A01

*Poster

Revisiting the concept of effective temperature for dilute active systems

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We revisit the concept of effective temperature in dilute systems of active particles. The interest in this topic has recently regrown due to the experimental possibility to design manmade artificial swimmers that emulate the ones that exist in the biological realm . In this work we explore a connection between the stationary non-Boltzmann distributions of run-and-tumble, noninteracting particles, moving in a conservative potential, and the corresponding distributions of passive, noninteracting, Brownian particles moving in the same potential, in a temperature-inhomogeneous source of heat. The nature of the non-Boltzmann distributions can be regarded as the effect of the inhomogeneous thermal bath through the assumption of the existence of local equilibrium that presumes the existence of a well defined local temperature. We apply these ideas to commonly used external potentials, namely, constant force field and the harmonic potential. Authors acknowledge financial support from DGAPA-UNAM-PAPIIT grants IN113114 and IA103615

*Poster

A Numerical Study of the Two-Dimensional Incompressible Toner-Tu Equation

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Active matter systems are driven out of equilibrium by the energy injection at the particle level. The Toner-Tu model is a stochastic continuum theory that captures the flocking behavior where many polar active particles move coherently through the short-ranged alignment interaction. Recently the incompressible case of the model has attracted some attention. The density-polarization coupling makes the phase transition discontinuous in the compressible Toner-Tu model that have been studied, but this mechanism does not work in the incompressible case. A perturbative dynamical renormalization group analysis found a continuous phase transition indeed, and further found the critical exponents of a new universality class [1]. The flocking phase in two dimensions can be mapped onto the exactly solvable (1+1)-dimensional Kardar-Parisi-Zhang equation [2]. These interesting but partial theoretical results call for a more comprehensive numerical study. We numerically simulate the two-dimensional incompressible Toner-Tu equation, compare it with the theoretical predictions, and study other non-trivial behavior of the model. The results on the phase transition properties, the dynamics and the steady-state features will be reported and discussed. [1] L. Chen, J. Toner, and C.F. Lee, New Journal of Physics 17, 042002 (2015). [2] L. Chen, C.F. Lee, and J. Toner, arXiv: 1601.01924 (2016).

*Poster

Fluctuation-dissipation relation in spin ice

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Over the last decade spin ice materials, such as $Dy_2Ti_2O_7$, have been at the centre of attention in the frustrated magnetism community. In particular, the development of the so-called Dumbbell model, which pictures the low energy excitations as magnetic charges interacting through a magnetic Coulomb force, has provided an elegant way to study these materials, thanks to a mapping from the easy-axis Ising spins on the pyrochlore lattice to charges on the dual diamond lattice. In parallel, some of the most significant progresses in non-equilibrium statistical mechanics in the last twenty years have come from the study of the fluctuation dissipation ratio when the system of interest evolves out of equilibrium. However, there is still no such study for spin ice. We fill this gap here. Using numerical simulations with local dynamics, we focus on the violation of the fluctuation-dissipation relation after a thermal quench, for several physical observables, such as the magnetization, the density of charges or the energy. This allows us to identify an aging regime in which we can extract effective temperatures and other characteristics of non-equilibrium thermodynamics.

*Poster

The solution of the BBGKY hierarchy of quantum kinetic equations with generalized Yukawa potential.

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In paper the evolution of N identical in mass and charge particles interactiong wia generalized Yukawa potential is investigated. The system of particles is considered in a finite area. Using the semi group theory, we prove the existence of a unique solution of the BBGKY hierarche of quantum kinetic equations

*Poster

Generalisation of the Eyring-Kramers transition rate formula to irreversible diffusion processes

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In the small noise regime, the average transition time between metastable states of a reversible diffusion process is described at the logarithmic scale by Arrhenius' law. The Eyring-Kramers formula classically provides a subexponential prefactor to this large deviation estimate. For irreversible diffusion processes, the equivalent of Arrhenius' law is given by the Freidlin-Wentzell theory. In this paper, we compute the associated prefactor and thereby generalise the Eyring-Kramers formula to irreversible diffusion processes. In our formula, the role of the potential is played by Freidlin-Wentzell's quasipotential, and a correction depending on the non-Gibbsianness of the system along the instanton is highlighted. Our analysis relies on a WKB analysis of the quasistationary distribution of the process in metastable regions, and on a probabilistic study of the process in the neighbourhood of saddle-points of the quasipotential.

*Poster

Thermalization and many-body localization in systems under dynamic nuclear polarization

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Dynamic nuclear polarization (DNP) is a technique used to substantially enhance the nuclear spin polarization and has important applications in magnetic resonance imaging (MRI). We have studied the role of dipolar interactions in the standard DNP protocol, and two regimes were found: in the strongly interacting regime, the out-of-equilibrium stationary state displays an effective thermodynamic behaviour characterised by a very low spin temperature; in the weakly interacting regime, it is not possible to define a spin temperature, and local resonances are fully responsible for the smaller levels of the nuclear polarization. As a result, its value strongly varies from sample to sample. Our central finding is that the nuclear polarization, while in the spin temperature regime, increases steadily upon reducing the interaction strength. Interestingly, the highest polarization is reached at a point where the establishment of a spin temperature is just about to break down due to the incipient many-body localization (MBL) transition.

*Poster

Transport properties of correlated fluids in confinement

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Correlations in confined systems (e.g. fluctuating fluids confined to films) give rise to a wealth of remarkable phenomena. Many equilibrium phenomena, e.g. the critical (thermal) Casimir forces, are well-understood theoretically and have been observed experimentally. Confined, correlated systems out of equilibrium, however, are less explored. In this work we consider a field theoretic dynamical model for correlated fluids (e.g. oil-water mixtures near / at the critical point) under confinement. In particular, we investigate the steady state in a sheared near-critical fluid film, in dependence on the separation of the plates and the bulk correlation length. Our approach, based on linear response theory for small shearing velocities, leads to a self-consistent formulation for the shear rate in the film. We derive analogues of the bulk Green-Kubo relations for inhomogeneous shearing, and show that effective transport coefficients (specifically the viscosity) are affected by confinement. We also address the dependence on the choice of dynamical model, since conservation laws strongly affect dynamical time-scales.

*Poster

Computing transitions rates in the 1D Allen–Cahn equation with a rare event algorithm, beyond Freidlin–Wentzell regime

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Metastability is common in condensed matter, phase transitions, and turbulence, where one can see transition between one coherent macrostate to another. For systems described by stochastic partial differential equations tra- ditional sampling is computationally prohibitive and limits physical studies, due to the rarity of the events and the large number of degrees of freedom involved. This is a major concern for many applications. For this reason, we turn to a method of importance sampling, which runs the natural dynamics of a stochastic system, and gives more weight to trajectories leading to transitions. Using an algorithm called Adaptive Multilevel Splitting, we iteratively compute the transition trajectories which bring the system from one metastable state to another as well as their dynamical properties. With this algorithm, we performed a thorough analysis of transitions in the stochastic Ginzburg–Landau–Allen– Cahn equation [1], a prototype of metastability in statistical physics and nonlinear dynamics. This gradient system is particularly amenable to large deviation mathematical results in the low temperature limit (Freidlin-Wentzell large deviation) [2] and to phenomenological descriptions beyond the Freidlin–Wentzell regime. The use of the algorithm allowed us to accelerate greatly the numerical computation of quantities such as the transition rates from one metastable state to another or the duration of transition trajectories. These results match and confirm the Freidlin–Wentzel theoretical analysis, proving that we can sample events and estimate faithfully transition rates, which correspond to return time of order 1013 relaxation times at a numerical cost close to 103 relaxation times. This algorithm is used to make computation for regimes for which the noise is not small enough to be in a Freidlin-Wentzell regime, but the transition keeps a large deviation type phenomenology. The results are compared to a phenomenological theory, based on a combination of large deviation analysis and results on the motion of diffusive fronts. The algorithm also gives a unique sampling of transition trajectories, way beyond what can be expected from direct numerical simulations. Distributions of durations of transition trajectories is then also studied. Comparison with a Gumble distribution (the mathematical prediction for systems with one degree of freedom) is discussed. We will also discuss the great opportunities opened by this type of algorithms for more complex systems, including systems without detailed balance, for instance turbulent flows. References [1] J. Rolland, F. Bouchet, E. Simonnet, Computing transition rates for the 1-D stochastic Ginzburg-Landau-Allen- Cahn equation for finite-amplitude noise with a rare event algorithm. J. Stat. Phys. 162, 277–311 (2016). [2] W.G. Faris, G. Jona-Lasinio, Large fluctuations for a nonlinear heat equation with noise. J. Phys. A: Math. Gen. 15, 3025–3055 (1982).

*Poster

Heat conduction and thermal rectification in mass-graded next nearest-neighbor FPU lattice

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In this work we study the thermal rectification efficiency, i.e. quantification of asymmetric heat flow, of a one-dimensional mass-graded anharmonic oscillator lattice both with nearest-neighbor (NN) and next-nearest-neighbor (NNN) interactions, being a modification of the model studied in a previous work [M. Romero-Bastida and Jaen Misael Arizmendi-Carvajal, extitJ. Phys. A: Math Theo. ref48, 115006 (2013)]. As for the heat conduction properties of this system we determined that the divergence exponent of thermal conductivity with system size grows as both the mass asymmetry and the strength of the NNN interaction increase, but with a lower value of the thermal conductivity compared to the corresponding NN case for each system size value considered. The system presents an increment of rectification with increasing mass asymmetry and temperature differences, as well as a seemingly saturated rectification value for the largest system sizes considered, which can be considered as an indirect evidence of a non-vanishing rectification efficiency in the thermodynamic limit. For fixed system size, average temperature, and temperature difference values the rectification reaches its maximum at a very precise value of the parameter that controls the strength of the NNN interactions. A possible explanation in terms of breathers pinned in the heavy side of the lattice is suggested.

*Poster

Simulation of Quantum Spin Dynamics by Phase Space Sampling of BBGKY Trajectories.

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Recent experimental developments in quantum simulators with lattice spins in ion traps have necessitated the search for numerical techniques that adequately describe their dynamics. While methods based on matrix product states have been successful with one-dimensional systems up to intermediate time-scales, computational methods of equivalent accuracy for larger dimensions remain elusive. I will present a novel method that is suitable for simulating the dynamics of quantum spin models of any dimension. The method samples the many body Wigner function and evaluates the evolution equations obtained from the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. Higher orders in the hierarchy allow for systematic refinements. Quantum correlations can be treated through both, the Wigner function sampling and the BBGKY evolution, bringing about highly accurate estimates of correlations and entanglement witnesses. The method is particularly suitable for nonintegrable systems, especially those with long-range interactions. I will demonstrate its efficacy by comparing with exact results, as well as other numerical methods. Finally, I conclude with outlooks into modelling the Lindblad dynamics of the collective scattering of classical light by cold quantum gases, especially phenomena like superradiance, as well as experimental corrections in lattice spin simulators due to decoherence.

*Poster

Kink confinement and Bethe-Salpeter equation in the Potts field theory

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Kink topological excitations are quite common in one-dimensional massive quantum field theories characterized by the spontaneously broken discrete symmetry. If such a system is perturbed by the external field that explicitly breaks the discrete symmetry, it induces the long-range attractive force between the kinks leading to their confinement into the bound states. In the Ising field theory, the masses of the resulting meson bound states at small magnetic fields have been studied to much details in the recent years by means of several perturbative techniques based on the Bethe-Salpeter equation. Similar perturbative approaches, which exploit the WKB method, and the solution of the two- and three-body quantum mechanical problems with the linear confining potential, have been applied later to determine the masses of mesons and baryons in the three-state Potts Field Theory (PFT). However, in the PFT these perturbative techniques were not justified by the more systematic Bethe-Salpeter equation approach, since the latter equation contains the four-kink form-factors of the magnetization operator, which were unknown for the PFT. I have obtained the explicit expressions for these form-factors, as well as the explicit form of the Bethe-Salpeter equation in the 3-state PFT using the general form-factor representations derived by Kirillov and Smirnov [1]. Obtained results provide a firm basis for the previously used heuristic techniques, and make possible to extend the kink confinement theory in the 3-state PFT beyond the leading order in the magnetic field. 1. N. Kirillov, F. A. Smirnov. Kiev Preprint ITF-88-73R (1988), in Russian.

*Poster

Analytical study of giant fluctuations and temporal intermittency in a mass transport model.

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We study a mass transport model on a one-dimensional lattice in which single particles are injected at the boundary, undergo driven diffusive transport through the lattice, aggregate on contact, with the resultant aggregates exiting from one or both boundaries [1]. We analytically find the probability distribution of the mass or number of particles in any region as well as the total mass M in the system, and demonstrate that M has a non-Gaussian probability distribution and exhibits giant fluctuations when movement of aggregates is diffusive. Furthermore, we characterise the non-self similar dynamics of the system using dynamical structure functions $S_n(t) = \langle [M(t) - M(0)]^n \rangle$, defined in analogy with structure functions of the velocity field in fluid turbulence. We explicitly calculate these for various boundary conditions and both driven and diffusive motion of particles, and find that these exhibit extreme anomalous scaling with time t, indicative of temporal intermittency– a characteristic feature of turbulent systems. Our work provides a rare example of a model where anomalous scaling exponents of structure functions (as well as boundary condition dependent logarithmic corrections) can be calculated analytically, a task which is generally difficult for most turbulent systems. [1] H. Sachdeva and M. Barma, J. Stat. Phys. **154**, 950 (2014).

*Poster

A field-theoretic approach to the May-Leonard cyclic population dynamics model

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Spatially extended stochastic population dynamics models with cyclic predation interactions display intriguing time evolution and spontaneous structure formation. We study a version of the May-Leonard cyclic competition model in d dimensions with diffusive particle propagation. We use the second-quantized Doi-Peliti formalism and ensuing coherent-state path integral representation to construct its continuum representation and explore its collective dynamics. Expanding the resulting action about the mean-field species concentrations enables us to compute the diagonalized harmonic propagators and hence 'masses', i.e., relaxation rates and eigenfrequencies of the fundamental modes. Furthermore, operating near the Hopf bifurcation point, we identify the validity range for the necessary time scale separation that allows us to project out the purely relaxing eigenmode. The remaining oscillating fields obey the complex Ginzburg-Landau equation, which is consistent with spiral pattern formation.

*Poster

Spontaneous Directional Motion of Shaped Nanoparticle before the Onset of Diffusive Brownian Motion

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In nanoscale space and pico- to nanoseconds enormous physical, chemical and biological processes take place, while the motions of involved particles/molecules under thermal fluctuations are usually analyzed using the conventional theory of diffusive Brownian motion based on both sufficiently long time averaging and assumptions of spherical particle shapes. Here, using molecular dynamics simulations, we show that asymmetrically shaped nanoparticles in dilute solutions possess spontaneous directional motion of the center of mass within a finite time interval. The driving force for this unexpected directional motion lies in the imbalance of the interactions experienced by their constituent atoms during the orientation regulation at timescales before the onset of diffusive Brownian motion. Theoretical formulae have been derived to describe the mean displacement and the variance of this directional motion. Our study potentially takes an important step towards establishing a complete theoretical framework for describing the motions of variously-shaped particles in solutions over all timescales from ballistic to diffusive regime.

*Poster

Floquet-Gibbs states for periodically driven open quantum systems

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A periodically driven quantum system, when coupled to a heat bath, relaxes to a non-equilibrium asymptotic state. In the general situation, the retrieval of this asymptotic state presents a rather non-trivial task. In order to describe the subclass of the systems, we introduce the Floquet-Gibbs state, i.e., a state whose density matrix is diagonal in the Floquet basis of the system Hamiltonian with the diagonal elements obeying a Gibbs distribution over the quasienergies. In the limit of an infinitesimal system-bath coupling strength, using the so-called rotating wave approximation (RWA), we obtain sufficient conditions for the realization of the Floquet-Gibbs state, and find that these conditions severely restrict a class of suitable systems attaining this Gibbs form [1].
Upon using the Magnus expansion [2], we employ the concept of a corresponding effective Floquet Hamiltonian. In doing so and without using the RWA, we demonstrate that the idea of the Floquet-Gibbs states can be extended to the realistic case of a weak, although finite system-bath coupling, herein termed effective Floquet-Gibbs states [3].
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*Poster

No-go theorem for Carnot efficiency with finite power

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The thermodynamic efficiency and power (extracted work per a unit time) are two of the main properties of heat engines, and thus much effort has been devoted to investigate the relation between these two. Carnot has established that an infinitely slow process, which implies zero power, leads to the maximum efficiency known as the Carnot efficiency. However, surprisingly its opposite, whether a heat engine with finite power attains the Carnot efficiency or not, has still been an open problem. Conventional equilibrium thermodynamics provides no restriction on the speed of processes. In addition, it has been clarified that at the level of formal analyses the linear irreversible thermodynamics does not prohibit devices operating reversibly (i.e., zero total entropy production) at finite power if time-reversal symmetry is broken [1].
This has triggered a number of studies based on specific dynamical models to investigate the relation between the power and efficiency for systems with broken-time reversal symmetry [2-5]. Most studies have arrived at the same result that within these specific models the Carnot efficiency and finite power are incompatible. A few studies have insisted the attainability of the Carnot efficiency with finite power, while these arguments contain ambiguous justifications and thus most researchers are not convinced these results. Our present state is that since existing researches are based on limited models in the linear response regime, this problem has still been under debate. To this end, a general theory without resorting specific models is strongly desired.
In this presentation, we demonstrate a general no-go theorem that the Carnot efficiency with finite power is prohibited even with broken time-reversal symmetry and even beyond the linear response regime. In our proof, the notion of *partial entropy production* plays a crucial role, which is the decomposition of the entropy production of the total system into the contribution of each individual transition [6]. By generalizing this idea, we rigorously prove that a Markovian heat engine never reaches the Carnot efficiency with finite power [7]. In addition, we derive a bound for power by using the efficiency, which clearly illustrate the trade-off between large power and high efficiency [8]. Since our argument does not resort specific models, our result will put a period on the debate as far as the heat baths are Markovian.
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*Poster

Free energy formalism for inhomogeneous nonlinear Fokker–Planck equations

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We introduce a free-energy formalism for a wide class of inhomogeneous nonlinear Fokker–Planck equations. In this formalism, the free-energy functional is expressed in terms of an entropic functional and an effective potential, both derived from the coefficients of the equation. We discuss the entropy production in this very general framework and, moreover, we show that, for a large class of inhomogeneous nonlinear Fokker–Planck equations a thermodynamical formalism can be introduced, in which the stationary distribution is associated to equilibrium.

*Poster

Generalized TASEP with a Slow Bond

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We revisit the slow-bond problem in one-dimensional (1D) totally asymmetric simple exclusion process (TASEP) [1] with modified hopping rates. It is well-known that TASEP can be mapped to a zero-range process (ZRP), where the condensation transition in ZRP corresponds the queuing/jamming transition in TASEP. Most recently, a conserved generalized interacting ZRP has been considered to discuss how the interaction bias on particle density of ZRP affects the condensation transition [2]. In our study, the modification of hopping rates at normal bonds are employed to suppress the queue caused by the reduced hopping at the slow bond. Based on the 1D nonequilibrium lattice-gas model analysis [3], we argue a schematic phase diagram and critical behaviors at the queuing transition, which are also numerically tested. 1] M. Ha, J. Timonen, and M. den Nijs, Phys. Rev. E 68, 056122 (2003); H. Soh, Y. Baek, M. Ha, and H. Jeong (in preparation). 2] A. Khaleque and P. Sen, Phys. Rev. E 93, 042102 (2016) 3] Priyanka and K. Jain, Phys. Rev. E 93, 042104 (2016)

*Poster

On the applicability of Fokker-Planck equation to the description of diffusion effect on nucleation

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The nucleation of islands in a supersaturated solution of surface adatoms is considered taking into account the possibility of diffusion profile formation in the island vicinity. It is shown that the treatment of diffusion-controlled cluster growth in terms of the Fokker-Planck equation is justified only provided certain restrictions are satisfied. First of all, the standard requirement that diffusion profiles of adatoms quickly adjust themselves to the actual island sizes (adiabatic principle) can be realized only for sufficiently high island concentration. The adiabatic principle is essential for the probabilities of adatom attachment to and detachment from island edges to be independent of the adatom diffusion profile establishment kinetics, justifying the island nucleation treatment as the Markovian stochastic process. Second, it is shown that the commonly used definition of the 'diffusion' coefficient in the Fokker-Planck equation in terms of adatom attachment and detachment rates is justified only provided these processes are statistically independent, which is generally not the case for the diffusion-limited growth of islands. We suggest a particular way to define the attachment and detachment rates that allows us to satisfy this requirement as well. When applied to the problem of surface island nucleation, our treatment predicts the steady-state nucleation barrier, which coincides with the conventional thermodynamic expression, even though no thermodynamic equilibrium is assumed and the adatom diffusion is treated explicitly. The effect of adatom diffusional profiles on the nucleation rate pre-exponential factor is also discussed.

*Poster

Nonlinear Relaxation Phenomena in Condensed Matter Metastable Systems

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Nonlinear relaxation phenomena in three different systems of condensed matter are investigated. (i) First, the phase dynamics in Josephson junctions is analyzed. Specifically, a superconductor-graphene-superconductor (SGS) system exhibits quantum metastable states, and the average escape time from these metastable states in the presence of Gaussian and correlated fluctuations is calculated, varying the noise source intensity and the bias frequency. Moreover the transient dynamics of a long-overlap Josephson junction (JJ) subject to thermal fluctuations and non-Gaussian noise sources, Lévy type, is investigated. Noise induced phenomena are observed, such as the noise enhanced stability and the resonant activation. The analysis of the time evolution of the order parameter highlights the influence of the noise induced solitons on the mean switching time behavior and the observation of breathers. (ii) Second, the electron spin relaxation process in n-type GaAs crystals driven by a fluctuating electric field and two different noise sources is investigated. Monte Carlo numerical simulations show, in both cases, an enhancement of the spin relaxation time by increasing the amplitude of the external noise. (iii) Finally, the stabilization of quantum metastable states by dissipation is presented. Normally, quantum fluctuations enhance the escape from metastable states in the presence of dissipation. We show that dissipation can enhance the stability of a quantum metastable system, consisting of a particle moving in a strongly asymmetric double well potential, interacting with a thermal bath. We find that the escape time from the metastable region has a nonmonotonic behavior versus the system-bath coupling and the temperature, producing a stabilizing effect.

*Poster

Brownian motion in periodic potentials: anomalous diffusion induced by symmetry and ergodicity breaking

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We consider *far from equilibrium* transport of an externally driven inertial Brownian particle moving in a *periodic* one-dimensional potential. As it was shown (Spiechowicz J. and Łuczka J., Phys. Rev. E 91, 062104 (2015)), the mean square deviation of the particle position from its average evolves in three distinct stages: initially as superdiffusion, next as subdiffusion and finally as normal diffusion in the asymptotic long time limit. Even though these anomalies are transient effects their lifetime is extremely sensitive to changes of the potential asymmetry parameter so that they may last many orders longer than characteristic time scales of the setup. The mentioned controllability of anomalous diffusion is related to *nonergodicity* of the setup and *ultraslow relaxation* of the Brownian particle velocity to its steady state. Similar sequence of the diffusional behaviour has been observed in various systems including, among others, colloidal particles in random potentials, glass forming liquids and granular gases. With a simple ratchet model we propose an entirely new mechanism standing behind such *diffusion anomalies* which involves breaking of *reflection symmetry* of the potential and *ergodicity* of the system.

*Poster

Generalized Langevin Equation for many probes in nonequilibrium environment

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Langevin equations describe the statistical fluctuations of mesoscopic systems at equilibrium, which are held in contact with a thermal bath. The results are in accordance with statistical mechanics since the fluctuations driving the system have probability given by Boltzmann principle, their correlations satisfy the fluctuation-dissipation theorem (FDT), and induce static correlation functions which conform to the equipartition theorem. Out of equilibrium the Langevin approach remains valid, under the assumption that the source of non-equilibrium does not affect appreciably the bath. Nevertheless, none of the previous properties survives when the source of non-equilibrium resides in the environment. Equilibrium arguments become unusable, and a reduced Langevin description must be found by other means, namely integrating out explicitly the dynamics of the off-equilibrium environment. We derive a generalized Langevin equations for many probe particles weakly interacting with a driven environment applying non-equilibrium linear response theory. Integrating out the fast degrees of freedom we obtain an expression for the noise and the friction perceived by the probes. They are related as in equilibrium via the fluctuation-dissipation relation. Nevertheless, due to the nonequilibrium nature of the bath, this relation presents new contributions.

*Poster

Semi-Markov approximation and algorithm for anomalous diffusion

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Anomalous Diffusion is typically modeled by a Continuous Time Random Walk (CTRW). Scaling limits of CTRWs constitute a less-well known example of Semi-Markov processes which have infinitely many renewals in finite time intervals (the renewal set is a fractal). We study these Semi-Markov processes and show how they can be embedded into a higher-dimensional Markov process. We then derive master equations for this Markov process which allow for a discrete numeric scheme, and thus for the computation of finite-dimensional distributions of CTRW limit processes.

*Poster

Dynamics of non-equilibrium bosonic systems in acoustic potentials

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We consider a system of microcavity exciton polaritons, hybrid light-matter quasi-particles emerging from the strong coupling between quantum well excitons and cavity photons in the semiconductor microcavities [1]. Recently, polariton quasi-condensation was observed in micrometer sized periodic slowly-moving tunable potentials created by coherent surface acoustic waves (SAW) [2] which resembles a standing sine-shaped wave. It was demonstrated that such SAW potentials can lead to various effects, including fragmentation of the condensate into an array of wires which move with the acoustic velocity. In spite of the success on the experiment side, the theoretical description is yet unclear and, moreover, a plethora of new interesting effects can be proposed. We apply a microscopic theory [3] to describe the behavior of polaritons in the potentials created by surface acoustic waves in one-dimensional system and show particle propagation, scattering, and binding in direct and reciprocal spaces at different temperatures and intensities of the SAW at resonant and incoherent excitation of the system. We also investigate the current crowding effect, similar to [4]. [1] Imamoglu, A., R. J. Ram, S. Pau, and Y. Yamamoto, 1996, Phys. Rev. A 53, 4250 [2] E.A. Cerda-Mendez, D. N. Krizhanovskii, M. Wouters, R. Bradlley, K. Biermann, K. Guda, R. Hey, P. V. Santos, D. Sarkar, and M. S. Skolnick, PRL 105,116402 (2010) [3] I. G. Savenko, T.C.H Liew and I.A.Shelykh, Phys. Rev Lett. 110 127402 (2013). [4] Phys. stat. solidi (c) 7, No 7-8, 2124-2126 (2010) DOI 10.1002/pssc.200983415

*Poster

Brownian motion on disordered landscapes

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We present a study of overdamped Brownian particles moving on a random landscape either static (spatial disorder) or made of dynamic and deformable obstacles (spatio–temporal disorder). Transport and diffusion are studied through the statistical moments of the ensemble of particle trajectories to be obtained by Langevin dynamics. Anomalies—if any—are characterized by the time exponents of these quantities. A static landscape models a solid medium where potential configurations do not change with time. In this milieu, we characterize and analyze the effects of three different disordered potentials. The anomaly in the transport is always of the subtransport type, but diffusion presents a greater variety of anomalies: both subdiffusion and superdiffusion are possible. In two dimensions we present a mixed anomaly: subdiffusion in the direction perpendicular to the force, and superdiffusion in the parallel direction. With regard to the spatio–temporal disorder, it is made of obstacles that move randomly, assemble, and dissociate following their own dynamics. This landscape may account for a soft matter or liquid environment in which large obstacles, such as macromolecules and organelles in the cytoplasm of a living cell, or colloids or polymers in a liquid, move slowly leading to crowding effects. This representation also constitutes a novel approach to the macroscopic dynamics exhibited by active matter media. The landscape dynamics are characterized by a Gaussian spatio–temporal correlation, with fixed time and spatial scales, and controlled obstacle concentrations. We have explored the motion of Brownian particles in the dynamical obstacle landscape for various values of the obstacle density ρ, correlation length (mean obstacle width) λ, and correlation time t_0. The main inferences of our work focus on the intermediate scenarios of landscapes of rather low densities of obstacles moving on a time scale between that of Brownian motion and the total observation time. In this scenario, the transient behavior of transport and diffusion over time scales shorter than t_0 mimics that of a static landscape. After time t_0 these anomalies disappear because of the motion of the obstacles and transport and diffusion coefficients reach asymptotic constant values.

*Poster

Non-Gaussianity in quantum conductors

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Nonequilibrium fluctuation through mesoscopic devices has been intensively studied in both classical and quantum regimes. It requires us to use a sophisticated scheme to measure the current fluctuations. In this work, we theoretically study the nonequilibrium transport through a quantum point contact (QPC) coupled to a detector RLC circuit. We show that the electron tunneling through the QPC generates non-Gaussian noise in the detector circuit. The dynamics of the detector circuit can be equivalently represented as a Langevin-like particle driven by the non-Gaussian noise.

*Poster

Unavoidable gapless edge state of bosonic Mott state trapped in two-dimansional optical lattices

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We theoretically study boundary properties of trapped bosonic Mott insulators in optical square lattices. By performing quantum Monte Carlo calculations, we show that a finite superfluid density almost always appears in the incommensurate-filling (IC) boundary surrounding the bulk Mott insulator at a very low temperature. In this IC boundary, both off-diagonal and density correlations exhibit a power-law decay. Our result clearly indicates that the gapless IC boundary state always emerges in any bosonic Mott insulators on optical lattices. Therefore, we can expect that if a topological insulating state in trapped cold-atom systems is realized, its boundary possesses at least two gapless modes (or coupled modes) of the above gapless state in the IC region and the intrinsic topologically-protected edge state.

*Poster

Measurement-based formulation of quantum heat engines and optimal efficiency of quantum heat engines

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One of the main interests in statistical mechanics is a quantum-mechanical foundaiton of thermodynamics. For this study, we need to clarify the difference between "heat" and "work" and the optimal performance of the heat engines, whose discussion is required to be based on the quantum theory. Unfortunately, these problems have not been solved with respect to the following two points. One is the lack of the consensus for the formulation of work extraction on quantum system. That is, two different communities adopted their own models, the internal model [1,2] and the full quantum model [3,4,5], and have less communication with each other. The other problem is solving the optimum efficiency of the heat engine with finite resource size as the maximization problem in quantum many body systems under the proper formulation of the quantum heat engine. Using the measurement theory [6], we firstly discussed the first problem [8]. We focus on the measurement effect for the heat engine because the amount of extracted work should be recognized by persons, and can be the starting point of the common consensus. Then, based on quantum measurement, we give a unified formulation of quantum heat engine [8]. Based on our formulation, we derive two trade-off relations that clarify a problem of the internal model [1,2]. In the internal model, we can hardly know the amount of the extracted work when the time evolution of the internal system is close to unitary due to the lack of the concept of measurement. Recently, Tasaki, one of the founders of the internal model, publicly agreed our claim and our model in his recent paper [10]. Next, based on the strong large deviation theory [7] and the above formulation of heat engine, we address the second problem, i.e., we derive the maximum efficiency and the minimal variance of quantum heat engines whose heat baths are n-particle systems [9]. Using our results, we evaluate the accuracy of the macroscopic thermodynamics for the heat engines with finite-size heat baths from the statistical mechanical viewpoint. [1] H. Tasaki, arXiv:cond-mat/0009244 (2000). [2] J. Kurchan, arXiv:cond-mat/0007360 (2000). [3] P. Skrzypczyk, et al, Nat. Comm. 5, 4185, (2014) [4] M. Horodecki and J. Oppenheim, Nat. Commun. 4, 2059 (2013). [5] F. G. S. L. Brandao, et al, PNAS, 112,3215(2015). [6] M. Ozawa, J. Math. Phys., 25, 79 (1984). [7] R. Bahadur and R. R. Rao, Ann. Math. Stat., 31, 1015 (1960). [8] M. Hayashi and H. Tajima, arXiv:1504 .06150 (2015). [9] H. Tajima and M. Hayashi, arXiv:1405.6457 (2014). [10] H. Tasaki, arXiv:1511.01999.(2015).

*Poster

Emergence of macroscopic slip of a simple fluid

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The dynamical behavior of a simple fluid is described by solutions to the Navier-Stokes equation with the no-slip boundary conditions. Here, the no-slip boundary condition means that a fluid velocity at solid surfaces is the exactly same as that of the solid surfaces. However, it has been known that there always exists the finite slip velocity at a molecularly smooth surface. This is indeed confirmed by numerical simulations and laboratory experiments. Nevertheless, the previous studies did not clarify whether this slip is macroscopic or microscopic. In this presentation, we first define the macroscopic slip by considering a large system size limit under shear flow. Then, we propose a phenomenological theory to understand the fluid slip at the solid surface. Based on the theory, we show that a simple fluid may exhibit a macroscopic slip with breaking the no-slip boundary condition as the result of a non-linear relation between the shear stress and the velocity at the surface. Finally, we argue a possibility of observing this phenomenon in laboratory experiments.

*Poster

Use of laminar interval distributions in characterization of spatiotemporal intermittency

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Since the concept of spatiotemporal intermittency (STI) was proposed by Kaneko [1], the distribution of the size of laminar clusters (laminar interval distributions) has been one of the central quantities to be investigated in literatures. It has also been playing a considerable role in experimental characterization of a transition to STI (in particular the measurements of correlation length) thanks to its high accessibility [2,3]. However, the interpretation of the experimentally observed distribution is not necessarily straightforward because (a) the relation between the correlation length (time) defined through characteristic length (time) of the decay in the laminar interval distribution and one defined through usual (density-density) correlation function has been unknown, and (b) a histogram constructed from the observation in a finite range may significantly underestimate the correlation length. In this contribution, we elucidate utility of the laminar interval distribution by addressing the two difficulties mentioned above. First, we argue, through numerical simulations of the contact process and scaling arguments with a help of independent interval approximations [4], that the above two correlation length are in proportion to each other in a case of directed percolation. This forms a theoretical background of empirical observations in experiments [2,3]. Then, we quantify a possible difference between a histogram constructed from a finite observation window and a genuine laminar interval distribution of the system via a numerical simulation on an alternating renewal process, where several methods of correction to the histogram are compared in light of their consistency. Generality of the conclusion obtained here is also discussed, if time permits.

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*Poster

Study of a two-species reaction-diffusion process by the non-perturbative renormalization group

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We consider the diffusive epidemic process (DEP), a two-species reaction-diffusion process defined as follow: the species A and B representing healthy and sick individuals diffuse on a lattice with diffusion coefficients D_A and D_B respectively and can undergo the reactions $A + B \to 2B$ (contagion) and $B \to A$ (recovery) with given rates [1]. This process exhibits a transition from an active state (where the density of B, n_B, is positive) to an absorbing state ($n_B = 0$) when lowering the total density. The critical physics depends only on the respective value of D_A and D_B but some questions are not settled yet, notably the order of the transition for $D_A > D_B$ [2,3,4]. We investigate this system using the non-perturbative renormalization group formalism. Whereas we recover previous results for $D_B = D_A$ and $D_A < D_B$, we find a new fixed point for $D_A > D_B$ which we hope may bring a conclusive answer to this issue.

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*Poster

Driven non-equilibrium systems modeled with Markov processes

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This poster will present result about a study of the current fluctuation of a motion of a particle on a ring, evolving with a driving force and the potential under the influence of a stochastic force. We derived the equation of motion with and without noise and solved it for various parameters. We analyzed an analytical and numerical stationary distributions. We also derived for this model the fluctuations properties of the current observable and looked at the driven process for these fluctuations. The resulting function tell us about how the fluctuations arise.

*Poster

Replica symmetry breaking in trajectories of a driven Brownian particle

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Diffusion in active environments have gradually attracted attention in recent studies of non-equilibrium physics and biophysics. Recent developments in experimental techniques enabled us to investigate trajectories of a tracer particle in active environments. Theoretically, a statistical mechanical framework of trajectories has also been developed, and the first-order transitions in the trajectory ensemble have been discovered in glassy systems. Although this framework was originally developed for general Markov processes, it is useful to characterize properties of trajectories of a tracer particle. Here, we report an anomalous diffusion characterized by replica symmetry breaking (RSB) in the trajectory ensemble. RSB is a concept which describes the low temperature phase of mean-field spin glass models, and is detected by the similarity between configurations of two independent and identical spin-glass systems (overlap). In the spin glass phase, the distribution function of the overlap takes a non-trivial form, reflecting the existence of several stable configurations. We apply this method of RSB detection to the trajectories of two tracer particles, and identify RSB by the existence of a non-trivial feature of the distribution function of the overlap. Concretely, we study an active environment obeying the noisy Burgers equation. The noisy Burgers equation was introduced as a toy model of turbulence, and it is equivalent to the Kardar–Parisi–Zhang (KPZ) equation, which has been extensively studied. In this study, we find that the overlap between the trajectories of two tracer particles obeys a non-trivial distribution, and we subsequently provide evidence to support the claim that this model exhibits RSB in the path ensemble. This result is published in Phys. Rev. Lett. [1].

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*Poster

Dynamic instability in a dissipative feedback process with time delay

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We investigate dynamic behaviors in a cold damping system with successive measurement and feedback processes. In this work, we consider a time-delayed protocol such that the feedback force depending on the measurement outcome is applied to the system not immediately, but after a delay time δ. When the protocol is applied over a finite interval Δ, the feedback force, which is intended to be a friction, may turn into an accelerating force in the last stage, implying that feedback protocols with long duration time fail in cooling the system. Moreover, the system temperature grows up to infinite when the protocol is applied longer than a threshold time interval ($\Delta > \Delta_c$). Interestingly, it is found that the reentrance behavior of threshold Δ_c develops depending on the time delay δ, which will be discussed in the context of Lyapunov exponent. We present the phase diagram showing unstable, stable warmed, and cooled regimes in terms of time scales and strength of feedback force.

*Poster

Comparing ballistic Landauer quantum transport to time-evolved Wigner functions

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Electronic devices such as transistors and diodes in operation are commonly driven far from equilibrium. Common length scales in the nanometer range mean quantum effects such as confinement, tunnelling and ballistic transport must be considered. Finding the behaviour of these systems in steady state is a formidable task. Which is why, in computational electronics, an approximation usually is made; two contacts are considered as large reservoirs in constant equilibrium, both at a different chemical potential witch drives a non-equilibrium flow through the device. This approach is the basis of commonly used methods such as the Landauer formula, quantum transmitting boundary methods (QTBM), and non-equilibrium Greens functions (NEGF). We contrast this approximation with the actual time evolution from a known state e.g. equilibrium, to the non-equilibrium steady state. The system is fully described by the Wigner function, a quasi-distribution function in phase space with the time evolution governed by the Wigner-Liouville equation. On the other hand, the Wigner function of the Landauer approach is constructed by Wigner-Weyl transformation of the approximate density matrix in the wavefunction basis. This enables a comparison of the steady state obtained from the Wigner-Liouville method to the Landauer/QTBM approximation. We validate the Landauer approach for several realistic potentials, in the presence and absence of both (quasi-)bound and resonant levels, the former of which are only weakly coupled to the contact reservoirs, whereas the latter are strongly coupled to both contacts.

*Poster

The harmonic oscillator in an active viscoelastic bath

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We investigate the rich behaviour of the harmonic oscillator in a viscoelastic heat bath which is pulled out of equilibrium by an active component. This model can be used to describe many biological systems such as a tracer particle diffusing in the cytosol. We use the formalism of the generalised Langevin equation to study this system both analytically and numerically. We observe various types of anomalous diffusion at different time-scales, while the distribution of the position always remains Gaussian distributed. We find an expression for the effective temperature when the system is in the nonequilibrium steady state. The velocity correlations are also discussed. As an extension to the model we modify the algorithm to study the escape rate in bistable potential and compare our results to existing theories.

*Poster

Wave effects in pulsed thermoelectricity in nanoscaled semiconductor films.

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Due to the progress in the microscaling techniques the thickness of thermoelectric layers may be reduced to values comparable to the phonon mean free path (PMFP) in the material. Modelling heat and electric charge transport at those length scales requires including nonlocal and memory effects. The relationship between transport, thermoelectric coefficients and size (nonlocality) can be theoretically obtained from the very principles of Irreversible Thermodynamics and Solid State Theory. Considering thermodynamic inertia (memory) in the internal energy leads to a heat transport equation which describes a wave-like behaviour of system's temperature. In this way, if the layer thickness is in the order of the PMFP the heat transport regime becomes of the wave type. In this work we analyse the effects of nonlocality and memory in the super cooling effect in a nanoscaled semiconductor layer under pulsed regime. Some conclusions are: i) the transient for the nanometric layer once the electric pulse is applied shows an oscillating decaying behaviour towards the stationary state, ii) this behaviour causes an extra cooling improving the thermal figure of merit compared with a micrometric layer, and iii) the system shows a set of parameters of the applied pulse of electric current optimizing the thermal figure of merit.

*Poster

Energy spectrum distorsion for non equilibrium systems

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The main question we try to answer with our work is: how non equilibrium conditions can affect the energy of a system? Particularly, this study is focused on the energy spectrum distorsions of harmonic oscillator chains in out-of-equilibrium conditions. Many questions have to be answered to deal with this problem. First of all, since there are many ways to describe this kind of systems, which is the model that can give the more detailed description of this phenomenon? For this reason we have first studied a single or a chain of two harmonic oscillators where the non equilibrium conditions were given by different approaches to check if any distorsion was actually visible. The choice of dealing at first with few degrees of freedom has been made because the aim was to get exact analytical solutions with the purpose of extrapolating some properties of the models with no approximations. Through these computations we realized that one has to be careful also in the choice of the right definition of heat flux. We will show that not all the ones commonly used can be useful in this case. Once the model had been set, we have studied it also through numerical simulations to check if with a higher number of degrees of freedom there is still a correspondence with the analytical results.

*Poster

Collective dynamics on a three-channel exclusion processes with Langmuir-Kinetics

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Collective dynamics on a three-channel exclusion processes with Langmuir-Kinetics Atul Kumar Verma and Arvind Kumar Gupta, Department of Mathematics, IIT Ropar, Ropar, Punjab, India-140001. Motor-proteins are molecular motors that can move along filaments to transfer cargoes to specific locations in cells and in this intracellular transport filaments work as macromolecular highways [1]. Movement of motor-proteins is an important aspect not only in understanding the bio-logical properties of a cell but also to get insight about some diseases like ciliary dyskinesias, situs inversus, retinitis pigmentosa, tumor suppression, left-right body determination etc. [2]. Motor-protein transport is a far from equilibrium process which in past decades is studied by using totally asymmetric simple exclusion process (TASEP) model [3] that is a paradigm of non-equilibrium processes. TASEP is a discrete nonequilibrium model which was first used for describing the kinetics of biopolymerization in 1968 [4]. It is also able to explain many non-equilibrium phenomena occurring not only in physics but also in many other applied areas [5] like protein synthesis, translation of mRNA and vehicular flow in traffic etc. In intracellular transport of molecular motors, attachment and detachment of motors occurs between the cytoplasm and the filament, which can be mimicked by Langmuir-kinetics. So, the goal of this study is to analyze, the effect of Langmuir kinetics on steady-state phase diagrams for three-channel exclusion processes with open boundary conditions under fully asymmetrically coupling environment. We define a parameter, namely binding constant which represents the ratio of attachment and detachment rates. We have derived various phase diagrams and density profiles for different values of binding constant using mean-field theory. Theoretical findings are validated using Monte-Carlo simulation which are found to be in good agreement with simulation results. References: 1. Howard, J., Clark, R.: Mechanics of motor proteins and the cytoskeleton. Appl Mech. Rev. 55, 39 (2002). 2. Kinesin molecular motors: transport pathways, receptors, and human disease. Proc. Natl. Acad. Sci. U.S.A. 98(13), 69997003 (2001). 3. An exactly soluble non-equilibrium system: the asymmetric simple exclusion process. Phys. Rep. 301(1), 6583 (1998). 4. MacDonald, C.T., Gibbs, J.H., Pipkin, A.C.: Kinetics of biopolymerization on nucleic acid templates. Biopolymers 6(1), 125 (1968). 5. Chowdhury, D., Schadschneider, A., Nishinari, K.: Physics of transport and traffic phenomena in biology: from molecular motors and cells to organisms. Phys. Life Rev. 2(4), 318352 (2005).

*Poster

Efficiency fluctuations of small machines

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A thermodynamic machine is a device designed either to generate mechanical work or to cool (or heat) by using a spontaneous current. At small size scale, the fluctuations of the current strongly influence the device behavior. In this context, the machine is ruled by the laws of stochastic thermodynamic: all thermodynamic variables become random variables and so does the efficiency used to characterized the performance of the machine. In this work, we revisit recent results on the stochastic efficiency assuming that three fluxes exist in the machine: an input, an output and some losses. In the long-time limit, we predict the shape of the large deviation function of the efficiency in two cases, namely with known or unknown losses. More precisely, we study the extrema of the efficiencies large deviation function. In particular, we connect the maximum of this function to a minimum of entropy production under constraint. We illustrate our results on a model of photoelectric cell made of two single level quantum dots.

*Poster

Some remarks on finite-reservoir finite-time thermodynamics within and beyond the linear response regime

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We will first briefly introduce our recent works on finite-reservoir finite-time thermodynamics [Phys. Rev. E 90, 062140 (2014); 93, 012120 (2016)]. In particular, in the case of a finite-sized hot reservoir and an infinite cold reservoir, the optimization problem of extracting the maximal amount of work from the hot reservoir for a given duration is found to be determined by a duration-dependent constant H, which plays the role similar to that of the Hamiltonian in classical mechanics. Within the linear response regime, H is equivalent to the entropy production rate σ, and then a quantity Φ can be further obtained, which sets a lower bound for energy dissipation of the finite-time process. We in this talk will show, for linear response, Φ can be used to directly optimize quite generic object functions that take the form of $P^m\eta^n$ or $mP-n\sigma$, where P is the power output and η is the thermodynamical efficiency. Moreover, we will address the geometric meaning of the optimized thermodynamical path in phase space. As is well known, for linear response, such optimized paths can be seen as geodesics in some space endowed with a metric constructed by second-derivatives of internal energy, Helmholtz free energy, or entropy, with respect to extensive variables. However, beyond linear response, constructing the metric this way does not generally guarantee the optimized path to be a geodesic. Thus we are confronted with two choices: to redefine the metric to always make the optimized path a geodesic, or to discard the "optimized path-geodesic" correspondence and work with a conventionally defined metric. We argue technically the second choice is more favored.

*Poster

Entropy production of nano systems with timescale separation

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Energy flows in bio-molecular motors and machines are vital to their function. Yet experimental observations are often limited to a small subset of variables that participate in energy transport and dissipation. Here we show, through a solvable Langevin model, that the seemingly hidden entropy production is measurable through the violation spectrum of the fluctuation-response relation of a slow observable. For general Markov systems with timescale separation, we prove that the violation spectrum exhibits a characteristic plateau in the intermediate frequency region. Despite its vanishing height, the plateau can account for energy dissipation over a broad timescale. Our findings suggest a general possibility to probe hidden entropy production in nano systems without direct observation of fast variables.

*Poster

Experimental Demonstration of the Fluctuation Theorem for Entropy Production in a Shear Flow

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The original fluctuation theorem was presented by Evans it et al. [1] in 1993 for the entropy production rate $sigma_au$ within a laminar shear flow. We report the first experimental demonstration of this theorem using particle tracking data for a small subsystem within a two-dimensional dusty plasma. A dusty plasma [2] consists of thousands of micron sized dust particles (melamine-formaldehyde microspheres) incorporated into a plasma of electrons, ions, and neutral gas. These microspheres are large enough to be tracked individually, using a video camera. Within the plasma, the microspheres accumulate a large negative charge so that the dust particles can be levitated in a single two-dimensional layer. The collection of microspheres is a driven-dissipative system that is heated by the lasers and simultaneously cooled by neutral gas friction. The random motion of the microspheres is found to mimic that of thermal equilibrium. We then apply two additional laser beams to drive a steady shear flow. Analyzing a subsystem of $N = 56$ microspheres within the shear flow, $sigma_au$ is found to fluctuate to negative values, with a probability that confirms the theorem,

$$fracp(sigma_{au} = -C)p(sigma_{au} = C) = expleft(-Cauight). \quad (1)$$

We experimentally determine a convergence time t_c. The original theorem requires the averaging time interval $auightarrowinfty$ for the two sides of the theorem to balance, but it does not quantify a finite time for this convergence. We measured a convergence time using the data from the same experiment, averaging over different values of au, and comparing the LHS and RHS of Eq. (1). The two sides are found to converge together with an e-folding time of $t_c = 0.047gamma^{-1}$, where $gamma$ is the shear rate. Work supported by the National Science Foundation, US Department of Energy, and NASA. [1] D. J. Evans, E. G. D. Cohen, and G. P. Morriss, Phys. Rev. Lett. ref 71, 2401 (1993). [2] R. L. Merlino and J. A. Goree, Phys. Today ref 57, No. 7, 32 (2004).

*Poster

Thermoelectric efficiency under a broken time-reversal symmetry and inelastic processes of the charge carriers

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Raising the efficiency of a thermoelectric device, which converts for instance wasted heat into useful electric power, is one of the most crucial issues for energy harvesting. Benenti *et al.* suggested that a magnetic field together with inelastic scattering of the charge carriers could enhance the efficiency [1]. Here we consider an Aharonov-Bohm ring threaded by a magnetic flux, incorporating electron-phonon inelastic scattering. The model has a quantum dot and three reservoirs; two electronic reservoirs and a bosonic one. Electrons are inelastically scattered by bosons at the quantum dot [2]. It can work as a thermoelectric heat engine, which generates electric power using the heat currents from the hotter reservoirs. We calculate various efficiencies for the model [3]. Setting one of the reservoirs as a probe, we calculate the two-terminal efficiency of generating power by an electronic heat current and the one by a phononic heat current. We calculate them under the effect of a magnetic field and find that both increase as the AB phase increases only when there exists a broken left-right symmetry. The result shows that we need inelastic scattering *and* a broken left-right symmetry, which Saito *et al.* suggested using another model [4]. Our device also allows for the examination of the three-terminal efficiencies. Based on our previous work, these are expected to improve the working conditions of the device [3]. Our investigations include the efficiency of generating power by both electric and phononic currents and the one of generating power and cooling one of the reservoirs by an electronic or a phononic heat current [3].

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*Poster

Reconstruction of energy landscapes for diffusing particles and observation of stochastic resonance in particle transport through microfluidic channels

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We use holographic optical tweezers to generate attractive potentials in microfluidic channels. The microfluidic channels connect two large reservoirs. Colloidal particles diffuse freely in the reservoir and single file in the channel. By using particles as probes, the potential energy landscapes in the channels can be accurately measured through the probability density function (PDF) analysis of the extracted trajectories. However the PDF method is not capable of detecting biases along a channel because it does not contain information of particles' moving directions. Here, we improve splitting probability (SP) to reconstruct potential energy landscapes in confining channels with limited amount of trajectories. We find that the potential energy landscape recovered from our SP based analysis is sensitive to bias down to $1k_BT$. In addition, we modulate attractive energy landscapes at a wide range of frequencies and observe stochastic resonance with a maximum of translocation rate. The optimized modulation frequencies are found in reservoirs with different concentrations of particles. Ref: [1]Pagliara, Stefano, Simon L. Dettmer, and Ulrich F. Keyser. "Channel-Facilitated Diffusion Boosted by Particle Binding at the Channel Entrance."Physical review letters 113.4 (2014): 048102. [2] Pagliara, Stefano, Christian Schwall, and Ulrich F. Keyser. "Optimizing diffusive transport through a synthetic membrane channel." Advanced Materials 25.6 (2013): 844-849.

*Poster

Microscopic Derivation of the Stokes Law from Hamiltonian Particle Systems

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—- Let us consider a macroscopic solute particle, such as a colloidal particle, immersed in a large number of solvent particles obeying a microscopic classical Hamiltonian. When solvent particles flow, the solute particle fixed spatially feels a force, which can be calculated by the Stokes law. The law is obtained by the hydrodynamics with the boundary condition on the surface of the solute particle, such as slip and stick boundary conditions. The Stokes law is believed to be valid for the macroscopic solute particle. It, however, remains unclear whether the boundary condition assumed in the law can be understood on the basis of microscopic Hamiltonian particle systems. —- Deriving microscopically the boundary condition in the Stokes law has been studied by theoretical and numerical methods. Exact derivation in a liquid state, however, is out of the scope of the previous studies. The exact derivation in a gas state has theoretically been studied, although the theories cannot be applied to a system in a liquid state. Some researchers have developed approximate liquid state theories, which cannot be employed for the exact derivation. There are many studies by molecular dynamics simulations providing numerical results, by which one cannot discuss exact derivation. —- In the present study, the boundary condition in the Stokes law is exactly derived in any state including a liquid for an isolated Hamiltonian system. The present study shows that the slip boundary condition is always obtained for the solute-solvent interaction depending only on a distance between solute and solvent particles. To other interaction systems, one can also apply the method developed in the present study. —- The boundary condition is derived at the large-solute limit in the Hamilton particle system. Since the limit is singular with respect to the distance from the solute particle, the whole space should be divided into the two regions. These are the regions far from and near the solute particle. In the two regions, the limit is separately taken. While the hydrodynamic equations are derived in the region far from the solute particle, the boundary condition is obtained in the region near the solute.

*Poster

Phonon lifetime in one dimensional chains

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We scrutinize the effects of the anharmonicity on phonon lifetime in one dimensional chains via molecular dynamic simulations. Our results demonstrate that the asymmetry of interaction potentials produce a significant impact on lifetimes of phonons, which the theories based on phonon Boltzmann equations fail to predict. We identify a new phonon-scattering mechanism induced alone by the asymmetry of the interaction potential and suggest a microscopic picture to understand such a new mechanism. More importantly, strong asymmetry combined with moderate (symmetric) nonlinearity will make most phonons exhibiting glasslike behaviors. Our findings provide a new insight to understand anharmonicity induced ultralow heat conduction in crystals, which is important in searching and designing more efficient thermoelectric materials.

*Poster

Topic 3: Quantum fluids and condensed matter-Posters

Thermal Transport at Crystalline Solid Interfaces

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Interfacial thermal conductance is of a great importance for many applications where thermal management at nanoscale is a vital issue [1]. That because at nanoscale, when the characteristic length of the system becomes comparable to the phonon mean free path, scattering at the boundary dominates thermal transport. In microelectronics for instance, there is a strong need to know how energy can be exchanged at separation distance of few nanometers where heat is primarily exchanged by acoustic waves for sub-nanometric gaps [2]. In this communication, we have performed lattice dynamics calculations on three dimensional solid/solid interfaces using ab initio interatomic force constants to predict interfacial phonon transmission as a function of both phonon frequency and wavevector. The transmission and thermal boundary conductances are calculated from an intensive statistical analysis of the probability of excited modes to be scattered in incoming and outcoming media. A spectral and angular analysis have been done to quantify the contribution of each phonon mode in a given scattering direction. The effect of interfacial bonding was studied at Si/Ge interface as well as the effect of the acoustic contrast at Si/heavy Si interface. Our results show that, in general, the transmitted thermal energy is not uniformly distributed over frequency and angle of transmission. In addition, we found that there is no critical angle but a spectral analysis of phonon transmission reveals a critical angle depending on the frequency. This can be used to devise high pass phonon filter via changing the orientation of the interface. In the case where the two solids separated by a nanometer scale gap, we also quantify the influence of phonon tunneling mediated by evanescent waves. References: [1] D. G. Cahill et al Appl. Phys. Rev. 1 011305 (2014). [2] V. Chiloyan, J. Garg, K. Esfarjani and G. Chen Nature Communications 6 6755 (2015)

*Poster

Phase Transition in Magnetic Nanodots with Potts Clock-Model and Dipolar Interaction: Localized and Mobile Spins

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We study the phase transition in magnetic nanodots using the q-state Potts clock model of inplane interaction J and interplane interaction J_z. In addition, we take into account a long-range dipolar interaction of magnitude D. The dot size is $NimesNimesN_z$ where N is the linear lateral size and N_z the thickness. For the localized spin model, using the steepest descent method which consists in minimizing the system energy we determine the ground-state spin configuration as a function of D/J. We show that the dot has stable vortex structures in a wide range of parameters. Monte Carlo simulations were carried out to study the phase transition of these vortex structures of the localized model. We also consider in this work the mobile spin model: putting the dot in an empty space and letting the spins evaporated under the effect of the temperature, we study the behavior of the evaporation and the melting. We show that in the gaseous phase (or liquid phase) the spins can form structures similar to nematic and smectic phases depending on various interaction parameters. Results are shown and discussed in the light of liquid crystals.

*Poster

Quantum phase transition in the evolution of $NO(X_2)Ar_n$ clusters $(n = 1 - 12)$: Equilibrium structures and stabilities

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We present pseudo-potential calculations of geometrical structures of stable isomers of $NO(X_2)Ar_n$ clusters (n=1-12). The NO molecule is perturbed by argon atoms in $NOAr_n$ clusters. For each cluster size considered, the global and a few energetically close $NOAr_n$ local minima are calculated using the Basin Hopping method of Wales et al.[1] which combines a Monte-Carlo exploration and deformation method. The reliability of our model was checked by deriving the potential energy cuts of $NOAr$ using an ab initio calculation based on multireference configuration interaction (MRCI) [2]. Our results reveal a good agreement for small configurations. For $NOAr$, we have obtained a triangular planar structure. In $NOAr_2$ cluster, both Ar atoms occupy the T-shaped positions relative to NO, and in $NOAr_3$ the third Ar atoms lies closer to the oxygen atom. The absolute minimum of $NOAr_4$ is a pyramidal with a square base. The stable structure of $NOAr_5$ was obtained arises by adding one Ar atom to an edge of the energetically optimal configuration of $NOAr_4$. The NO molecule lies in an axial site of the $NOAr_6$ pentagonal bipyramid, also in the $NOAr_7$ capped pentagonal bipyramid. It lies on the principal rotation axis in $NOAr_8$, $NOAr_9$ and $NOAr_{10}$, but in $NOAr_{11}$ it lies in the open face. An icosahedron structure is found for $NOAr_{12}$, in which the first solvation shell is completed. Our results reveal that a transition in the couple NO coordination from 8 (square antiprism) to 12 (icosahedrons) occurs for n = 11.We note also that the couple NO usually lie in the surface of the Arn subsystem, or are partly submerged in it with the closest Ar atoms forming T shaped units. Generally, the predicted global minima for $NOAr_n$ are based on the lowest minima of Ar_{n+1}, with NO playing the role of a surface atom. In addition, our results agree very well with the available experimental and theoretical findings on $NOAr_n$ clusters [3]. The obtained structures are also similar to those previously found for the open-shell systems Cl_2Ar_n [4] but different from those for the closed shell systems $HFAr_n$ [5] and $HClAr_n$ [6]. This can be explained by the fact that $NOAr$, like Cl_2Ar and unlike $HFAr$ and $HClAr$, has a T-shaped equilibrium structures. [1] D. J. Wales and J. P. K Doye, J. Chem. Phys. A, 101, 5111 (1997). [2] H. Hammami, F. E. Ben Mohamed, and M.Ben El Hadj Rhouma, J. Chem. Phys. (submitted) (2015). [3] F. Y. Naumkin and D. J. Wales, Mol. Phys. 98,219(2000). [4] F. Y. Naumkin and D. J. Wales, Computer Physics Communications 145, 141 (2002). [5] S. Liu, Z. Bacic, J. W. Moskowitz and K. E. Schmidt, J. Chem. Phys . 100, 7166 (1994). [6] D. T. Anderson, S. Davis and D. J. Nesbitt, J. Chem. Phys. 107, 1115 (1997).

*Poster

Large-scale Quantitative Analysis of Graphene Structures by Statistical Properties of Morphology

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Quantitative analysis of graphene structures is a very important issue in material science especially numerous results were generated by simulation or experiment. However, analyzing these messy data is mostly by some software packages so far. Not only the task is very labor intensive but also the result is susceptible to errors and is usually lack of objectivity. Therefore, fast and accurate analyzing tools are crucial and very desirable. Recently, we developed a computational workflow which can get characteristic quantities of graphene structures from their morphology in a very efficient way. These characteristic quantities (called Characteristic Indexes) are, for example, distribution of bond length, distribution of bond angle, and distribution of torsion angle, etc. After Characteristic Indexes of graphene structures were obtained, isomap and modularity methods are applied to classify their structures and to get its structural phase diagram. The isomap method can defined the similarity between graphene structures by geodesic paths in a high-dimensional manifold as well as the modularity method can find the best community structure of classification by optimization, i.e., to maximize the intra module connections as many as possible and to minimize the inter module connections as few as possible. With these tools, large-scale graphene morphological structures, their annotations as well as quantified characteristics, and classifications can be facilely and reliably retrieved as useful data.

*Poster

Boltzmann equation with double-well potentials

Silvia Chiacchiera * [1], Tommaso Macrì, Andrea Trombettoni

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We study the dynamics of an interacting classical gas trapped in a double-well potential at finite temperature. Two model potentials are considered: a cubic box with a square barrier in the middle, and a harmonic trap with a gaussian barrier along one direction. The study is performed using the Boltzmann equation, solved numerically via the test-particle method. We introduce and discuss a simple analytical model that allows to provide estimates of the relaxation time, which are compared with numerical results. Finally, we use our findings to make numerical and analytical predictions for the case of a fermionic mixture in the normal-fluid phase in a realistic double-well potential relevant for experiments with cold atoms. [pre-print: arXiv:1601.07543]

*Poster

Shear Viscosity of Quasi 2D Dipolar Bose-Fermi Mixtures with Long-Range Interactions

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Low temperature shear viscosity of a spin polarized two-component quasi 2D dipolar Fermi gas with long-range $1/r$ interaction in the Bose-Einstein condensation (BEC) limit, where the system can be considered as dimers and the unpaired fermions, is calculated by means of the Kubo formalism. By taking into account the dimer-atom, dimer-dimer, and atom-atom interactions in the self-energies the viscous relaxation time ($au_{eta} = (au_{DA}^{-1} + au_{DD}^{-1} + au_{AA}^{-1})^{-1}$) is determined. Since, the relaxation rates due to these interactions au_{DA}^{-1}, au_{DD}^{-1} and au_{AA}^{-1} varies respectively as T, T^2, and T in the low temperature limit $To0$, the dimer-atom and atom-atom interactions play the dominant role to the shear viscosity and the shear viscosity varies as T^{-1}. For small polarization the effect of dimer-dimer interaction is important ($au_{DA}, au_{AA} >> au_{DD}$), and the shear viscosity changes as the standard T^{-2} behviour. In this case, the temperature behavior of the dimer relaxation rate unaffected by $1/r$ interaction and the contact, dipole-dipole, and $1/r$ interactions play the same role in the temperature dependence of the shear viscosity. Our results have important consequences for developing experiments and theoretical researches on the transport properties of ultracold gases with repulsive or attractive long range $1/r$ interaction.

*Poster

Berezinskii–Kosterlitz–Thouless transition in dynamical coupled fields

Laurent De Forges De Parny * [1], Adam Rançon, Tommaso Roscilde

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At finite temperature, two spatial dimensions is known to be a marginal dimension in statistical physics for models with continuous symmetry, such as the XY model with $U(1)$ symmetry. Indeed, due to the special role played by the long-wavelength fluctuations, the finite-temperature physics and critical phenomena are qualitatively and quantitatively different from the mean-field prediction, which completely fails, and the $U(1)$ continuous symmetry remains unbroken. Nevertheless, two different phases exist: a low-temperature quasi-ordered phase with power law correlation and a high-temperature disordered phase with exponential correlation. The transition between these two phases is called Berezinskii–Kosterlitz–Thouless (BKT) transition, transition of infinite order associated with the unbinding of pairs of topological excitations (vortices and antivortices) at a critical temperature. The case of coupled fields received little attention despite its relevance in condensed matter physics. Motivated by the physics of coupled atomic and molecular Bose-Einstein condensates, we investigate a classical coupled XY model with $U(1)$
times
mathbbZ$_2$ symmetry capturing the critical properties of the quantum ultracold atom-molecule mixtures. The asymmetric coherent coupling between atoms and molecules clearly leads to a complex interplay between the phenomena of quasi-condensation of atoms and molecules, and to the possibility of quasi-condensation transitions which are not realized in the context of monoatomic quantum fluids. The
mathbbZ$_2$ can lead to a finite-temperature Ising transition, associated with quasi-phase locking between the atoms and the molecules. On the other hand, the $U(1)$ symmetry has an associated BKT transition towards quasi-condensation of atoms or molecules. The existence of the two transitions (Ising and BKT) is found to depend crucially on the population imbalance between atoms and molecules: when the molecules are majority in the system, their BKT quasi-condensation transition occurs at a higher temperature than that of the atoms; the latter has the unconventional nature of an Ising quasi-phase-locking transition, lacking a finite local order parameter below the critical temperature. When the balance is gradually biased towards the atoms, the two transitions merge together to leave out a unique BKT transition, at which both atoms and molecules acquire quasi-long-range correlations, but only atoms exhibit conventional BKT criticality, with binding of vortex-antivortex pairs into short-range dipoles. The molecular vortex-antivortex excitations bind as well, but undergo a marked crossover from a high-temperature regime in which they are weakly bound, to a low-temperature regime of strong binding, reminiscent of their transition in the absence of atom-molecule coupling.

*Poster

Symmetry, density profile and momentum distribution for 1D strongly interacting multi-component Fermi gases

Jean Decamp * [1], Pacome Armagnat, Bess Fang, Mathias Albert, Anna Minguzzi, Patrizia Vignolo

[1] Institut Non Lineaire de Nice – France

We consider a mixture of one-dimensional strongly interacting Fermi gases up to six components, subjected to a longitudinal harmonic confinement. In the limit of infinitely strong repulsions we provide an exact solution which generalizes the one for the two-component mixture. We show that an imbalanced mixture under harmonic confinement displays partial spatial separation among the components, with a structure which depends on the relative population of the various components. Furthermore, we provide a symmetry characterization of the ground and excited states of the mixture introducing and evaluating a suitable operator, namely the conjugacy class sum. We show that, even under external confinement, the gas has a definite symmetry which corresponds to the most symmetric one compatible with the imbalance among the components. We also study the properties of the momentum distributions, focusing on the asymptotic behavior, which is closely related to the interaction energies.

*Poster

Disorder Effects in Extreme Type-II Superconductors at High Magnetic Fields

Sasha Dukan * [1]

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Within a T-matrix approximation for a homogenous superconductor, we investigate the influence of nonmagnetic impurities on the behavior of the density of states as scattering potential crosses from the weak (Born) to the strong (unitary) limit in a strongly-coupled superconductor in a magnetic field. We calculate the tunneling conductance between a scanning tunneling microscope tip and the surface of an extreme type-II superconductor in a high magnetic field and at zero temperature. We find that in the presence of disorder the differential conductance becomes finite at zero bias and develops a nonlinear dependence on the bias voltage. We apply our theory to calculate the differential conductance of a borocarbide superconductor in the mixed state.

*Poster

Bose-Hubbard model with long-range interactions

Thibaut Flottat * [1], Laurent de Forges de Parny, Frédéric Hébert, Valery Rousseau, George Batrouni

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We present a numerical study of a bidimensional Bose-Hubbard model with competing short- and long-range interactions, using quantum Monte-Carlo simulations and mean field methods. We determine exactly the phase diagram at unit filling and analyse phases properties of the system at zero temperature. We found three distinct phases : a Mott insulator, a superfluid, a charge density wave and the coexistence of the two last which could be a supersolid.

*Poster

Targeting Eigenstates by "Simulated Measurements" using a Decoherence based Nonlinear Schrödinger Equation

Oliver Furtmaier * [1], M. Mendoza

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Inspired by the idea of mimicking the measurement on a quantum system through a decoherence process to target specific eigenstates based on Born's law instead of the hierarchy of eigenvalues, we transform a Lindblad equation for the reduced density operator into a nonlinear Schr´odinger equation to obtain a computationally feasible simulation of the decoherent dynamics in the open quantum system. The method shows an exponential convergence and its computational costs scale linearly for sparse matrix representations of the involved Hermitian operators. Symmetries of the problem can be incorporated either in the initial state of the dynamics or explicitly using the symmetry operators in the evolution equation. As an application of the method we discuss *parallel eigenstate towing*, which relies on the adiabatic principle to follow the progression of an arbitrary subset of eigenstates along a perturbation strength increase with the intention to explore for instance the effect of interactions on these eigenstates.

*Poster

Liquid 3He on graphite: theoretical calculations

M.C. Gordillo * [1], J. Boronat

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We performed diffusion Monte Carlo calculations of ^{3}He on fully corrugated graphite. We found that at densities lower that 0.006 Å^{-2} the system is a very dilute gas, that at that density is in equilibrium with a liquid of density 0.014 Å^{-2}. Our prediction agrees very well with the extant experimental data and disagrees with the results of previous purely 2D calculations.

*Poster

Entanglement and concurrence in a quantum critical spin 1/2 quasi-one dimensional Heisenberg antiferromagnet compound $[Cu(\mu\text{-}C_20_4)(4\text{-}NC_5H_4NH_2)_2(H_2O)]_n$

Jaiswal-Nagar Deepshikha * [1], Arya Mohan, Ranjeet Singh, Neeraj K. Rajak

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Magnetisation measurements were done on single crystals of $[Cu(\mu\text{-}C_20_4)(4\text{-}NC_5H_4NH_2)_2(H_2O)]_n$, a spin 1/2 quasi-one dimensional Heisenberg antiferromagnet known to be quantum critical with external magnetic field as the control parameter. Single crystals were grown using slow diffusion and gave an R value of 1.14, pointing to the excellent quality of the crystals. Fitting to Bonner-Fischer model for 1 T gave a value of J/k_B as 3.12 and g as 2.3 that matched very well with published data. ξ_T shows an increase when T decreases (suggesting ferromagnetism) till a temperature T_{Cross} where it starts to decrease. T_{Cross} seems to show an oscillatory behavior with H. The fingerprint of quantum criticality is captured very well by the quantum entanglement. We have been able to extract entanglement as well as concurrence- an entanglement witness, from susceptibility data as a function of field and temperature. The value of concurrence at 1.9 K and 0.02 T is 0.42, in excellent agreement with theoretical predictions for a two spin correlation. Curiously enough, entanglement also shows an oscillatory behavior with field suggesting a possible correlation with magnetic order.

*Poster

Exchange symmetry, fluctuation-compressibility relation, and thermodynamic potentials of quantum liquids

Ji-Hyun Kim * [1], Yu Rim Lim, Seong Jun Park, Sanggeun Song, Gil-Suk Yang, Young-Gui Yoon, Jaeyoung Sung

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Liquid helium does not obey the Gibbs fluctuation-compressibility relation, which was noted more than six decades ago. However, still missing is a clear explanation of the reason for the deviation or the correct fluctuation-compressibility relation for the quantum liquid. Here we present the fluctuation-compressibility relation valid for any grand canonical system. Our result shows that the deviation from the Gibbs formula arises from a nonextensive part of thermodynamic potentials. The particle-exchange symmetry of many-body wave function of a strongly degenerate quantum gas is related to the thermodynamic extensivity of the system; a Bose gas does not always obey the Gibbs formula, while a Fermi gas does. Our fluctuation-compressibility relation works for classical systems as well as quantum systems. This work demonstrates that the application range of the Gibbs-Boltzmann statistical thermodynamics can be extended to encompass nonextensive open systems without introducing any postulate other than the principle of equal a priori probability.

*Poster

Linking number cascade in non-Abelian quantum turbulence

Michikazu Kobayashi * [1]

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I investigate quantum turbulence comprised of non-Abelian vortices, the topological charge of which is characterized by the non-Abelian group. Different from classical-fluid turbulence and Abelian quantum turbulence, non-Abelian quantum turbulence conserves the total linking number of vortex lines during its dynamics. The resulting energy spectrum of turbulence differs from the famous Kolmogorov spectrum, and is determined by the linking number cascade in the inertial range instead of the energy cascade.

*Poster

Ab initio calculation of fundamental properties of SrTe1-xOx alloys in Rock-salt structure

Salima Labidi * [1], M. Labidi, J. Zeroual, K. Klaa

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Structural, electronic, optical and thermodynamic properties of the SrTe1-xOx alloys ( ) in rock-salt phase are calculated using the full potential augmented plane wave (FP-LAPW) method within density functional theory. The exchange-correlation potential for structural properties was calculated by the standard local density approximation (LDA) and GGA (PBE) and the new form of GGA (WC) which is an improved form of the most popular Perdew-Burke-Ernzerhof (PBE), while for electronic properties, in addition to LDA and GGA correction, Engel and Vosko GGA (EVGGA) scheme was also applied. The results show that the use of WC in our calculations is more appropriate than GGA and LDA and gives a good description of structural properties such as lattice parameters and bulk modulus. Our investigation on the effect of composition on lattice constant, bulk modulus, and band gap for ternary alloys shows almost nonlinear dependence on the composition. In addition to FP-LAPW method, the composition dependence of the refractive index and the dielectric constant was studied by different models. On the other hand, the thermodynamic stability of this alloy was investigated by calculating the excess enthalpy of mixing as well as the phase diagram.

*Poster

Synchronization of cascaded optomechanical cavities

Matthieu Labousse * [1], Eduardo Gil-Santos, Arthur Goetschy, Ivan Favero, Cristiano Ciuti

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Synchronization of nonlinear oscillators arise in many different configurations and can imply a wide range of self-organization effects. At a quantum level, synchronization of mechanical modes have been for long a challenge. A fruitful strategy relies on light radiation pressure which couples mechanical motions with electromagnetic modes in a nonlinear way. What was initially a fundamental limitation in optical interferometry for gravitational detectors has been turned into a fundamental field called now optomechanics [1]. The recent developments of optomechanical devices at the microscopic scale have paved the way to efficient, tunable and precise light-mediated mechanical effects. This can be achieved for example by engineering micrometer-sized disk cavities whose radius varies with the radiation pressure. In return, the resulting change in optical length impacts the cavity modes and the mechanical motion might ultimately enters into self-oscillatory regimes. Optomechanical networks are now platforms for studying synchronization and light-mediated self-organization at small scale [2,3]. In this talk, I will present a very recent theoretical and experimental investigation of cascaded optomechanical disks, which are unidirectionally coupled trough an optical waveguide. The system is implemented in a single semiconductor chip and its scalability makes this system an excellent candidate for the investigation of large complex metamaterials. After briefly discussing the experimental setup, I will focus on our very recent theoretical investigations and discuss the synchronization properties of such a system. [1] Aspelmeyer et al., Rev. Mod. Phys. 86 (2014). [2] Zhang et al., Phys. Rev. Lett. 109 (2012). [3] M. Ludwig and F. Marquardt, Phys. Rev. Lett. 111 (2013)

*Poster

Distribution of zeros in the rough geometry of fluctuating interfaces

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We study numerically the correlations and the distribution of intervals between successive zeros in the fluctuating geometry of stochastic interfaces, described by the Edwards-Wilkinson equation. For equilibrium states we find that the distribution of interval lengths satisfies a truncated Sparre-Andersen theorem. We show that boundary-dependent finite-size effects induce non-trivial correlations, implying that the independent interval property is not exactly satisfied in finite systems. For out-of-equilibrium non-stationary states we derive the scaling law describing the temporal evolution of the density of zeros starting from an uncorrelated initial condition. As a by-product we derive a general criterion of the Von Neumann's type to understand how discretization affects the stability of the numerical integration of stochastic interfaces. We consider both diffusive and spatially fractional dynamics. Our results provide an alternative experimental method for extracting universal information of fluctuating interfaces such as domain walls in thin ferromagnets or ferroelectrics, based exclusively on the detection of crossing points.

*Poster

Dispersion relation for interface ripplons in segregated Bose-Einstein condensate mixtures

Chang-You Lin * [1], J.O. Indekeu, V. T. Nguyen, T.H. Phat

[1] KU Leuven – Belgium

The localized low-energy interfacial excitations, or Nambu-Goldstone modes, of phase-separated binary mixtures of Bose-Einstein condensates are investigated analytically by means of a double-parabola approximation (DPA) to the Lagrangian density in Gross-Pitaevskii theory. The DPA allows one to obtain nontrivial analytic expressions for the excitations underlying capillary waves or "ripplons", and to derive their dispersion relation directly from the Bogoliubov-de Gennes equations. (Submitted to Physical Review A.)

*Poster

Demixing and Temperature effects in mixtures of two Bosonic species

Fabio Lingua * [1], Vittorio Penna, Barbara Capogrosso Sansone, Marco Guglielmino

[1] Politecnico di Torino – Italy

We investigate the properties of phase separation in a mixture of two bosonic species by means of path-integral quantum Monte Carlo by the two-worm algorithm. The mixture is trapped in a square optical lattice at different filling and temperature conditions. The work is focused on the study of the ground-state phase diagram where various quantum phases can arise depending on the interplay between intra-and inter-species interactions. Demixed phases, characterized by spatial separation of the two species, are studied in details determining under which conditions they can be stabilized. The influence of temperature, filling factor and harmonic trap on phase separation is also investigated. An interesting dependence of the degree of demixing from temperature has been found, suggesting new ways to measure the temperature of a two-component bosonic mixture.

*Poster

Destruction of quantum entanglement and non-linearity of quantum mechanics

A.V. Melkikh * [1]

[1]Ural Federal University – Russia

A number of experiments in which the entanglement plays an important role (EPR, Wheeler's delayed choice, Hardy's paradox) is considered. It has been shown that a complete theoretical explanation of these experiments is possible only within the framework of quantum field theory. In particular, we show that only in the framework of quantum field theory the phenomenon of destruction of entangled quantum states may be properly explained. The complete system of equations for fields and particles is written and analyzed. The most important property of this system is its non-linearity (see, [1]). Wherein, Schr?dinger equation is a special case of such a system for a situation in which quantization of fields is insignificant. It is shown that only the processes of creation and annihilation of particles are "truly random" and only they can lead to the destruction of quantum entanglement. These processes are in the basis of mechanisms of relaxation of the isolated system to equilibrium. References 1. Melkikh, A.V., 2015. Nonlinearity of quantum mechanics and the solution of the problem of wave function collapse. Communications in Theoretical Physics. V.64, issue 1, 47-53.

*Poster

Ab initio DFT investigation of complex structured metamaterials based on graphene and hexagonal boron nitride

Tudor Luca Mitran * [1], George Alexandru Nemnes

[1]Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH) – Romania

By considering periodic screw dislocations induced in graphene, hexagonal boron nitride and hybrid graphene - hexagonal boron nitride, novel metamaterials with new and interesting properties can be developed. These materials are characterized by studying the topological configuration, stability, electronic and vibrational properties of their relaxed atomic configurations with the help of ab initio density functional theory (DFT) simulations. We also propose a metamaterial based on a graphene-boron nitride hybrid that makes use of graphene's high electrical conductance and boron nitride's large bandgap in order to produce an intense magnetic field at the nanoscale when connected to an external power source. In order to determine the current density that is further used for the estimation of the magnetic field, ballistic transport simulations are performed. Possible practical applications are envisioned for the proposed metamaterials, such as their use in electronic, thermoelectric and sensing applications.

*Poster

Spin Wave Propagation in Helical Magnet

Shin Miyahara * [1]

[1] Fukuoka University – Japan

A helical magnet is a typical magnetoelectric multiferroics where there is a strong coupling between magnetization and electric polarization. Such a coupling induces an electro active spin wave excitation and such a spin wave may show novel features as a spin-wave spin current. We clarify the dynamics of the spin-wave spin current in a helical magnet.

*Poster

Phase transitions and ordering structures of a model of chiral helimagnet in three dimensions

Yoshihiko Nishikawa * [1], Koji Hukushima

[1] Department of Basic Science, the University of Tokyo – Japan

We study a classical Heisenberg spin model of chiral helimagnet with the Dzyaloshinskii–Moriya (DM) interaction in three dimensions by large-scale Monte Carlo simulations up to about 10^6 spins. The DM interaction breaks the chiral symmetry of the system and induces a helical structure into the system in the low temperature region. Without magnetic fields, the system shows a continuous phase transition with the critical exponents of three-dimensional extitXY model. On the other hand, in the presence of a magnetic field perpendicular to the helical structure, it is found that the criticality of the system changes depending on the intensity of the magnetic field and the specific heat and the uniform magnetic susceptibility diverges at the transition temperature when the intensity of the magnetic field is sufficiently large. This means that a multicritical point exists in the phase diagram of the system.

*Poster

Critical behavior in the presence of an order-parameter pinning-field

Francesco Parisen Toldin * [1], F. F. Assaad, S. Wessel

[1]Institute for Theoretical Physics and Astrophysics, University of Wuerzburg – Germany

We apply a recently proposed simulation scheme that employs a local order-parameter pinning field to study quantum critical phenomena in the two-dimensional square-lattice bilayer quantum Heisenberg model. Using a world-line quantum Monte Carlo approach, we show that for this model, the pinning-field approach allows to locate the quantum critical point over a wide range of pinning-field strengths. However, the identification of the quantum critical scaling behavior is found to be strongly affected by the presence of the pinning-field. In order to further elucidate the scaling behavior in this situation, we also study a classical lattice model by means of Monte Carlo simulations and refined finite-size scaling considerations. A renormalization group analysis exhibits the presence of an important crossover effect from the zero pinning-field to a critical adsorption fixed point. In line with field-theoretical results, we find that at the adsorption fixed point the short-distance expansi on of the order-parameter profile exhibits a new universal critical exponent. This also suggests the presence of slowly-decaying scaling corrections, which we analyze in detail.

*Poster

Generalized Quantum Entropies

M. Portesi * [1], G. Bellomo, G.M. Bosyk, F. Holik, P.W. Lamberti, S. Zozor

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We study the properties of quantum generalized entropies inspired in the family of (h, ϕ)-functionals given by Salicrú for classical distributions. The quantum versions comprise some known cases as von Neumann and others, and provide a plethora of entropies the behaviour of which we analyze under the action of quantum operations. For given subfamilies of the quantum (h, ϕ)-entropies, the problem of detection of quantum entanglement is addressed and the application as measures of quantum correlations for bipartite systems is discussed. Sho Sugiura

*Poster

Entanglement threshold values

Luis Roa Oppliger * [1], Ariana Muñoz, Gesa Gruening, Robinson Gómez, Gautam Rai, Matthias Hecker

[1]Universidad de Concepción – Chile

We have addressed the protocols for quantum teleportation and for entanglement swapping when the main channel is an special mixed state. In both schemes demand threshold values in order to observe quantum features in the outcomes of the protocols. In our work we present the specific analytical values of those entanglement threshold values as function of the parameters of the channel.

*Poster

Universal equation of state for strongly interacting Fermi gas: fit with geometry of thermodynamics

George Ruppeiner * [1]

[1] New College of Florida – United States

Strongly interacting Fermi gasses at low density possess universal thermodynamic properties that have seen very precise ultralow temperature measurements in ^{6}Li atoms tuned to Feshbach resonance. In this talk, I present fits to measured thermodynamic properties, with fitting functions produced by the geometry of thermodynamics. The fits were done in two sections, joined at the second-order phase transition. The high temperature normal phase was fit with ideal gas like terms, and the low temperature superfluid phase was fit with power law expressions showing divergences at absolute zero [G. Ruppeiner, J. Low Temp. Phys. **181**, 77 (2015)]. Four free parameters were varied, and three recent data sets [L. Luo and J. E. Thomas, J. Low Temp. Phys. **154**, 1 (2009), M. J. H. Ku, A. T. Sommer, L. W. Cheuk, and M. W. Zwierlein, Science **335**, 563 (2012)] were fit with an overall precision of about $\chi^2 = 1.7$. The result is an explicit equation yielding the complete unitary thermodynamics over the entire range of data, including the phase transition, and with a power law extrapolation to absolute zero having Bertsch parameter $\xi_B = 0.368(5)$. Results also suggest that methods based on geometry of thermodynamics can model universal equations of state of strongly interacting systems relatively simply and with no need of any explicit microscopic models.

*Poster

Phase Transition driven by Skyrmion Destruction and Quantum Fluctuations in a Helimagnetic Thin Film under an Applied Field

El Hog Sahbi * [1], Hung T.Diep

[1] LPTM (CNRS/UCP) – France

We study in this paper properties of a helimagnetic thin film of Heisenberg spins under a magnetic field $\vec{H}$ applied along the c axis perpendicular to the film surface. The helimagnetic structure of our model comes from the competition between the ferromagnetic nearest-neighbor interaction J_1 and the antiferromagnetic next-nearest-neighbor interaction J_2 along the c axis. The inplane interaction is taken as J_1 for simplicity. In our study we consider both classical and quantum Heisenberg spin models. We first determined by minimizing the interaction energy the ground-state (GS) configuration as a function of H. We show that the spin configuration along the c axis is highly non uniform and has the characteristics of a skyrmion. The film is a collection of identical skymions sandwiched between the two surfaces. In each skyrmion, the structure is symmetric between the two surfaces in z spin components. Using Monte Carlo simulations, we show that when the temperature increases the layers with large perpendicular xy components undergo a transition to a disordered state, breaking therefore the skyrmion structure. Detailed results on layer susceptibilities for varying H will be shown and discussed. At low temperatures, we study effects of quantum fluctuations using the Green's function method. We show that quantum fluctuations at $T = 0$ result in non-uniform spin contractions of layers near the surface. At low T, there are crossovers of layer magnetizations due to the competition between quantum fluctuations and thermal effects. The spin-wave spectrum is also shown as a function of H, T and $J - 2$.

*Poster

Bose-Einstein condensation of the mixtures of interacting bosons and fermions in the self-consistent field model

S. Shulga * [1], Yu. Poluektov

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The model of Bose-Einstein condensation is constructed with account of interparticle interactions in mixed systems of bosons and fermions, on the basis of the self-consistent field method [1]. This work is a generalization of the model of Bose-Einstein condensation of pure bosonic system based upon the same method [2]. As we describe the condensation of the Bose subsystem we turn into zero, in contrast to most theories, the effective chemical potential that differs from the true one by the presence of terms responsible for interparticle interaction. Thus, the true chemical potential is not zero both for normal and condensed states, and remains a good thermodynamic variable in both cases. All of this permits to avoid several difficulties inherent in the model of ideal gas, such as fulfilment of thermodynamical relations and infiniteness of the particle number fluctuation. We considered in detail the case of δ-like interaction that gives the possibility to express all thermodynamical values analytically, in terms of the special Stoner functions. The thermodynamics of condensed state is constructed, behavior of the system around the critical temperature is considered, influence of admixture of fermions to the character of the phase transition is studied.
[1] Yu.M. Poluektov Ukr. J. Phys. 50 (2005) 1303 [arXiv:1303.4913].
[2] Yu.M. Poluektov, arXiv:1602.02746v1.

*Poster

Unavoidable gapless edge state of bosonic Mott state trapped in two-dimansional optical lattices

Takafumi Suzuki * [1], Masahiro Sato

[1]Graduate School of Engineering, University of Hyogo – Japan

We theoretically study boundary properties of trapped bosonic Mott insulators in optical square lattices. By performing quantum Monte Carlo calculations, we show that a finite superfluid density almost always appears in the incommensurate-filling (IC) boundary surrounding the bulk Mott insulator at a very low temperature. In this IC boundary, both off-diagonal and density correlations exhibit a power-law decay. Our result clearly indicates that the gapless IC boundary state always emerges in any bosonic Mott insulators on optical lattices. Therefore, we can expect that if a topological insulating state in trapped cold-atom systems is realized, its boundary possesses at least two gapless modes (or coupled modes) of the above gapless state in the IC region and the intrinsic topologically-protected edge state.

*Poster

Bayesian Model Selection of $NiGa_2S_4$ Triangular Lattice with Boltzmann Factor

Hikaru Takenaka * [1], Kenji Nagata, Takashi Mizokawa, Masato Okada

[1] University of Tokyo – Japan

We propose a method for inducting the Boltzmann factor to extract effective classical spin Hamiltonians from mean-field-type electronic structural calculations by means of the Bayesian inference [1]. This method may enable the results of mean-field-type electronic structural calculations and those from magnetic experiments to be compared seamlessly because the Boltzmann factor takes into account the finite temperature effect. The method is applied to a NiS_2 triangular lattice in $NiGa_2S_4$ with a spin disordered ground state. Unrestricted Hartree-Fock calculations for the spin configurations of 16 Ni sites led to the estimation that the superexchange interaction between the nearest neighbor sites is ferromagnetic, which is consistent with magnetic experiment results. [1]H. Takenaka, K. Nagata, T. Mizokawa, and M. Okada, J. Phys. Soc. Jpn. 83, 124706, (2014).

*Poster

Measure synchronization in a two species bosonic Josephson junction

Jing Tian * [1], Haibo Qiu, Li-bin Fu

[1] Xi'an university of posts and telecommunications – China

Measure synchronization (MS) in a two-species bosonic Josephson junction (BJJ) is studied based on semi-classical theory. Six different scenarios for MS, including two in the Josephson oscillation regime (0 phase mode) and four in the self-trapping regime (π phase mode), have been clearly shown. Systematic investigations of the common features behind these different scenarios have been performed. We show that the average energies of the two species merge at the MS transition point. The scaling of the power law near the MS transition has been verified, and the critical exponent is 1/2 for all of the different scenarios for MS. We also illustrate MS in a three-dimensional phase space; from this illustration, more detailed information on the dynamical process can be obtained. Particularly, by analyzing the Poincare sections with changing interspecies interactions, we find that the two-species BJJ exhibits separatrix crossing behavior at MS transition point, and such behavior depicts the general mechanism behind the different scenarios for the MS transitions. The new critical behavior found in a two-species BJJ is expected to be found in real systems of atomic Bose gases.

*Poster

Structure properties of MoS2-Graphene Heterostructures under static and cyclic bending loading

An-Cheng Yang * [1], Nan Yow Chen Wen Jay Lee

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Molecular dynamics (MD) simulations are performed to investigate the structure properties of finite-size MoS2-Graphene heterostructures under different static and cyclic bending loading at different working temperature. The structure properties are quantified by means of interfacial flatness and the cross section profile. Both MoS2 and Graphene are generally regarded as flexible material. In this study, difference between two types of graphene are validation. We will show that MoS2-Graphene heterostructures can be bent repeatedly through large angles without undergoing catastrophic failure. The range of responses to this high-strain deformation is also estimated and discussed.

*Poster

Topic 4: Disordered and glassy systems-Posters

TAP equations for two models of jamming: negative perceptron and soft spheres in high dimension

Ada Altieri * [1], Silvio Franz, Giorgio Parisi

[1] "Sapienza" Università di Roma and Université Paris-Sud / Paris-Saclay – Italy

In the last years the study of glassy materials at low temperature has attracted significant interest, both from a theoretical and an experimental point of view. Much attention has concentrated on systems formed by an athermal assembly of repulsive particles with finite-range interactions, where one can observe - upon increasing density - a jamming transition, corresponding to a rigid arrangement of particles which cannot freely move and flow. We present a parallel derivation of the Thouless-Anderson-Palmer (TAP) equations and of an effective thermodynamic potential for the soft spheres and the negative perceptron in high dimension. Both models are continuous constrained satisfaction problems with a critical jamming transition characterized by the same exponents. Varying the number or the type of satisfied/violated clauses one could jump between two different phases, from a SAT region (with at least one configuration in agreement with all the requested constraints) to an UNSAT region (where all the constraints cannot be verified simultaneously). Our analysis reveals that a power expansion of the Gibbs potential up to the second order represents a successful framework to approach the jamming points from the SAT phase. This allows us to obtain the spectrum of the Hessian matrix and understand the leading behavior of the dominant eigenvalue. A pivotal outcome is that the effective thermodynamic potential has a subleading logarithmic contribution, which turns out to be dominant in an appropriate scaling regime. Our approach is quite general, independent from the specific form of the potential energy and directly applicable to other interesting models.

*Poster

Lattice sphere packing: the importance of being perfect

Alexei Andreanov * [1], Antonello Scardicchio, Salvatore Torquato

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Sphere packing is an old (optimisation) problem at the intersection of mathematics, physics and computer science. The formulation of the problem is very simple - what is the densest arrangement of spheres in a given Euclidean dimension. Despite that, the solution proved to be very hard to find, even approximately. The proofs for d=2,3 were only established in 20th century, while in higher dimensions our knowledge remains limited despite over a hundred years of research. The complexity of the problem originates from its combinatorial optimisation nature and the failure of our intuition in high dimensions. While there is a large body of results from (pure) mathematics, I am going to present some new results in lattice sphere packing based on a theory by Voronoi and methods of statistical mechanics. I will also discuss the decorrelation principle, a recent conjecture, that has important implications for the problem of packing.

*Poster

Light scattering properties of percolation clusters

Jean-Christian Anglès D'auriac * [1], Pierre-Étienne Wolf

[1] Institut Néel – France

The mechanisms of evaporation of fluids from disordered nanoporous materials are still debated. In a lattice model description, evaporation can occur either through a collective process of invasion percolation starting from the sample surface, or through a local process of cavitation, that is thermally activated nucleation of vapor bubbles, or from a combination of both. We discuss how light scattering measurements, which probe spatial correlations of the fluid density, can confirm the validity of such a lattice model and discriminate between these processes. To this aim, we investigate by numerical simulations in two and three dimensions the scattering properties of invasion percolation, a problem not yet discussed to our knowledge. Our results reveal under which conditions the inter-correlations between different clusters can be neglected, and the structure factor, or correlation function, accounted for by suitable averages over the cluster size distribution characteristic of the percolation problem. Our results explain the behavior observed in a recent experiment (F. Bonnet et. al, EPL 101, 16010, 2013).

*Poster

Soft modes and two-level systems in Spin Glasses

Marco Baity-Jesi * [1], Víctor Martín-Mayor, Giorgio Parisi, Sergio Pérez-Gaviro

[1] CEA Saclay – France

Several types of disordered systems display an excess of soft modes with respect to the Debye prediction. The origin and universality of these modes is not yet fully understood. Being spin glasses an epitome of the disordered system, we are interested in understanding how much of this behavior extends to a spin glass model. This would help us to understand the extent of the universality of phenomena such as the boson peak, and it would consitute new grounds for their understanding. Thus, we study the three-dimensional Heisenberg spin glass, the prototypical model with continuous spins. We investigate the properties of the inherent structures that are obtained by an instantaneous cooling from infinite temperature. We do find that the density of states g(w) exhibits localized soft plastic (non-Debye) modes and reaches zero as w^4. Further, when perturbing the system by adding a force along the softest mode, one reaches very similar minima of the energy, separated by small barriers, that appear to be good candidates as classical versions of Anderson's two-level systems. References: Marco Baity-Jesi, Victor Martin-Mayor, Giorgio Parisi, Sergio Perez-Gaviro, Phys. Rev. Lett. 115, 267205 (2015) Marco Baity-Jesi, Victor Martin-Mayor, Giorgio Parisi, Sergio Perez-Gaviro, in preparation.

*Poster

Population annealing algorithm tests and improvements

Lev Barash * [1], Martin Weigel, Michal Borovsky, Lev Shchur

[1] Landau Institute for Theoretical Physics – Russia

We revise the recently proposed population annealing algorithm for computational statistical physics and propose modifications and improvements.

*Poster

Edwards approach for random close packings of non-spherical particles

Adrian Baule * [1], Romain Mari, Lin Bo, Louis Portal, Hernan A. Makse

[1] Queen Mary University of London – United Kingdom

Random packings of objects of a particular shape are ubiquitous in science and engineering. However, such jammed matter states have eluded any systematic theoretical treatment due to the strong positional and orientational correlations involved. Here, a mean field theory based on a statistical treatment of the Voronoi volume in the spirit of the Edwards ensemble approach [1] is discussed, which allows for the calculation of the random close packing fractions of non-spherical particles [2]. This approach captures in particular the density peaks observed in simulations of different classes of non-spherical shapes. A phase diagram is presented that describes packings of elongated shapes such as spherocylinders and dimers in terms of an analytic continuation from the spherical random close packing [3]. [1] A. Baule, F. Morone, C.S. O'Hern, and H. A. Makse, arXiv:1602.04369 (2016) [2] A. Baule, R. Mari, L. Bo, L. Portal, and H. A. Makse, Nature Commun. 4, 2194 (2013) [3] A. Baule and H. A. Makse, Soft Matter 10, 4423 (2014)

*Poster

Thermal conductivity of glass-forming liquids

Pranab Jyoti Bhuyan * [1], Rituparno Mandal, Pinaki Chaudhuri, Abhishek Dhar and Chandan Dasgupta

[1]Indian Institute of Science – India

We carry out a detailed study of the thermal transport properties of glass-forming liquids. The spectrum of harmonic excitations is obtained from the eigenvalues of the Hessian matrices of the inherent structures. The eigenvalues and eigenfunctions of the Hessian matrix are used to calculate the low-temperature thermal conductivity of a model glass-forming system. The results of this calculation have been validated from comparisons with those obtained from equilibrium molecular dynamics simulations in which the thermal conductivity is calculated using the Green-Kubo equation. It shows that there is a strong correlation between the thermal conductivity and the energy of the relevant potential energy minima. This study provides explanations of some of the features observed in simulation results for the temperature-dependence of the thermal conductivity of glass-forming liquids.

*Poster

Record Dynamics as the Origin of Aging

Stefan Boettcher * [1], Dominic M. Robe, Paolo Sibani, Peter Yunker

[1] Emory University – United States

We provide a unified description of "aging", the increasingly sluggish dynamics widely observed in the jammed state of disordered materials, in terms of record dynamics. Structural evolution in aging materials requires ever larger, record-sized rearrangements in an uncorrelated sequence of intermittent events (avalanches or quakes). According to record statistics, these (irreversible!) rearrangements occur at a rate $\sim 1/t$. Hence, in this log-Poisson statistics, the number of events between a waiting time t_w and any later time t integrates to $\sim \ln(t/t_w)$, such that any observable inherits the t/t_w-dependence that is the hallmark of pure aging. Based on this description, we can explain the relaxation dynamics observed in a broad range of materials, such as in simulations of low-temperature spin glasses and in experiments on high-density colloids and granular piles. We have proposed a phenomenological model of record dynamics[†] that reproduces salient aspects of the experiments, for example, persistence, intermittency, and dynamic heterogeneity. Here, we compare the predictions of the model with the data available from experiments by Yunker, et. al.[‡].

*Poster

[†]N Becker, et. al. Mesoscopic model of temporal and spatial heterogeneity in aging colloids 2014 *J. Phys.: Condens. Matt.* http://arxiv.org/abs/1401.6521v1

[‡]P Yunker, et. al. Irreversible rearrangements, correlated domains, and local structure in aging glasses 2009 *Phys. Rev. Lett.* http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.103.115701

Configurational ovelap, effective potentials and the coexistence of localized and de-localized states in structural glass formers.

Jean-Marc Bomont * [1], Jean-Pierre Hansen Giorgio Pastore

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We consider two weakly coupled replicae of a dense system of N atoms interacting via a repulsive inverse-power potential, and calculate the mean value of the configurational overlap Q of the two replicae as well as its mean-square fluctuation, using the hyper-netted chain (HNC) integral equation for the pair structure of this symmetric "binary mixture". The Helmholtz free energy per particle $f(\rho, T; \epsilon_{12})$ and its Legendre transform or effective potential W(rho,T; Q) [1] are determined as functions of temperature T (at fixed density rho) and the inter-replicae coupling ϵ_{12} or its conjugate variable Q. Analysis of the $\epsilon_{12}(Q)$ and $W(Q)$ curves shows that the two-replicae system undergoes a Landau transition between weak overlap (delocalized) and high overlap (localized) states below a critical temperature T_{cr}. The extrema of $W(Q)$ correspond to the $\epsilon_{12} - > 0$ limit; the minima are associated with a delocalized super-cooled liquid (L) and a localized glass phase (G_2), while the intermediate maximum may be associated with an unstable glass phase G_1 predicted in our earlier work [2]. The Landau transition associated with a discontinuity of the mean overlap order parameter [1,3,4] may be considered as a precursor to the ideal (or "random first order") glass transition between the L and G_2 phases, which occurs at a temperature $T_{RFOT} < T_{cr}$, and is characterized by the vanishing of the configurational entropy [1,3,4] and by a weak discontinuity of the molar volume, implying that the ideal glass transition is a weakly first-order thermodynamic phase transition which requires an infinite long equilibration time. In view of the thermodynamic inconsistency of the HNC closure, we have repeated our calculations on the basis of the thermodynamically self-consistent Rogers-Young (RY) closure which confirm the qualitative predictions of the HNC results, but with significant quantitative differences. [1] M. Cardenas, S. Franz and G. Parisi, J.Chem.Phys. 110, 1726 (1998) [2] J.M. Bomont, J.P. Hansen and G. Pastore, J. Chem. Phys. 141, 74505 (2014) and 142, 107105 (2015) [3] L. Berthier, Phys. Rev. E 88, 022313 (2013) [4] G. Parisi and B. Seoane, Phys. Rev. E 89, 022309 (2014)

*Poster

Extended Plefka Expansion for Stochastic Dynamics

Barbara Bravi * [1], Peter Sollich, Manfred Opper

[1] King's College London – United Kingdom

We propose an extension of the Plefka expansion, which is well known for the dynamics of discrete spins, to stochastic differential equations with continuous degrees of freedom and exhibiting generic nonlinearities. The scenario is sufficiently general to allow application to e.g. biochemical networks involved in metabolism and regulation. The main feature of our approach is to constrain in the Plefka expansion not just first moments akin to magnetizations, but also second moments, specifically two-time correlations and responses for each degree of freedom. The end result is an effective equation of motion for each single degree of freedom, where couplings to other variables appear as a self-coupling to the past (i.e. memory term) and a coloured noise. This constitutes a new mean field approximation that should become exact in the thermodynamic limit of a large network, for suitably long-ranged couplings. For the analytically tractable case of linear dynamics we establish this exactness explicitly by appeal to spectral methods of Random Matrix Theory, for Gaussian couplings with arbitrary degree of symmetry.

*Poster

First-order transition and strong correlations: a model for glasses?

Olivier Cépas * [1]

[1] Institut Néel – France

The glass transition occurs near a first-order transition from a liquid to a solid, both states with correlations. We address the issue of strong correlations by studying a classical model of closely-packed dimers which represent interacting molecules, that can move collectively on a lattice. This model has a first-order phase transition to a "solid" phase, at thermodynamic equilibrium. The dynamics involve however collective motion of larger and larger scales in the supercooled phase which resemble in some aspects that of a glass-forming supercooled liquid. I will discuss how it fits with and differs from Adam and Gibbs' 1960's arguments and the phenomenology of glasses.

*Poster

Dielectric spectroscopy of a stretched polymer glass : heterogeneous dynamics and plasticity

Caroline Crauste-Thibierge * [1], Roberto Perez-Aparicio, Denis Cottinet, Loic Vanel ,Paul Sotta, Jean-Yves Delannoy, Didier R. Long, Sergio Ciliberto

[1] Laboratoire de Physique, Univ Lyon, Ens de Lyon, Univ Claude Bernard, CNRS – France

We study the dielectric relaxation of polycarbonate (PC) at room temperature under imposed strain rate $\dot{\gamma}$, above the yield stress and up to 13% strain. We find that the dielectric response of stretched PC behaves as if it was heated up at a temperature just below its glass transition temperature $T_g \approx 423$ K for PC. Indeed, in the frequency range of our experiment (10^{-2} Hz and 10^3 Hz), the dielectric response of the stretched PC at room temperature superimposes to the dielectric response of PC at a temperature $T_a(\dot{\gamma}) < T_g$, which is a function of strain rate. Specifically we observe that at T_a the dominant relaxation time $\tau_\alpha(T_a)$ of PC at rest is related to $\dot{\gamma}$ in such a way that: $\tau_\alpha(T_a) \sim 1/\dot{\gamma}$ at and beyond the yield point. In our experiment $10^{-5}s^{-1} < \dot{\gamma} < 10^{-3}s^{-1}$, the temperature shifts $T_g - T_a$ are of a few K. The mechanical rejuvenation modifies the dielectric response at frequencies smaller than 10Hz, whereas for higher frequencies the spectrum is only slightly modified.

*Poster

Conformal invariance in Correlated Random Surfaces

Caio P. de Castro * [1], M. Lukovic, Roberto F. S. Andrade, Hans J. Herrmann

[1]Eidgenössische Technische Hochschule (ETH) Zurich and Universidade Federal da Bahia (UFBA) – Switzerland

There exist many examples of random surfaces in nature such as random Gaussian surfaces and turbulence vorticity fields, whose symmetries have been studied extensively, revealing the presence of conformal invariance. Through the Fourier Filtering Method, any long-range spatial correlations can be detected by analyzing the Fourier coefficients of the surface. From there it is possible to determine the corresponding Hurst exponent and consequently establish the presence of scale invariance. In particular, we go further by investigating conformal invariance using the iso-height lines extracted from such distinct surfaces in the framework of Schramm-Löwner Evolution (SLE).

*Poster

Belief-Propagation Guided Monte-Carlo Sampling

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We describe a new Monte Carlo sampling algorithm using Belief Progation as a guiding method to update whole sub-graphs of a given system at once. In our work, we show that this new method is thermalizing faster than the usual Monte Carlo single spin flip and also that it is less sensitive to frustration (PRB 2014) . Another advantage of our method is that it gives a good approximation of the free energy directly at a given temperature thanks to Belief Propagation. In this presentation, I will describe the principle of the algorithm on tree sub-graphs and then how it can be extended to loopy sub-graphs.

*Poster

From the hopping crystal to the cluster glass

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At low enough temperature, a monodispersed ensemble of particles with ultrasoft interactions exhibits an ordered self-assembled cluster-crystal structure. We explore the out-of-equilibrium dynamics for a two-dimensional version of such systems. For small enough temperatures following a quench, the suppression of thermally-activated particle hopping hinders the ordering process of the crystal and results in an exotic crystal-to-glass transition via an abrupt loss of both long-range orientational order and local hexatic order. We provide a microscopic explanation of the mechanism for glass formation in terms of an effective self-induced polydispersity in the cluster occupation following the thermal quench, as a result of suppressed hopping at low temperature. Our findings are likely to be observed in a wide variety of experiments ranging from cold atoms to colloids and vortices in superconductors.

*Poster

New method of the thermodynamic perturbation theory for calculation the Helmholtz free energy of simple liquid metals

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The thermodynamic perturbation theory (TPT) is widely used for investigating the structure and thermodynamics of liquid and amorphous substances [1]. There are two groups of the TPT methods: methods of the high temperature approximation (HTA) proposed by Zwanzig [2] and methods of the field theory (FT). In the HTA the entropy and structure functions of the entire system are respectively equal to those of the reference system. The FT approximations allow avoiding these equivalences and giving the correction to the HTA Helmholtz free energy obtained in a general form by Itoh [3]. In the present work, the HTA+FT formalism is developed for liquid metals described by the nearly-free-electron approximation for the case when the HTA method is the variational one [4] and the FT method is the random phase approximation (RPA) [5]. The hard-spheres (HS) reference system is used. The different ways of the HS diameter defining are studied for liquid sodium. The work is supported by the Russian Government assignment N 0396-2015-0076. [1] N.E. Dubinin, N.A. Vatolin and V.V. Filippov, Rus. Chem. Rev., v. 83 (2014), p. 987 (erratum: Rus. Chem. Rev., 84 (2015), C01). [2] W. Zwanzig, J. Chem. Phys., v. 22 (1954), p. 1420. [3] M. Itoh, J. Phys. C: Solid State Phys., v. 20 (1987), p. 2483. [4] G.A. Mansoori and F.B. Canéeld, J. Chem. Phys., v. 51 (1969), p. 4958. [5] J. Woodhead-Galloway, T. Gaskell and N.H.March, J. Phys. C: Solid State Phys., v. 1 (1968), p. 271.

*Poster

Avalanche phenomena and shear localization near the creep fracture limit in amorphous plasticity

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The plastic behavior of bulk metallic glasses (BMGs) at room temperature is characterized by strong shear localization after yield, leading to quasi-brittle fracture. However, there is evidence of high plastic deformation at the microscopic scale in form of intermittent flow, known as avalanches. A key challenge in understanding the plastic behavior of BMGs is to establish statistical links between the microscopic avalanches and the macroscopic brittleness. To this end, it is useful to coarse-grain the important aspects from the atomistic scale in a mesoscopic model without fully resolving the atomic motions, being thus computationally more efficient. A common approach is to consider plastic activity as a sequence of spatially and temporally localized events, known as shear transformations. Amorphous plasticity arises as a stochastic phenomenon, consequence of the elastic interaction of a large number of shear transformations, whose self-organization together with strain softening leads to the formation of macroscopic shear bands that results in specimen failure. Using a finite element-based elastoplastic model which accounts for multi-axial stress states in a stochastic model of shear transformation activation, we simulate the processes that lead to failure in finite size samples. We characterize the failure process with statistical measures and find that, under creep conditions, the avalanche distributions become power-law distributed with non-universal exponents as the fracture strain is approached, even at stresses well below the zero-temperature flow stress. We study how loading conditions, temperature and strain softening affect the avalanche statistics and the shear localization process.

*Poster

Spatio-temporal patterns in ultra-slow creep dynamics

Laura Foini * [1]

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*Poster

Direct evidence for strong crossover of collective excitations and positive sound dispersion in the supercritical state

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Supercritical state has been viewed as an intermediate state between gases and liquids with largely unknown physical properties. However, it was recently shown that supercritical state of matter can be separated into two regimes - rigid-like liquid and dense gas [1,2,3]. The line demarcating these regimes was named Frenkel line after Russian scientist J. Frenkel. Here, we address the important ability of supercritical fluids to sustain collective excitations. We directly study propagating modes on the basis of correlation functions calculated from extensive molecular dynamics simulations and find that the supercritical system sustains propagating solid-like transverse modes below the Frenkel line but becomes devoid of transverse modes above the line where it supports longitudinal modes only. Important thermodynamic implications of this finding are discussed. We directly detect positive sound dispersion (PSD) below the Frenkel line where transverse modes are operative and quantitatively explain its magnitude on the basis of transverse and longitudinal velocities. PSD disappears above the Frenkel line which therefore demarcates the supercritical phase diagram into two areas where PSD does and does not operate [4]. The work was supported by Russian Science Foundation (Grant No 14-22-00093). [1] V.V. Brazhkin, A. G. Lyapin, V. N. Ryzhov, K. Trachenko, Yu.D. Fomin, and E. N. Tsiok, Phys. Usp. 55, 1061 (2012). [2] V. V. Brazhkin, Yu. D. Fomin, A. G. Lyapin, V. N. Ryzhov, and K. Trachenko, Phys. Rev. E 85, 031203 (2012). [3] V. V. Brazhkin, Yu. D. Fomin, A. G. Lyapin, V. N. Ryzhov, E. N. Tsiok, and Kostya Trachenko, Phys. Rev. Lett. 111, 145901 (2013). [4] Yu. D. Fomin, V. N. Ryzhov, E. N. Tsiok, V. V. Brazhkin, and K. Trachenko, arXiv: 1507.06094 (2015).

*Poster

Splitting of the Universality Class of Anomalous Transport in Crowded Media

Thomas Franosch * [1], Markus Spanner, Felix Höfling, Sebastian C. Kapfer, Klaus R. Mecke, G.-E. Schröder-Turk

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The basic paradigm of complex transport in disordered structures has been formulated originally by H.A. Lorentz as the motion of a tracer particle in a random structure of arrested scatterers. A striking prediction is the emergence of subdiffusive motion, concomitantly, the model exhibits a localization transition [1] which has also been found in fluids confined to porous host structures [2-4] and, at intermediate time scales, also in nanoporous silica melts [5] or in size-disparate mixtures [6,7]. The localization transition is driven by a continuum percolation transition of the underlying geometry. Upon increasing the excluded volume, the spanning cluster in the accessible space is diluted until, at a critical excluded volume fraction, it becomes a fractal structure and the mean-square displacement of a tracer on the critical spanning cluster becomes anomalous. While for structural properties, lattice and continuum percolation belong to the same universality class, the dynamic universality class describing transport splits, since in the case of continuum percolation long-range transport depends on the passage through arbitrarily narrow channels. In this talk we provide an overview of the physics of the Lorentz model, in particular, we relax idealizing assumptions of the Lorentz model to investigate the robustness of the critical dynamics near the localization transition [8]. First, we introduce obstacle correlations by using frozen-in hard-sphere fluids as realistic host structures, thereby changing the statistics of channel widths for the tracer particle. Second, we gradually change the microscopic dynamics from ballistic to Brownian which affects the rules how narrow channels in the system are probed. Our results confirm that the microscopic dynamics can dominate the relaxational behavior even at long times in striking contrast to glassy dynamics. [1] F. Höfling, T. Franosch, and E. Frey, Phys. Rev. Lett. 96, 165901 (2006); M. Spanner, S. K. Schnyder, F. Höfling, Th. Voigtmann, and T. Franosch, Soft Matter 9, 1604 (2013). [2] V. Krakoviack, Phys. Rev. Lett. 94, 065703 (2005); Phys. Rev. E 84, 050501 (2011). [3] J. Kurzidim, D. Coslovich, and G. Kahl, Phys. Rev. Lett. 103, 138303 (2009). [4] K. Kim, K. Miyazaki, and S. Saito, Europhys. Lett. 88, 36002 (2009). [5] Th. Voigtmann and J. Horbach, Europhys. Lett. 74, 459 (2006). [6] Th. Voigtmann and J. Horbach, Phys. Rev. Lett. 103, 205901 (2009). [7] A. J. Moreno and J. Colmenero, Phys. Rev. E 74, 021409 (2006); J. Chem. Phys. 125, 164507 (2006). [8] M. Spanner, F. Höfling, S.C. Kapfer, K.R. Mecke, G.-E. Schröder-Turk, and T. Franosch, Phys. Rev. Lett. 1116, 060601 (2016).

*Poster

Driven interfaces: from flow to creep through model reduction

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The response of spatially extended systems to a force driving their steady state out of equilibrium is strongly affected by the presence of disorder. We focus on the mean velocity induced by a constant force applied on one-dimensional interfaces. In the absence of disorder, the velocity is linear in the force. In the pres- ence of disorder, it is widely admitted and experimentally and numerically verified that the velocity presents a stretched exponential dependency in the force (the so-called 'creep law'), which is out of reach of linear response or more generically of direct perturbative expansions at small force. In dimension one, there is no ana- lytical derivation of such a law, even from a theoretical physical point-of-view. We propose an effective model with two degrees of freedom, constructed from the full spatially extended model, that captures many aspects of the creep phenomenology. It provides a justification of the creep law form of the force-velocity characteristics, in a quasi-static approximation. It allows to capture the non-trivial effects of short- range correlations in the disorder. It enables us to establish a novel phase diagram where the creep law manifests itself in a critical point in the force – system-size plane, from which arises a line describing the crossover between the linear-response regime and the creep regime.

*Poster

Nonlinear scaling variable at the lower critical dimension: Scaling in the 2D random field Ising model

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We systematically analyze the nonlinear invariant scaling variables at bifurcations in the renormalization-group flow, and apply our methods to the two-dimensional random-field Ising model (RFIM). At critical points, the universal scaling functions are usually written in terms of homogeneous invariant combinations of variables, like Lt^{nu} in the finite-size scaling form for the magnetization $M(T|L)$
$simt^{-beta}M(Lt^{nu})$, where t
$proptoT_c - T$. The renormalization-group flow to third order for the RFIM has a pitchfork bifurcation in two dimensions, leading to an exponentially diverging correlation length,
xi
$proptoexp^{1/2At^2}$. The invariant scaling combination suggested by this form is $L/$
xi
$simL/exp^{1/2At^2}$. Our analysis, inspired by normal-form theory, proposes that this exponential divergence can take a richer, more general scaling form. We explore possible consequences for simulations.

*Poster

Distinct Structural and Dynamical Difference between Supercooled and Normal Liquids of Hydrogen Molecules

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Nuclear quantum effects of hydrogen nuclei such as zero-point energy and nuclear delocalization significantly influence dynamical and structural properties of condensed hydrogen systems as reflected in the broad radial distributions and rapid diffusions. We will report the first computational study on real-time dynamics of vapor-pressure hydrogen molecular liquids, solids, and supercooled liquids exhibiting strong nuclear quantum effects which have been hardly accessible by use of previous computational and theoretical methods like density functional theory and semiquantum molecular dynamics simulations with path integrals.[1-5] For example, in vapor-pressure hydrogen solids, the hexagonal close-packed lattice structures and the stable lattice phonon modes with the reasonable frequency were successfully reproduced by the current method. The discrete jumps of the librational frequency, average H-H bond length as well as the H-H vibration frequency at the liquid-solid phase transition were computationally found and physically rationalized in comparison with liquid and high-pressure solid hydrogen systems.[2] Further, we recently realized supercooled hydrogen liquids which have not been stably observed in low-temperature experiments, and demonstrated that the hydrogen supercooled liquid is not a simply cooled liquid but rather exhibits intrinsic structural and dynamical properties including a precursor of tunneling and superfluidity of hydrogens which neither normal hydrogen liquid nor solid possesses.[1] All of the insights and information we obtained will provide a milestone for planning low-temperature experiments of metastable hydrogen systems like glassy and superfluid states and for identifying and characterizing various unknown hydrogen phases at low temperatures, which will open a new avenue of hydrogen material research. [1] Hyeon-Deuk K. and Ando K., Phys. Chem. Chem. Phys. (Communication), 18, 2314 (2016) [2] Hyeon-Deuk K. and Ando K., J. Chem. Phys. (Communication), 143, 171102 (2015) [3] Hyeon-Deuk K. and Ando K., Phys. Rev. B, 90, 165132 (2014) [4] Hyeon-Deuk K. and Ando K., J. Chem. Phys. (Communication), 140, 171101 (2014) [5] Hyeon-Deuk K. and Ando K., Chem. Phys. Lett., 532, 124 (2012)

*Poster

Granular force chain orientation characterizing disorder-induced metastable relaxation

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Order-disorder transitions represent one of the most important concepts in statistical physics. In this study, this concept is applied to a typical athermal system, granular matter. The crystalline (ordered) structure resulting from densely packed monodisperse grains gives way to a disordered structure when polydisperse grains are introduced in the granular pack. In such granular packs, configurational structure is supported by a set of grain-contact networks called "force chains". Whereas force-chain structure is related to the grain configuration, it also possesses an orientational degree of freedom. This situation is similar to liquid crystal nematic phases where molecular positions are random but their orientations exhibit an ordered state; configurational structure and orientational order can be independent. Therefore, a quantification of the orientational order is necessary for the proper characterization of the order-disorder transition in granular matter. In this study, we experimentally measure structural parameters (packing fraction and coordination number) and force-chain orientational order parameter in granular order-disorder transition by using bidisperse photoelastic materials. By comparing these parameters, we find that the force-chain orientational order parameter is much more sensitive than structural parameters, in order to characterize the granular pack's order-disorder transition followed by metastable relaxation by external perturbation.

*Poster

Decoupling phenomenon and replica symmetry breaking in the glass transitions of binary mixtures of particles

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We investigate the glass transition for the binary mixtures of Harmonic spheres on the high dimensional limit. Our study is based on the replica liquid theory which allows us to calculate the free-energy even in the glass phase. We show that when the size ratio between large and small particles is far from unity, there arises the partially frozen phase in which only large particles are frozen while small particles are mobile. Further, we find that even for the fully frozen phase in which all particles are frozen, there are two kinds of distinct phases. One of which is characterized by the one-step symmetric breaking and the other is by the two-step replica symmetric breaking.

*Poster

Transient shear banding in supercooled liquids

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Supercooled liquids and other soft glassy systems show characteristic spatial inhomogeneities in their local dynamical properties. Using detailed molecular simulations, we find that supercooled liquids also show transient shear banding in start-up of steady shear flow as has been observed for many soft glassy systems. We verify that the onset of transient shear banding coincides quite well with the appearance of a stress overshoot for temperatures in the supercooled regime. We find that the slower bands adapt less well to the imposed deformation and therefore accumulate higher shear stresses than the fast bands. Our results also indicate that the shear rates of the fast and slow bands are adjusted such that the local dissipation rate is approximately the same in both bands.

*Poster

Dynamic Facilitation in Binary Hard Disk Systems

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We investigate numerically the applicability of dynamic facilitation (DF) theory for glass-forming binary hard disk systems where supercompression is controlled by pressure. By using novel efficient algorithms for hard disks, we are able to generate equilibrium supercompressed states in an additive non-equimolar binary mixture, where micro-crystallization and size segregation do not emerge at high average packing fractions. Above an onset pressure where collective heterogeneous relaxation sets in, we find that relaxation times are well described by a "parabolic law" with pressure. We identify excitations, or soft-spots, that give rise to structural relaxation, and find that they are spatially localized, their average concentration decays exponentially with pressure, and their associated energy scale is logarithmic in the excitation size. These observations are consistent with the predictions of DF generalized to systems controlled by pressure rather than temperature.

*Poster

Asymptotic scaling behavior of self-avoiding walks on critical percolation clusters

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We study self-avoiding walks on three-dimensional critical percolation clusters using a new exact enumeration method. It overcomes the exponential increase in computation time by exploiting the clusters' fractal nature. We enumerate all $\simeq 10^{1200}$ conformations of walks with over 10^4 steps, far more than has ever been possible in previous studies (that is over 200 times more steps – over 10^{1000} times more conformations). The scaling exponent ν for the end-to-end distance turns out to be smaller than previously thought and appears to be the same on the backbones as on full clusters. We find strong evidence against the widely assumed scaling law for the number of conformations and propose an alternative, which perfectly fits our data. N. Fricke and W. Janke, Phys. Rev. Lett. **113**, 255701 (2014).

*Poster

Exploring the quasibrittle process zone with real-space RG

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Cracking in quasi-, or disordered, brittle materials like cement is poorly understood. Strong finite-size effects and a large microcracked process zone complicate analysis and characterization of these materials and thwart direct numeric methods. Recently work by Shekhawat and Sethna took a major step toward resolving inconsistencies in the theory of quasibrittle fracture using RG crossover ideas. We look to extend that model to the scaling of stress and damage in the quasibrittle process zone using an inhomogeneous real-space RG. In our picture, cracks at small scales appear percolation-like, while sufficiently course-grained cracks are sharply defined. These regimes are connected by a crossover characterized by variably sized damage clusters, corresponding to microcracking.

*Poster

Zero-temperature directed polymer in random potential on 4+1 dimension

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Zero-temperature directed polymer in random potentials on 4+1 dimension is described. The energy fluctuation $\Delta E(t)$ of the polymer grows as t^{β} with $\beta = 0.159 \pm 0.007$ as function of polymer length t and ΔE follows $\Delta E(L) \sim L^{\alpha}$ at saturation with $\alpha = 0.274 \pm 0.009$, where L is the system size. The dynamic exponent $z = \alpha/\beta \approx 1.72$ is obtained. The estimated values of exponents satisfy the scaling relation $\alpha + z = 2$ very well. Our results show that the upper critical dimension of the Kardar-Parisi-Zhang Equation is higher than $d = 4 + 1$ dimension.

*Poster

Structure and dynamics of a fluid in a quenched disordered potential

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Quenched disordered environments represent a very useful paradigm for the study of thermodynamics and transport phenomena in a variety of physical systems of great interest. Thus, structural and chemical randomness is a hallmark of many inorganic natural systems, such as porous rocks or soil, and manufactured materials, such as controlled porosity glasses, and has a strong influence on the static and dynamical properties of the fluids adsorbed or confined in them [1]. Also, in the realm of biological systems, concepts such as the macromolecular crowding in the cell interior and membranes and its consequences have often been illustrated and investigated through models displaying some kind of quenched randomness [2]. A lot of the work done on the topic has considered the disorder as due to randomly placed immobile obstacles or interaction sites. Here, we take a more minimalistic route by describing the disordered environment as not ensuing from immobile discrete bodies, but as a continuous random external potential energy field, chosen with Gaussian statistics for simplicity, in which a hard-sphere fluid is plunged. Experimental work has been done on the subject, recording the dynamics of colloids in a random optical potential [3,4,5], and the mode-coupling theory (MCT) for quenched-annealed systems [6,7] can be shown to be easily transposable to fluids in this kind of disorder. This last observation is the basis of our study. The structural properties required as input by the dynamical calculations are studied in the framework of liquid-state integral equation theories combined with the replica trick. Although the system looks rather simple, we are faced in some parameter domains with serious and unusual failures of well established schemes of the theory of simple liquids such as the hypernetted chain (HNC) closure and the exponential (EXP) approximation of the optimized cluster theory (OCT). The possible causes and consequences of these results will be briefly discussed, as these approaches are among the most popular for the study of fluids in disordered environments and glassy systems. The liquid-glass transition and other dynamical properties are studied within the MCT framework. The dynamical phase diagrams predicted by the theory will be reviewed and critically discussed. Some interesting phenomena appear, such as the great dependence of the phase diagrams on the potential correlation length, or the emergence of complex patterns in the time dependence of quantities such as the diffusion exponent. Comparison with available experiments and simulations will be attempted, and similarities and discrepancies will be discussed.

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*Poster

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Colloidal crystallization under spherical confinement

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Geometrical confinement can drastically modify the properties of liquids and crystals because of the appearance of finite-size effects and the enhancement of interface interactions [1,2]. Spherical confinement is of particular interest since the curvature governs the degree of frustration inside the system [2-3]. Recently, large icosahedral crystals were obtained through spherical confinement of nanoparticle suspensions although such a structure is not an equilibrium state in bulk systems [4].

In our work, monodisperse colloidal suspensions were embedded within emulsion droplets and observed by confocal microscopy experiments. The experimental system was characterized in terms of Yukawa interaction potentials fitted to radial distribution functions with molecular dynamics simulations [5-6]. It is reasonable to imagine that at a given size of the confinement, when increasing the packing fraction, one should get better crystallization [3]. Remarkably, spherical confinement appears to suppress crystallization. Indeed, using order parameters to identify crystals [7], we observe much less structure crystalline than in the corresponding simulations. By demonstrating the existence of a reentrant behaviour for crystallization in this model system, our work provides insights for the microscopic mechanisms of crystallization under spherical confinement. Thus, it is relevant for the design of small crystalline structures.

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*Poster

Driving Rate Dependence of Avalanche Statistics and Shapes at the Yielding Transition

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Amorphous systems, such as grains, foams or metallic glasses, respond to slow driving with strongly intermittent avalanche dynamics, which is typically evidenced in the time series of deviatoric stress tensor. In the limit of vanishing deformation rate we approach the so-called "yielding transition", which whether can be characterized as a continues dynamical phase transition, belonging to a specific universality class, is still under debate. The analysis of avalanche statistics close to yielding has therefore a particular relevance. We study stress time series caused by plastic avalanches in athermally sheared disordered materials. Using particle-based simulations and a mesoscopic elasto-plastic model[2], we analyze size and shear-rate dependence of the stress-drop durations and size distributions together with their average temporal shape. We find critical exponents different from mean-field predictions, and a clear asymmetry for individual avalanches. We probe scaling relations for the rate dependency of the dynamics and we report a crossover towards mean-field results for strong driving[1]. [1] C.Liu, E.E.Ferreo, F.Puosi, K.Martens, J-L.Barrat, Phys. Rev. Lett. 116, 065501 (2016) [2] A.Nicolas, J-L.Barrat, Phys. Rev. Lett. 110, 138304 (2016)

*Poster

Near optimal structure and parameter learning in Ising model

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Ising model is a graphical model representing stationary statistics of binary variables associated with nodes of a graph. They are used to represent systems in various fields such as statistical physics, computational biology, or image processing. However, the structure or parameters of the graphical model are often unknown a priori and have to be learnt from experimental data. In this talk, we consider the problem of inferring the underlying graph and parameters of the Ising model defined on an arbitrary topology from a collection of independent configurations. We suggest a new statistical physics inspired reconstruction method that is computationally efficient and achieves perfect graph structure recovery with a near information theoretical optimal number of samples. We provide mathematical guarantees that our consistent and convex estimator recovers couplings in a number of samples that is small with respect to the system size and couplings strength, outperforming the state of the art algorithms. Importantly, the reconstruction algorithm remains efficient in the low-temperature regime, and can be generalized to graphical models with higher-order interactions and alphabets.

*Poster

Quantum transition in disordered Weyl fermions from $2+\varepsilon$ and $4-\varepsilon$ expansions.

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After discovering graphene the materials with relativistic-like spectrum of electronic excitations have become a popular subject which currently drives several hot topics in physics. Among them there are three dimensional materials which have been recently identified as Weyl semimetals and which provide a new universality class of phase transitions. The Weyl semimetallic phase is topologically protected against small perturbations such as the presence of disorder. For a weak disorder, the system remains in a semimetallic phase: the density of states vanishes linearly at the band crossing, where electronic transport is pseudoballistic. However, for a critical disorder strength a transition occurs towards a diffusive metallic phase, characterized by a finite density of states at the nodal point. This transition has been studied numerically and using renormalization group in d = 2 + eps without consensus on the values of the critical exponents. We reconsider this problem in view of relevance of disorder correlations and rare events. We find that the renormalization flow generates new terms in $d = 2 +$
varepsilon and propose an alternative route based on a $4 -$
varepsilon expansion. Our method allows one to calculate the critical exponents in a systematic way opening an interesting perspective on several issues related to the transition.

*Poster

Local Entropy and Coupling Methods for Optimization Problems

Carlo Lucibello * [1], C. Baldassi, A. Ingrosso, L. Saglietti, R. Zecchina

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The ubiquitous problem of cost function minimization greatly benefited in the last decades from the connection with ground state search in statistical mechanics systems. Physics' inspired Monte Carlo methods, such as Simulated Annealing and Parallel Tempering, and heuristics, such as Belief Propagation, proved to be higly effective in dealing with rough free energy landscapes. Here we present a slightly different mapping for the minimization problem, where the Gibbs weight is modified with the addition of a bias towards configurations having an high local entropy. For integer bias exponents, the resulting partition function is that of a replicated system with an attractive coupling among replicas. This leads to a general prescription that can be applied to many existing algorithms, resulting sometimes in huge improvements in their performances. I will discuss the performance of Simulated Annealing and Belief Propagation on the replicated system for the problems of binary perceptron and KSAT. Bibliography: [1] C Baldassi, A Ingrosso, C Lucibello, L Saglietti and R Zecchina. Subdominant Dense Clusters Allow for Simple Learning and High Computational Performance in Neural Networks with Discrete Synapses. PRL 2015. [2] C Baldassi, A Ingrosso, C Lucibello, L Saglietti and R Zecchina. Local entropy as a measure for sampling solutions in Constraint Satisfaction Problems. JSTAT 2016.

*Poster

Soft modes and localization in the ground state of the random field XY model

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Spin glass XY model (i. e. $m = 2$ dimensional spin vectors) on Bethe lattice is studied at $T = 0$ when a random field is present. The spectral properties of the Hessian matrix of Bethe free energy are then examined, in order to study the lowest-energy excitations of the system. Two critical values of the external field H are detected, such that below Hc_1 the smallest eigenvalues of the Hessian go to zero, while at $Hc_2 < Hc_1$ the corresponding eigenvectors become delocalized. Furthermore, for $H < Hc_1$ the spectral density shows a power-law lower-band edge, and the related exponent is measured.

*Poster

Connection between athermal jamming and the glass transition

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Since the jamming transition at zero temperature has many similarities with the glass transition, the fundamental question is whether the glass transition density in the limit of vanishing temperature is same as the jamming density. We explore the energy landscape of repulsive spheres and determine the local minima that can be reached without crossing energy barriers and those that are obtained with a protocol that includes random crossings of energy barriers. We tune the probability of such random events as a parameter that is similar to the temperature to find out the transition density for a given temperature from an non-overlapping to an arrested state. We show that the glass transition at vanishing temperature occurs at a density lower than the athermal jamming density.

*Poster

Preparation of stable glass of phenolphthalein made by vapor-deposition and its thermal characterization

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Recently many previous studies suggested that the glass which is more stable than ordinary liquid quenched glass is formed by depositing molecules at 0.7 - 0.9 times of ordinal glass transition temperature (T_g). We investigated the deposition temperature dependence of the stability of vapor-deposited phenolphthalein glass. Variance of glass transition temperatures and heat capacities of vapor-deposited glass measured by differential scanning calorimeter told us that most stable glass was formed with 313K equivalent to 0.87 T_g and deposited phenolphthalein glass was immediately crystalized just after glass transition unlike liquid quenched glass. These results suggest that structure of stable glassy state which is formed by vapor deposition essentially differs from that of liquid quenched glass.

*Poster

Local structure of supercooled cyclohexane extracted from molecular dynamics simulations

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A new phase transition is observed for cyclohexane in a silica nano-pore from heat capacity measurements by an adiabatic calorimeter. The transition temperature is 154K, independent of a pore diameter. The transition is different from that observed in a bulk system and is suggested a liquid-liquid phase transition. To elucidate the origin of the new phase transition, we examined a local structure of supercooled cyclohexane by Molecular Dynamics (MD) simulations. We prepared two systems: (i) cyclohexane confined in a silica-nano pore and (ii) bulk cyclohexane. The quenching rate obtained by numerical simulation, which is estimated as 10^{11} K/sec, is rapid enough to obtain a supercooled state even in a bulk system. A force field adopted for amorphous silica was developed by Schulten and his co-workers [E. R. Cruz-Chu et. al., J. Phys. Chem. B 110, 21497 (2006)]. A CHARMM35 force field was used for cyclohexane. All the MD simulations were conducted with NAMD 2.10 in the isothermal-isobaric (NPT) ensemble at 1 atm and a variety of temperatures. Icosahedron-like local structures were observed in a supercooled cyclohexane both of the systems (i) and (ii). In the system (ii), the fraction of the structures increases as a temperature decreases and becomes constant around 170K. In the system (i), on the other hand, the fraction of the structures is not sensitive to temperature. It is also ascertained that a more variety of local structures were contained in a pore than in a bulk system.

*Poster

Pressure-Induced Bulk-Melting in Water Ice

Clemens Moritz * [1], Christoph Dellago

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Apart from its rich phase diagram of thermodynamically stable phases, water ice can also be found in glassy phases called amorphous ices. While often produced by rapid cooling, such ices also form when ice Ih cooled to 77 K is subjected to pressures on the order of 1 GPa in a process called pressure induced amorphization (PIA) [1]. Based on experimental evidence as well as on results from molecular simulation, multiple transition mechanisms have been proposed for this process: thermal and mechanical melting, as well as a cross-over scenario between the two [2,3]. However, direct simulations suffer from an inherent bias towards mechanical melting due to the disparate timescales accessible in simulation and experiment. We approach the subject of PIA by studying pressure-induced bulk-melting in water ice using computer simulations employing the TIP4P/Ice water model [4]. In particular, we use path-based rare-event techniques such as transition interface sampling (TIS) [5] to sample dynamical trajectories of melting events at successively lower temperatures and increased pressures in an effort to overcome the timescale problems of molecular simulation. These calculations allow us to investigate the transition mechanism by analysing the resulting trajectories, thereby elucidating the influence of increased pressure and reduced temperature on the formation of defects within the crystal structure. [1] O. Mishima, L.D. Calvert, and E. Whalley, Nature 310, 393 (1984). [2] T. Strässle, S. Klotz, G. Hamel, M. Koza, and H. Schober, Phys. Rev. Lett. 99, 175501 (2007). [3] J.S. Tse and D.D. Klug, Phys. Chem. Chem. Phys. 14, 8255 (2012). [4] J.L.F. Abascal, E. Sanz, R. García Fernández, and C. Vega, J. Chem. Phys. 122, 234511 (2005). [5] T.S. van Erp, D. Moroni, and P.G. Bolhuis, J. Chem. Phys. 118, 7762 (2003).

*Poster

Beating by order the amorphous lower limit of thermal conductivity

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The way in which ordered and disordered structural organizations impact properties of materials with identical chemical composition at the same external thermodynamic conditions is a key issue. Consider heat transfer, a process of paramount importance in physics and material science. The value measured in the amorphous glassy structure is considered as a lower limit for the thermal conductivity of any material. Indeed, in this case phonons strongly interact with disorder, and their lifetimes reach the minimum time scale allowed by thermal fluctuations at the given temperature. Smart design at the nano-scale, however, is known to allow reducing the thermal conductivity even below the amorphous limit, as demonstrated in recent breakthrough experiments. The mechanisms contributing to these observations still have not been completely rationalized in a coherent picture. In this talk I will address this point. We have studied by classical Molecular Dynamics computer simulation model systems, formed by binary mixtures of soft spheres with different masses, for a few values of the mass heterogeneity [1]. The vibrational spectra and the low temperature thermal conductivity have been investigated in the two cases where the masses are distributed at random positions (glass) or organized in fully ordered intercalated structures (super-lattices). I will show that, by controlling the width of the ordered domains in the latter case, the thermal conductivity in the direction of the replication pattern can be tuned to reach a value lower than that associated to the completely disordered structure. In this case, the different domains act as filters in complementary non-overlapping regions of the vibrational spectrum, therefore significantly suppressing the total phonons transport in the direction of the replication pattern. I will elucidate the critical role played by the interfaces, and show how to directly modify these latter to tune heat transfer even further.
[1] "Beating the amorphous limit in thermal conductivity by super-lattices design" Hideyuki Mizuno, Stefano Mossa, and Jean-Louis Barrat Scientific Reports 5, 14116 (2015) - doi:10.1038/srep14116

*Poster

Influence of the aspect ratio and boundary conditions on universal finite-size scaling functions in the athermal metastable two-dimensional random field Ising model

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This work [1] studies universal finite size scaling functions for the number of one-dimensional spanning avalanches in a two-dimensional (2D) disordered system with boundary conditions of different nature and different aspect ratios. To this end, we will consider the 2D Random Field Ising Model at $T = 0$ driven by the external field H with athermal dynamics implemented with periodic and forced boundary conditions. We have chosen a convenient scaling variable z that accounts for the deformation of the distance to the critical point caused by the aspect ratio. In addition, assuming that the dependence of the finite size scaling functions on the aspect ratio can be accounted by an additional multiplicative factor, we have been able to collapse data for different system sizes, different aspect ratios and different types of the boundary conditions into a single scaling function $hatmathcalQ$. [1] 'Influence of the aspect ratio and boundary conditions on universal finite-size scaling functions in the athermal metastable two-dimensional random field Ising model', Víctor Navas-Portella and Eduard Vives, Phys. Rev. E 93, 022129 (2016)

*Poster

Tracking sub- and super-diffusion with subordinated Lévy processes by inverting Pulsed Field Gradient Nuclear Magnetic Resonance signal

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Molecular motions of water or chemicals flowing through complex media are sometimes badly described on the basis of Brownian motion. Indeed, these motions are sometimes enhanced or hindered by physico-chemical properties of the surrounding medium, or by complex flow domain geometry[1]. Disregarding memory effects or possibly very rapid displacements may severely limit the liability of any prediction and our ability in cotrolling industrial or therapeutic devices. Lévy processes provide a wide variety of models accounting for sub- and super-diffusion, and PFG NMR measures the characteristic function of molecular displacements. Analytical methods are available for to invert PFG NMR signals by assuming displacements distributed by any specified infinitely divisible law, and interrupted by pauses of random duration represented by any Lévy subordinator [2]. Moreover, thus obtained subordinated Lévy processes have probability density functions that satisfy partial differential equations for which an increasing number of simulation methods becomes available. The analytical approach to displacement characteristic functions of subordinated Lévy processes helps us inverting PFG NMR signals : for each class of Lévy process and each class of subordinator we can find the parameters of the latter and of the parent the best adapted to a series of signals recorded during different prescribed durations, but at very small scale. Later, if other measurements using other techniques are performed at larger scale, they check whether a model apparently valid at small scale persists at larger scale. Measurements performed in water flowing through porous media illustrate the general method [3][4].

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*Poster

Coarsening dynamics of a granular lattice gas

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We studied experimentally and theoretically a granular gas on a square lattice. This particular geometry allows the clustering of particles on selected sites and modifies the usual gaseous behavior that characterizes driven granular materials. While most studies only focus on the stationary regime (obtained after a long period of shaking), we investigated the evolution of the system beginning with particular initial positions. We observed that our system transits from a fast regime characterized by frequent particles exchanges to a slow regime where its dynamics are dictated by the formation and the stability of the trapping sites. Our work addresses fundamental questions concerning dynamical regimes encountered in a dilute dissipative system.

*Poster

Equilibrium sampling of hard spheres up to the jamming density and beyond

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We implement and optimize a particle-swap Monte-Carlo algorithm that allows us to thermalize a polydisperse system of hard spheres in three dimensions up to unprecedently-large volume fractions, where standard algorithms and experiments fail to equilibrate[1]. We show that no glass singularity intervenes before the jamming density, which we determine by a non-equilibrium compression from a dilute fluid[1,2]. We demonstrate that equilibrium fluid and non-equilibrium jammed states can have the same density, showing that the jamming transition cannot be the end-point of the fluid branch[1]. Instead, we obtain a very wide range of the jamming density(around 65-70%) which is so-called J-line[3,4,5]. All jammed states in the J-line maintain the isostatic condition(the averaged contact number is six) and share a critical exponent characterizing near contact value of the radial distribution function, which is consistent with a prediction of a mean-field theory[6]. Furthermore, we examine the hyperuniformity which is vanishing of the density (volume fraction) fluctuation at the long wave length limit[7]. We find that higher density jammed states show stronger fluctuation at longer wave length[5]. This observation suggests that the hyperuniformity is violated at the jammed states[5,8,9]. [1] L. Berthier, D. Coslovich, A. Ninarello, and M. Ozawa, arXiv:1511.06182 (2015) [2] N. Xu, J. Blawzdziewicz, and C. S. O'Hern, Phys. Rev. E 71, 061306 (2005) [3] P. Chaudhuri, L. Berthier, and S. Sastry, Phys. Rev. Lett. 104, 165701 (2010) [4] M. Ozawa, T. Kuroiwa, A. Ikeda, and K. Miyazaki, Phys. Rev. Lett. 109, 205701 (2012) [5] L. Berthier, D. Coslovich, A. Ninarello, and M. Ozawa, (in preparation) [6] P. Charbonneau, J. Kurchan, G. Parisi, P. Urbani, and F. Zamponi, Nat. Comm. 5, 3725 (2014) [7] C. E. Zachary, Y. Jiao, and S. Torquato, Phys. Rev. Lett. 106, 178001 (2011) [8] A. Ikeda and L. Berthier, Phys. Rev. E 92, 012309 (2015) [9] Y. Wu, P. Olsson, and S. Teitel, Phys. Rev. E 92, 052206 (2015)

*Poster

Avoiding Total Confusion by the Hub of Brain Networks.

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Hopfield model is an artificial neural network which exhibits an autoassociative memory retrieval. Hopfield model on fully connected networks exhibits an errorless retrieval up until a storage threshold, after which none of the information is retrieved, i.e. total confusion. This feature of the model is unsatisfactory, for example, in the perspective of the enormously high storage capacity of human brain. We observe that Hopfield model on scale-free networks suppresses total confusion and enhances the retrieval quality in the glassy phase, when the degree exponent *gamma* of the network approaches two. We check the error rate on several real neural networks with heavy-tailed degree distributions and obtain similar results to analytic calculations near $gamma = 2$.

*Poster

Length scales of heterogeneous dynamics and the breakdown of the Stokes-Einstein relation in square well model liquid

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The breakdown of the Stokes-Einstein relation is a well known phenomenon that occurs in glass forming liquids, and is generally believed to be a consequence of heterogeneous dynamics, whereby the dynamics of the liquid becomes progressively more correlated spatially as temperature decreases. Although heterogeneous dynamics has been widely studied to understand growing length scales in glass forming liquids, the length scales involved in determining the breakdown of Stokes-Einstein relation are not adequately understood. We investigate the breakdown of the Stokes-Einstein (SE) relation by probing the dynamics at different length scales (wave numbers k) to identify a length scale beyond which the Stokes-Einstein relation becomes valid. The crossover length is defined by performing a systematic study of the SE relation for timescales associated with the self intermediate scattering function ($\tau(k,T)$) and diffusivity (D). For a given temperature this length is estimated from the wave number k such that the SE relation breaks down for $\tau(k,T)$ below that temperature. Our results show that the T- dependent crossover length can be identified with the heterogeneity length scale. We also show that, in the presence of the breakdown of the SE relation, the Adam-Gibbs relation applies to diffusion but not for relaxation times.

*Poster

Fluctuation-Dissipation ratio and static-dynamics equivalence: the JANUS II perspective.

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JANUS II, our custom made computer is the fastest device ever for the simulation of spin-glasses in three dimensions Janus II has just entered into full operation and our first study with it regards Aging dynamics as revealed by the study of the violations of the Fluctuation-Dissipation Theorem. In this context, Janus II gives access to new, unexplored dynamic regimes where new, unexpected results are observed. Specifically, we study the non-equilibrium Fluctuation-Dissipation Theorem (FDT) violations for the Edwards-Anderson model in 3 dimensions, as a way to investigate equilibrium properties of spin glasses [0]. Thanks to the special purpose computers JANUS [1] and JANUS II [2], we carried on simulations for very large systems, up to a lattice size of L=160, avoiding in this way the always bothering finite size scaling effects. And for very long simulation times, permitting us to investigate unexplored dynamical regimes from huge to small t/tw ratios (being $t + t_w$ up to 2^{35} MCS for L=160). Our accurate results show that the static-dynamic dictionary proposed by Barrat-Berthier in 2001 [3], in agreement afterwards with our group when using correlation functions [4], does not work properly for FDT studies in 3 dimensions, suggesting different behaviors depending on the time regime. [0] To be appeared very soon in arXiv. [1] Janus Collaboration: F. Belletti et al., Comp. Phys. Comm. 178, 208-216 (2008). [2] Janus Collaboration: M. Baity-Jesi, et al., Comp. Phys. Comm. 185, 550-559 (2014). [3] A. Barrat and L. Berthier, Phys. Rev. Lett. 87, 087204 (2001). [4] Janus Collaboration: R. Alvarez Banos et al., Phys. Rev. Lett. 105, 177202 (2010); R. Alvarez Banos et al., J. Stat. Mech. 2010, P06026 (2010).

*Poster

Energy diffusion in the ergodic phase of a many body localizable spin chain

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The phenomenon of many-body localization in disordered quantum many-body systems occurs when all transport is suppressed despite the excitations of the system being interacting. We report on the numerical simulation of autonomous quantum dynamics for disordered Heisenberg chains when the system is prepared with a strong inhomogeneity in the energy density. Using exact diagonalisation and a dynamical code based on Krylov subspaces we are able to simulate dynamics for up to $L = 26$ spins. We find, as expected, the breakdown of equilibration of the energy profile as the system enters the many-body localized phase. However, in the ergodic phase we also find a large region in parameter space where the energy dynamics remains diffusive but where spin transport has been previously evidenced to occur only sub-diffusively. This suggestive finding points towards a peculiar ergodic phase where particles do not diffuse but energy does, reminiscent of the situation in amorphous solids.

*Poster

A Boltzmann transport approach to the diffusivity of supercooled liquids

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While the dynamics of structural glasses is conveniently described as a collection of jumps in between the inherent structures (ISs) of the potential energy landscape, quantitative relations between the ISs statistical features and energetic profile, and the structural relaxation, are missing. Here we introduce a theoretical framework to connect ISs and dynamical properties of structural glasses, and we validate it against numerical dynamics simulations of a model system. Deep in the glassy phase, when a structural glass does not diffuse, its dynamics is the superposition of normal modes of oscillation. At finite temperature, ISs non-harmonicities lead to phonon-phonon scattering events that promote energy barrier crossing and diffusion. To estimate the diffusivity we assume the system to cross an energy barrier by moving along an eigendirection, and describe the dynamics along each eigendirection as that of a particle performing a deterministic motion in a given eigenfrequency dependent potential $V(\omega)$, punctuated by 'collisions' resetting the velocity to a random value taken from the equilibrium Maxwell distribution. The collisions represent phonon scattering events and occur with a rate $1/t_c$, where t_c is the typical phonon intercollision time in the relaxation time approximation. In this framework, each eigenfrequency ω has its own diffusion coefficient $d(T, \omega, t_c)$, and the overall diffusion coefficient is obtained averaging over the density of states, $D(T, t_c) = \int d(T, \omega, t_c) g(\omega) d\omega$. We have validated this approach focusing on a system of Harmonic spheres at volume fraction $\phi \simeq 0.65$, as previous results [1][**?**] suggest $V(\omega)$ to be well approximated by an ω^4 potential, with the amplitude of the energy barrier scaling as $\Delta E(\omega) \propto \omega^4$. We have determined the diffusion coefficient $d(T, \omega, t_c)$ by starting from the description of the 1d motion of a particle in a ω^4 potential, as a function of the intercollision time and of the temperature. The dependence of t_c exhibits a crossover we explain via the identification of the events mostly contributing to the diffusion. Then, we have derived the temperature dependence of the diffusion coefficient $D(T)$ integrating over the density of states, assuming the phonon intercollision time t_c to coincide with the ballistic time. Our theoretical predictions reproduce molecular dynamics simulation results, including the presence of an onset temperature marking a crossover in $D(T)$, and represent the first quantitative connection between the properties of the energy landscape of a supercooled liquid, and its relaxation dynamics.

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*Poster

Nanoporous amorphous carbon ensemble for electrode applications.

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In recent years, the theoretical study of amorphous nanoporous carbon structures has become a central part of the research and development of many kind of electrochemical devices . This knowledge is fundamental to overcome technical difficulties that arise measuring the exact topology of electrodes based on this materials. Obtaining such carbon structures may be useful to understand electrochemical processes such as: intercalation and electric double layer formation and lead us to develop a more efficient kind of organic devices. Using molecular dynamics simulations with the Tersoff potential implemented in LAMMPS software, we generated more than 1200 nanopurous structures with densities ranging between the critical and the triple point densities of carbon. The sampling procedure consists in simulate heating ramps in the supercells, from the coexistence phase to a point close to the liquid transition. Then select intermediate structures to apply a sudden quenching to room temperature. The result may be presented in a three-dimensional phase space with surface area, volume fraction and density as variables. In this space, at least, three different phases arise: a graphitic-like phase where graphene sheets bending outward and intercalate, a nano-foam phase where no graphite like structure is visible and a sponge-like phase rich in extitsp carbon bonding state. This data may be useful for multiscale simulations of porous carbons.

*Poster

Self-sustained clusters in spin glasses

Jacopo Rocchi * [1], David Saad, Chi Ho Yeung

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We introduce the notion of self-sustained clusters in Ising models. These clusters are defined by the property that for each spin in the cluster, in-cluster field contribution dominates over the field induced by out-cluster spins. Such clusters are primarily effected by the in-cluster configuration and are stable with respect to out-cluster fluctuations.The existence of self-sustained clusters sheds light on the microscopic manifestation of metastable states and the emergence of frozen variables in certain constraint satisfaction problems. We discuss results obtained for the SK model and present new results obtained for the p-spin model with p=3, which corresponds to the 3-XORSAT problem in the zero temperature limit; where the energy landscape undergoes an ergodicity breaking transition at a higher temperature than the true spin glass transition point. The analysis employs the (double) replica method to compute the entropy of macroscopic self-sustained clusters as a function of the temperature and their sizes.

*Poster

Suppression of crystalline order by competing liquid structures

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In a molecular liquid, the local structure characteristic of the crystal is likely to be particularly stable, and one can expect that it will accumulate on cooling. However, other non-crystalline structures can also be stable in the liquid, and compete with the accumulation of crystalline order. On what conditions can such a competition stabilize the supercooled liquid to the point of dynamical arrest? We tackle this question using a lattice model where both the crystalline order and the non-crystalline structures are explicitly specified in terms of local configuration of binary spins. We show that in order to efficiently suppress crystallization, the non-crystalline structure should be energetically and entropically favoured. Importantly, we demonstrate that it must also geometrically antagonize crystalline order. We quantify this effect in terms of overlap of structures: crystal-"agonist" structures with good overlap with the crystal tend to facilitate crystallization, while crystal-antagonist ones tend to impede it dramatically by increasing the surface tension.

*Poster

Cooperative strings and glassy interfaces

Thomas Salez * [1], Justin Salez, Kari Dalnoki-Veress, Elie Raphaël, James A. Forrest

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We introduce a minimal theory of glass formation based on the ideas of molecular crowding and resultant string-like cooperative rearrangement, and address the effects of free interfaces. In the bulk case, we obtain a scaling expression for the number of particles taking part in cooperative strings, and we recover the Adam-Gibbs description of glassy dynamics. Then, by including thermal dilatation, the Vogel-Fulcher-Tammann relation is derived. Moreover, the random and string-like characters of the cooperative rearrangement allow us to predict a temperature-dependent expression for the cooperative length of bulk relaxation. Finally, we explore the influence of sample boundaries when the system size becomes comparable to the cooperative length. The theory is in agreement with measurements of the glass-transition temperature of thin polymer films, and allows to quantify the temperature-dependent thickness of the interfacial mobile layer.

*Poster

Stress relaxation and the distribution of the shear modulus in amorphous solids

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The relaxation of stress in an amorphous solid depends on the complex collective motions typically described as non-affine displacements. These collective motions, largely absent in crystals, are the result of the coupling of the stress with the spatial distribution of broken symmetries that characterise the amorphous structure. These non-affine displacements can produce significant stress relaxation without involving activated processes, they exhibit high sensitivity to the thermal history of the solid and they can reveal features of amorphous configurations that are hidden from direct examination of the structures. This talk will examine a number of poorly understood aspects of the shear modulus of amorphous materials below their glass transition Tg using computer simulations. Topics will include the temperature dependence of stress relaxation below Tg and the inherent mechanical variability of amorphous solids as measured by the distribution of shear moduli of an ensemble of glasses.

*Poster

Circular Coloring of Regular Random Graphs

Christian Schmidt * [1], Lenka Zdeborová

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Circular coloring is a constraints satisfaction problem where colors are assigned to nodes in a graph in such a way that every pair of connected nodes has two consecutive colors (the first color being consecutive to the last). We study circular coloring of random graphs using the cavity method. Our most interesting results concern the case of 5-circular coloring of random 3-regular graphs. While this case is found colorable, we conclude that the description via one-step replica symmetry breaking is not sufficient. We observe that simulated annealing is very efficient to find proper colorings for this case in times linear in the system-size. 5-circular coloring of random 3-regular graphs thus provides a very interesting case of a problem where the ground state energy is known (to be exactly zero) yet the space of solutions requires full-step replica symmetry breaking. Identifying such a case is interesting for both numerical and rigorous future studies of the properties of the full-replica symmetry breaking in diluted systems.

*Poster

Avoiding problematic quantum first-order phase transitions in quantum annealing

Yuya Seki * [1]

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Quantum annealing (QA) is a quantum computation model to solve combinatorial optimization problems.Although some advantages of QA has been reported, QA still has a difficulty of exponentially long running time to solve certain problems.In order to circumvent the difficulty, we extend QA such that QA avoids problematic first-order quantum phase transitions.To this end, we first introduce antiferromagnetic transverse interactions in addition to the original transverse-field term.We have confirmed that problematic first-order phase transitions in a simple ferromagnetic model and a spin-glass model can be avoided thanks to the antiferromagnetic term.We discuss quantum entanglement which is considered to be related to the efficiency of QA for these models.Next, we investigate the efficiency of QA using qudit.We have confirmed that the order of phase transitions varies depending on the degeneracy of qudit and quantum transition between the degenerate states.These results suggest that we can achieve speed-up of QA by extending it as described above.

*Poster

Study of replica-symmetric metastable minima in the long-range 1-d diluted power-law decay Heisenberg spin glass: a Hessian approach.

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There is considerable current interest in finding concrete connections between spin glasses and structural glasses [1]. It has been argued in recent work [2] that the study of soft modes in Heisenberg spin glasses provides the opportunity to contrast with similar phenomenology in weakly connected amorphous solids [3]. Other recent work (including those of current authors) has shown the profitability of studying vector spin glasses by the application of random magnetic fields - specifically, work involving one of the authors showed [4] that under the appplication of a random magnetic field, there is the so-called de Almeida-Thouless line of phase transitions also for mean-field vector spin glasses. Here we look at a long-range one dimensional Heisenberg spin glass where by tuning a power-law parameter, one has access to a range of universality classes from mean-field-type to short-range. We concentrate on the zero-temperature version of this problem, and identify metastable minima of the Hamiltonian and study its Hessian across a range of universality classes specified by an exponent [4]. Numerical evidence for a lack of replica symmetry breaking amongst the metastable states generated will be presented. We also discuss some curious features of spin-glass susceptibility and the excellent agreement between analytical and numerical calculations of the density of states.

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*Poster

Piece-wise linear elasticity

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Quasi-static strain-controlled measurements of stress vs strain curves in macroscopic amorphous solids result in a nonlinear looking curve that ends up either in mechanical collapse or in a steady-state with fluctuations around a mean stress that remains constant with increasing strain. It is therefore very tempting to fit a nonlinear expansion of the stress in powers of the strain. We argue here that at low temperatures the meaning of such an expansion needs to be reconsidered. We point out the enormous difference between quenched and annealed averages of the stress vs. strain curves, and propose that a useful description of the mechanical response is given by a stress (or strain) dependent shear modulus for which a theoretical evaluation exists. The elastic response is piece-wise linear rather than nonlinear. Materials designated as "amorphous solids" span a large class of non-crystalline materials that exhibit an elastic response to small strains or stresses. In this class one finds "tough" materials like metallic glasses as well as "soft" materials like foams, with many intermediate (in strength) materials in between. All this host of materials display initially a linear response to a quasi-static external loading (strain γ_{ij} or stress σ_{ij}) with a shear modulus that relates the stress to the strain. Omitting tensor indices for notational simplicity one writes

$$\sigma = \mu\gamma \ , \quad \gamma \ll 1 \ , \tag{4}$$

with μ being the shear modulus. Viewing stress vs. strain curves one is tempted to present them before the onset of the steady state as a nonlinear expansion, referred to as ?nonlinear elasticity?, in the form (again with tensor indices omitted)

$$\sigma = \mu(\gamma = 0)\gamma + B_2(\gamma = 0)\gamma^2 + B_3(\gamma = 0)\gamma^3 + \dots \ . \tag{5}$$

It is already known that at zero temperature T = 0 the nonlinear coefficients do not exist and diverge in the thermodynamic limit. Later we will also show that this is the case also for finite temperature. Thus the question arise, how to explain the apparent non-linear behavior of the stress. We will show that in fact one should consider the elastic response of amorphous solids between plastic events, and there one can invariably define a ?piece-wise linear? elastic response with shear modulus that is strain-dependent. This theory holds for low but finite temperatures, and gives an expression to calculate this strain-dependent shear-modulus. In order to support this theory, we performed numerical simulations of glasses using the Kob-Andersen model, in which point particles interact via a Lennard Jones potential. For each system size 100 samples were made, and then strained in finite temperature, letting the system to reach a steady-state after each strain increment (Thermal QuasiStatic ? TQS). The stress vs. strain curves were then analyzed, and it was shown that the true nature of the shear modulus can be faithfully explained with the piecewise strain dep. Modulus, without needing higher order coefficients. Furthermore, this approach can also explain the finite non-zero shear modulus appearing in the "steady-state regime" after the sample has yielded. The key ingredient in this analysis is the distinction between "quenched average", in which the shear modulus is calculated for each sample in the ensemble separately and then averaged, and "annealed average", in which all stress-strain curves were averaged, and then the slope was calculated. We show that the right way to look at the shear modulus is that of the quenched average.

*Poster

Generalization of Darcy's law for yield stress fluids in porous media: From avalanche statistics to the flow-rate regimes

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Non-Newtonian fluids have practical applications in very different domains. Indeed, polymer mixture, paints, slurries, colloidal suspensions, emulsions, foams or heavy oil present complex rheologies. Among the large number of different non-Newtonian fluids an important class of behavior is represented by the yield-stress fluids, viz. fluids that require a minimum of stress to flow. Yield stress fluids are usually modelled as a Bingham fluid or by the Herschel-Bulkley equation. Simulating flow of a Bingham fluid in porous media still remains a challenging task as the yield stress may significantly alter the numerical stability and precision. In the present work, we use a Lattice-Boltzmann TRT scheme to determine this type of flow in a synthetic porous medium. Different pressure drops
$DeltaP$ have been applied in order to derive a generalization of the Darcy's equation. Three different scaling regimes can be distinguished when plotting the flow rate q as function of the distance to the critical pressure
$DeltaP -$
$DeltaP_c$. In this presentation, we will investigate the importance of the heterogeneities on these flowing regimes. First, we will investigate the statistical properties of the flowing areas of yield stress fluid in porous media. We will demonstrate that the size probability distribution of the unyielded clusters follows a power-law decay with a large size cut-off. This cut-off is shown to diverge following a power-law as the imposed pressure drop tends to a critical value. These scaling laws allow to account for the quadratic relationship between the pressure gradient and velocity Finally, we propose a simple model to understand the critical behavior of path opening during flow of a yield stress fluid in porous media. This model can be mapped to the problem of a contact line moving in an heterogeneous field. Close to the critical point, this line presents an avalanche dynamic where the front advance by a succession of waiting time and large burst events. These burst events are then related to the non-flowing (
emphi.e. unyielded) areas. Remarkably, the statistics of these areas reproduce the same scaling laws as in the direct numerical simulations.

*Poster

Performance of quantum annealing hybridized thermal annealing

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The quantum annealing has been considered as a high-performance computation method to obtain the best solution of combinatorial optimization problems. Recently the quantum annealing has been attracted attention in not only scientific fields but also industry since hardwares realizing the quantum annealing has been developed. A main issue in the quantum annealing is to understand when to use or when not to use the quantum annealing. Depending on types of combinatorial optimization problems, the performance of the quantum annealing is worse than that of the thermal annealing. We propose a new type of quantum annealing method in which we control not only the quantum fluctuation but also thermal fluctuation. We confirm that our method is better than the thermal annealing and the "conventional" quantum annealing for some combinatorial optimization problems.

*Poster

Static and dynamic aspects of a stepped liquid film as studied by MD simulations

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Thin liquid films have attracted considerable attention over the past twenty yeas due to their numerous applications applications. As several experimental and theoretical studies have revealed, molecular mobility and dynamics in confined environments substantially deviates from the corresponding behavior in the bulk.In recent approches in liquid films exhibiting some surface topography, the relaxation of the excess surface energy was exploited in order to probe viscoelastic and glassy effects[1,2]. The present contribution is inspired by experimental and theoretical studies in stepped polymer films and addresses static and dynamic aspects of a supercooled Lennard-Jones stepped film. Through the use of molecular dynamics simulations, we elucidate the factors that govern the mobility and relaxation of the step below the bulk glass transition temperature. References [1] J.D McGraw, N.M. Jago and K. Dalnoki-Veress, Soft Matter,7, 7832 (2011) . [2] Y. Chai, T. Salez, J.D. McGraw, M. Benzaquen, K. Dalnoki-Veress, E. Raphael and J. Forrest, Science, 343, 6174,(2014).

*Poster

Liquid-liquid transition in confined cyclohexane

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A new type first-order phase transition on the confined cyclohexane into pores with a diameter of nm scale was examined by adiabatic calorimetric and X-ray powder diffraction measurements and numerical investigation. Calorimetric measurements showed the strange nature of the pore size dependence of this transition. Transition enthalpy indicated emergences of transition were restricted in between about 1.5 nm to 3.0 nm and took maximum enthalpy at the pore size of 2.5 nm. The value of maximum enthalpy were about 60 J mol^{-1} which is about 1000 times less than ordinary phase transition. On the other hand, transition temperature becomes 154 K, which is insensitive to pore size. These insensitivities of the transition temperature on the pore size and smallness of transition enthalpy could be associated with the emergence of the local structure. We thought the confined cyclohexane showed the transition into ordered liquid phase. In fact, numerical investigations on the cyclohexane indicated the increasing of the icosahedron-like structures and these findings are consistent with temperature dependences of X-ray diffraction intensities those indicate development of a structural correlation around 0.3 nm at lower temperatures. In this talk, we will demonstrate further experimental results and comparison with numerical investigations.

*Poster

Relation between structure of blocked clusters and relaxation dynamics in kinetically constrained models

Eial Teomy * [1], Yair Shokef

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In a liquid all the particles are mobile, while in a glass only some of them are mobile at any given time. Although overall the structure is amorphous in both cases, the difference is that in glasses there are local structures that inhibit the movement of particles inside them. We investigate these structures by considering the minimum number of particles that need to move before a specific particle can move. By mapping the dynamics of the particles to diffusion of mobile vacancies, we find a general algebraic relation between the mean size of the structures and the mean persistence time, which is the time until a particle moves for the first time. The exponent relating these two quantities depends on the system's properties. In [1] we investigated this relation analytically and numerically in several kinetically-constrained models: the Fredrickson-Andersen, Kob-Andersen and Spiral models. These models are either lattice gas models or Ising-like models, in which a particle can move or a spin can flip only if the local environment satisfies some model-dependent rule. Due the discrete nature of these models and relative simplicity, we were able to analytically find the relation between the structure and the dynamics and found an excellent agreement between our analytical results, our numerical simulations, and the heuristic arguments presented above. In these simple models, the minimum number of particles that need to move before a specific particle can move is easily found by using a culling algorithm, also called bootstrap or threshold percolation. [1] E. Teomy & Y. Shokef, Physical Review E 92, 032133 (2015).

*Poster

Minimal cooling speed for glass transition in a simple solvable energy landscape model

Javier Toledo * [1], Isaac Perez Castillo, Gerardo G. Naumis

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The minimal cooling speed required to form a glass is obtained for a simple solvable energy landscape model. The model, made from a two-level system modified to include the topology of the energy landscape, is able to capture either a glass transition or a crystallization depending on the cooling rate. In this setup, the minimal cooling speed to achieve glass formation is then found to be related with the crystallization relaxation time, energy barrier and with the thermal history. In particular, we obtain that the thermal history encodes small fluctuations around the equilibrium population which are exponentially amplified near the glass transition, which mathematically cor- responds to the boundary layer of the master equation. The change in the glass transi- tion temperature is also found as a function of the cooling rate. Finally, to verify our analytical results, a kinetic Monte Carlo simulation was implemented.

*Poster

Correlation between structure, dynamics and mechanical response in glassy systems

Hua Tong * [1], Hajime Tanaka

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The central problem in the study of glass-forming liquids and the disordered solids after the glass transition lies in the understanding of the structural origin of a set of peculiar behaviors in their dynamics, mechanical response, and also vibrational modes. Using molecular simulations in several widely used model glass systems, we demonstrate that the intuitive picture about the correlations between strcuture and other properties is largely incorrect. We show in detail that the underlying structure can totally decouple with the mechanical response and the low-temperature dynamics, even in highly ordered solids. The role of the long-range stress correlation in the inherent structure played in the glassy dynamics is studied and alternative explanations in contrast to recent literatures are discussed.

*Poster

Avalanches and diffusion in an elasto-plastic automata with realistic near-field interactions

Botond Tyukodi * [1], Craig Maloney, Damien Vandembroucq

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We present results on an elasto-plastic automaton model of an athermal amorphous solid under shear. We study four different variants of the model with two different loading geometries and two different stochastic prescriptions (random yield thresholds or random strain amplitudes). We perform a finite size scaling analysis for the avalanche size distribution and single-site displacement statistics. The avalanche size distribution in all four cases is inconsistent with mean-field depinning results. For three of the four variants, the distribution is consistent with previous results from atomistic simulations and other related elasto-plastic models. The fourth seems to exhibit different scaling properties and may lie in a different universality class. The mean-squared displacement and the plastic strain fluctuations exhibit a pronounced dependence on the microscopic ingredients of the model and is completely non-universal. These results show that while certain microscopic ingredients of the model may be irrelevant for the individual avalanches, they may exhibit a profound impact on long-time correlations and long-lived shear localization.

*Poster

The long memory of glass surfaces

Damien Vandembroucq * [1], Bruno Bresson, Coralie Brun, Xavier Buet, Matteo Ciccotti, Jeôme Gateau, Marco N. Petrovich, Francesco Poletti, David J. Richardson, Botond Tyukodi, Gilles Tessier

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Glass remembers its liquid past. Nothing is closer to the structure of a vitreous material than a snapshot of the liquid before glass transition. In a similar way, the surface of a glass remembers its past as a liquid interface. Over a wide range of length scales, from the nanometer up to the millimeter range, the ultra-low roughness of a fire-polished glass surface (RMS rouhness about 0.2-0.4 nm) results from the superposition of frozen capillary waves. Here we show that a glass surface can also remember the direction of the flow to which the liquid was submitted. Performing high precision Atomic Force Microscopy (AFM) roughness measurements on the inner glass interfaces of photonic band-gap fibres and hollow capillary fibres produced by fibre drawing, we show that their roughness is clearly anisotropic with an overall amplitude below the expected equilibrium thermodynamic limit. This attenuation of capillary modes is reminiscent of recent results obtained with sheared liquid interfaces.

*Poster

Gauge Theory of Glass Transition: description of liquid–glass transition as a critical phenomenon

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The Gauge Theory of Glass Transition (GTGT) was recently developed [1-2]. The old idea of the gauge field description of glass transition underlies in this theory [3-5]. In GTGT is assumed that there are two key conditions for the implementation of glass transition. First of all, we believe, that the glass transition has common nature with the second order phase transition, which is spontaneous breaking continuous symmetry and starting an ordering process in the system structure. On the other hand, in contrast to the phase transition this ordering process stops because of frustration, which arises in this process. The presence of frustration is the second key condition for glass transition. The frustration gives rise to production of vortexes (disclinations in undercooled liquids [6, 7]) in the structure, which prevents the growth of the ordered regions. The nonequilibrium dynamics of the slowing vortex system, which takes into account the interaction of these vortexes with order parameter fluctuations, can be described in terms of the gauge field theory. This allows to get the theory analogous to the dynamical theory of phase transition [1-2], and gives the self-consistent description of glass transition, describing broad spectrum of its properties. [1] M.G. Vasin, J.Stat.Mech., 2011, P05009 (2011). [2] M.G. Vasin, Theoretical and Mathematical Physics, 174(3), 406-420 (2013). [3] E.I. Dzyaloshinskii and G.E. Volovik, J.Physique 39, 693-700 (1978). [4] J.A. Hertz, Phys.Rev.B 18, 4875-4885 (1978). [5] N. Rivier, Revista Brasileira de Flsica, 15 (4), 311-378 (1985). [6] N. Rivier, D.M. Duffy, J.Physique 43, 293-306 (1982). [7] R. Nelson, Phys.
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,B 28, 5515-5535 (1983).

*Poster

Characteristics of force networks in shear jamming

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Structure plays a significant role in the rigidity of granular packings. In the absence of friction, a collection of spheres jam at the random close packings density (RCP) $\phi_j \approx 0.64(3D)$. When subjected to athermal quasistatic shearing, an assembly of soft spheres interacting via a repulsive harmonic potential at densities below ϕ_j develops geometric features similar to jammed packings at ϕ_j, both in three and two dimensions. We demonstrate using discrete element method (DEM) simulations that the structure of sheared steady state (SS) packings can support jamming in the presence of friction, for a range of densities below ϕ_j [1]. Further two densities were identified as relevant for the shear jamming (SJ) phenomenon. The first density identified from the average contact number Z ($Z \approx 4$) and the distributions of contact forces, coincides with the previously identified random loose packing density (RLP) $\phi_{RLP} \approx 0.55$. The second density is $\phi_c = 0.58$, which was also reported previously as the density where shear jamming occurs [2, 3].
Independent of DEM simulations we obtain force balance solutions for a given steady state geometry by defining a suitable energy function. The force solutions are obtained using the constrained minimization method [4]. We obtain force balance solutions for the SS packings above $\phi = 0.55$, which is the lower density limit for shear jamming. We characterize the force solutions above and below $\phi_c = 0.58$, to understand the relevance of this density to the shear jamming phenomenon.

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*Poster

Shear induced solidification of athermal systems with weak attraction

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We find that unjammed packings of frictionless particles with rather weak attraction can always be driven into solid-like states by shear. The structure of shear-driven solids evolves continuously with packing fraction from gel-like to jamming-like, but is almost independent of the shear stress. In contrast, both the density of vibrational states (DOVS) and force network evolve progressively with the shear stress. There exists a packing fraction independent shear stress σ_c, at which the shear-driven solids are isostatic and have a flattened DOVS. Solid-like states induced by a shear stress greater than σ_c possess properties of marginally jammed solids and are thus strictly-defined shear jammed states. Below σ_c, states at all packing fractions are under isostaticity and share common features in the DOVS and force network, although their structures can be rather different. Our study reveals the significance of the shear stress in determining properties of shear-driven solids and leads to an enriched jamming phase diagram for weakly attractive particles. Zheng W, Liu H, Xu N. Shear induced solidification of athermal systems with weak attraction[J]. arXiv preprint arXiv:1603.02390, 2016.

*Poster

Topic 5: Biological Physics-Posters

Intransitivity, coexistence and synchronization in four species cyclic games

Jeferson Arenzon * [1], Alessandra Lütz, Charlotte Rulquin, Sebastián Risau-Gusman

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The Rock-Paper-Scissors (RPS) game and its generalizations with $calS > 3$ species are well studied models for cyclically interacting populations. Four is, however, the minimum number of species that, by allowing other interactions beyond the single, cyclic loop, breaks both the full intransitivity of the food graph and the one predator, one prey symmetry. Ref. [1] have shown the existence, on a square lattice, of two distinct phases, with either four or three coexisting species. In both phases, each agent is eventually replaced by one of its predators but these strategy oscillations remain localized as long as the interactions are short ranged. Distant regions may be either out of phase or cycling through different food web subloops (if any). Upon replacing a minimum fraction Q of the short range interactions by long range ones, there is a Hopf bifurcation and global oscillations become stable [2]. Surprisingly, to build such long distance, global synchronization, the four species coexistence phase requires less long range interactions than the three species phase, while one would naively expect the contrary. Moreover, deviations from highly homogeneous conditions ($chi = 0$ or 1) increase Qc and the more heterogeneous is the food web, the harder the synchronization is. By further increasing Q, while the three species phase remains stable, the four species one has a transition to an absorbing, single species state. The existence of a phase with global oscillations for $calS > 3$, when the interaction graph has multiple subloops and several possible local cycles, lead to the conjecture that global oscillations are a general characteristic, even for large, realistic food webs. oindent [1] Lütz it et al, J. Theor. Biol. ref 317 (2013) 286 oindent [2] Rulquin and Arenzon, Phys. Rev. E. ref 89 (2014) 032133

*Poster

Mutations and heterogeneity in tumor progression

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Genetic mutations cause changes in the membrane proteins which result in cell phenotype variations. There are mutations which affect the tissue cohesion, or reduce the constraints among cells increasing the possibility of cell migration and the type of cell-to-cell interactions adopted by cancer cells during the invasion of the tissue. Other mutations facilitate the intravasation into, and extravasation from, the blood vessels which favor the formation of circulating tumor cells capable of reaching secondary sites far from the primary site. Mutations can increase the cancer stemness which make cancer cells capable of forming metastatic colonies or not easily recognizable by the immune system. Many mutations, instead, produce cell instabilities and decrease the survival probability of cancer cells. In the framework of cellular automaton, we show the role of heterogeneity on cancer stemness and how the order of mutations affect the migration process of the cancer cells dividing the cell population of the tumor in subpopulations which differ in capability of developing metastases and times of invasion of the tissues.

*Poster

Complex arrhythmias and intermittency: Spontaneous desynchronisation processes of reticulated networks of excitable cells.

Guillaume Attuel * [1], Hussein Yahia

[1] INRIA – France

Following a singularity analysis of intracardiac " f waves " recordings in humans, surprisingly showing features of fully developed turbulence, we reassess complex arrhythmias and fibrillatory processes theoretically. The myocardium is generally supposed to be a syncytium of cells, meaning a continuous medium with rather smooth properties. In this framework, cardiac electrical contractions are the result of reaction-diffusion propagating fronts in excitable state. In fact, broad singularity spectra with negative exponents and heavy tails of amplitude probability distributions point to large deviations and intermittency, strictly incompatible with excitability. Following an original idea by Y. Pomeau on the onset of turbulence as an intermittent contamination process, we looked for a mechanism leading to a modulation of front trains. Thus, we speculate on a possible synaptic plasticity. This introduces a phase degree of freedom in cell cycles. The nucleation of desynchronised islands of cells follows. This is unknown biologically as far as we know. The plasticity follows an instability of the flow of chemical messengers. An adimensional number exists, that enables to explore parameter space. In other words, desynchronisation of the network of cells contaminates the whole myocardium. Transitions between states are observed, that is reminiscent of the context of coupled maps for instance. This helps to describe some clinically intriguing facts such as spontaneous or induced transitions between complex arrhythmias. Furthermore, from this new perspective, another long standing physiological question named remodelling, which describes how the substrate deteriorates as long as the arrhythmia lasts, is discussed as a slow reconfiguration of the network, either as ageing or a kind of deleterious synaptic learning. We end by discussing a generalisation of this argument involving gauge symmetries in such driven systems and the emergence of strong disorder.

*Poster

Disorder and compressive sensing in the olfactory system

Vijay Balasubramanian * [1], Kamesh Krishnamurthy, Ann Hermundstad, Thierry Mora, Aleksandra Walczak

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The olfactory system of animals is charged with identifying and discriminating familiar and novel odors which are complex mixtures drawn from a very high dimensional space of volatile molecules (perhaps 10^6 or more). Thus, the olfactory system must invest a limited number of receptor types (O(100) in fly, O(300) in human, O(1000) in mouse) wisely to sense a much higher dimensional and highly variable signal. A key simplifying property of natural odors is their sparsity – a typical odor contains of only 50-100 molecular components. We demonstrate that the nervous system exploits this sparsity by using disordered responses of olfactory receptors followed by randomness in circuit projections to the central brain. The resulting information representation packs high dimensional olfactory data into a small number of neural responses. The theory makes striking new predictions, e.g. that arbitrary and small subsets of cortical neurons can provide complete representations of odor space to support complex animal behaviors. This prediction can be tested by optogenetic manipulation of the olfactory cortex. In light of these results, we argue that the olfactory ciruit pathway should be regarded as a novel scheme for compressive sensing of odors that developed through natural selection.

*Poster

Colonization dynamics of Salmonella Typhimurium in mice

Florence Bansept * [1], Emma Slack, Roland Regoes, Raphael Voituriez, Claude Loverdo

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Our work aims at developping a stochastic model for the colonization of an organism by bacteria, applied to experimental data on mice colonization by Salmonella Typhimurium. One of the purposes of the model is to extract some biologically relevant parameters (probability for the bacteria to settle in the organism, growth and death rates) from quite indirect experimental data. A first simple model of populations dynamics was tested and proved to be insufficient to explain all the collected data. We therefore developed a more complex model with two subpopulations growing at different rates. Although it allows to get qualitatively closer to the experimental observables, it is still quantitatively insufficient. Other hypotheses are being tested to explain the data, and in the future, other questions will be investigated through this system, such as the effect of vaccination.

*Poster

Heterogeneous motility facilitates the persistence of cooperation

Marianne Bauer * [1], Jörg Martin, Steffen Rulands, Erwin Frey

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The presence of cooperation in nature is a fundamental, still unsolved problem in modern biology. We study the evolution of cooperation in populations exhibiting heterogeneous motility. We show that under these circumstances cooperation can persist under surprisingly harsh conditions. We identify three distinct parameter regimes which are characterized by the possibility for the persistence of cooperation and the average motility dominating at large times.

*Poster

The effects of ultraviolet radiation on the activation of pathogenic bacteria

Maamar Boukabcha * [1], AEF. Djemai, AEK. Ali Benamara

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Highly pathogenic bacteria contaminated the different fruits. Contaminates present in tomatoes. Are responsible for its contamination. The distinction of these types is a very difficult challenge in the tomato industry. It has therefore become necessary to develop methods to inactivate these pathogens in order to ensure the quality of the tomato. It is in this framework that integrates our work whose general objective is to study the inactivation of Escherichia coli bacteria species by ultraviolet radiation type C By studying the effect of different doses of radiation on inactivation of Escherichia coli bacteria. We noticed that the radiation dose high (very near the source of radiation bacteria), has an efficient effect of the inactivation. Furthermore, its effectiveness depends on the physical factors. Indeed, it increases proportionally with increasing duration of exposure such radiation. The presence of radiation in the environment improves the efficiency of the energy treatment in inactivating pathogenic bacteria E.coli. This study demonstrates the potential use of the combination with radiation or energy with distance from its source to inactivate highly pathogenic E.coli bacteria. The apparatus used for this purpose is provided with a UV lamp. In fact, the physical characterization of the UV lamp used in the tests demonstrated that the lamp outputs of 254 nm. Moreover, this device can process samples and remotely controlled time. Finally, the listing operation colonies after UV exposure type C are performed. UV rays are responsible for the bactericidal action. The different results obtained in our experiment confirm the sensitivity or the effect of different strains tested to UV radiation. We plan to continue this study to other types of bacteria to test the validity of the proposed model in this work. Keywords: Inactivation, UV radiation type C, pathogenic bacteria, Escherichia coli, Model.

*Poster

How do hidden units shape effective connections between neurons?

Braden Brinkman * [1], Tyler Kekona, Fred Rieke, Eric Shea-Brown, Michael Buice

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A major challenge in neuroscience is understanding how "hidden units" – neurons or other influences not observed in an experiment – influence the behavior of the observed neurons. Much work has been done on the inferring network interactions from data, but it remains unknown how hidden neurons shape the inferred network interactions. Using non-perturbative renormalization group techniques from non-equilibrium statistical physics, we have developed a theoretical framework to predict how effective connections in subsampled networks depend on the true connections in the full network. Beyond calculating effective connections, this approach can be systematically expanded to study how hidden units generate effective noise in subsampled networks. Our formalism applies to any number of neurons. As an example, we apply this framework to a network of 3 spiking neurons described by a generalized linear model (GLM) with rates driven by a neuron's own filtered spiking activity and the filtered spiking activity of neurons from which it receives input. By approximating the subsampled network as a GLM with effective spike-filters corrupted by Gaussian noise, we can analytically calculate how hidden units transform the filters and give rise to correlations in the effective noise. Based on our 3-neuron results, we conjecture that for general networks within this framework the filter between neurons i and j is modified by corrections from every path that neuron i can send a signal to neuron j through hidden units.

*Poster

Patterns following ecological extinctions

Guy Bunin * [1]

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The structure of ecological networks and its relation to the corresponding dynamics is a central question in ecology. We study networks of species that have not gone extinct under the dynamics, in popular ecological models such as the multi-species Lotka-Volterra equation. The results reveal surprising connections to patterns suggested in the context of neural networks.

*Poster

Stochastic lumping analysis on the fluctuations relations between hierarchical kinetic networks and its application to chemotaxis

Cheng-Hung Chang * [1], De-Ming Deng, Yi-Ta Lu

[1] Institute of Physics, National Chiao-Tung University – Taiwan

Kinetic networks are widely used to study complex biological systems. Since the selection of these networks for a real system is usually not unique, a concern is raised whether and under which conditions non-unique hierarchical schemes can consistently account for unique fluctuation data measured in experiments. To clarify these questions, we introduce stochasticity into the traditional lumping analysis, generalize it from rate equations to chemical master equations and stochastic differential equations, and extract the fluctuation relations between kinetically and thermodynamically equivalent networks. Under intrinsic noises, we prove the duality of indistinguishability in the mean and fluctuations between those networks, which justifies the legitimate use of low-dimensional models in the studies of macromolecular fluctuations. Under extrinsic noises, we derive various basic kinds of fluctuation relations for kinetically equivalent networks, which provides basic knowledge for model selection. As an example, the theory is demonstrated on a Langevin equation for the conformational fluctuations of proteins, which becomes a generalization of Bialek's formalism for studying the physical limits of biological sensing. In additional to its broad applicability, e.g., in structural and systems biology, the result may shed light on the hierarchical fluctuations of general extensive variables in Keizer's canonical theory. [J. Chem. Phys. 142, 184103 (2015) and preprint (2016)]

*Poster

Sensing correct ligands in a noisy environment

Shang-Yuan Chang * [1]

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To probe the environment, a cell needs to discriminate different kinds of ligand, and often different ligands have similar structure and affinity to the same receptor. It is crucial that in such very noisy environment a cell can recognize the correct ligand with high prevision. We show that spatial arrangement of the receptors and related molecules, such as receptor clusters that expel inhibitors can have great influence on this precision detection problem. More specifically, spatial physical interaction serves as a distinct mechanism to amplify the weak signal from few correct ligands, resulting cell sensing with high sensitivity.

*Poster

Planar and flipping motion of gliding bacteria

Hsuan-Yi Chen * [1], Mei-Hsien Tu, Hirofumi Wada

[1] National Central University – Taiwan

I will present a model for the gliding motion of bacteria Flavobacterium johnsoniae on a flat surface. With no flagella and cilia, a Flavobacterium johnsoniae moves on a solid surface by the transportation of protein adhesins SprB along a closed helical loop on its surface. As a result, on average at every instance about half of the adhesins in contact with the solid surface move toward one direction, and the other half of them move toward the opposite direction. Our main findings include: (i) The onset of gliding movement is accompanied by a symmetry-breaking in the distribution of closed adhesins on the helical track. (ii) Gliding bacterium switches moving direction from time to time, this is because when a group of closed adhesins reaches one of the cell poles, the bacterium has a finite probability to reverse its gliding direction. (iii) Experimentally observed flipping motion is likely a result of inhomogeneous distribution of adhesins along the track.

*Poster

Temporal Fluctuations of Protein SERS Spectra

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Keywords: Surface Enhanced Raman Spectroscopy, optical biosensor, microfluidics, protein detection, single molecule experiments, temporal fluctuations. Proteins can be viewed as molecular machines that control our vital cellular functions. Understanding its dynamics is a fundamental problem which can have a huge impact in disease diagnosis. Indeed, many misfolded proteins have been linked to the development of certain diseases such as Alzheimer. Since several years, single molecule spectroscopy has developed into a well-suited technology for detecting biomarkers at very low concentrations and for exploring protein dynamics. It is in this spirit that we propose an advanced optical nanobiosensor[1,2,3] based on Surface Enhanced Raman Spectroscopy combining plasmonic and microfluidic chips to study protein folding at the single protein level. Due to the high selectivity and sensitivity of our biosensor, we are able to probe the complex behavior of these macromolecules. Statistical analysis of spectra fluctuating both in intensity and wavenumber is a crucial task to extract new information unreachable using more classical ensemble methods[4]. The label free detection of proteins and aptamer-protein interactions illustrate how the decoding of the spectra fluctuations can be used to monitor with time the changes in the degree of freedom and conformation adopted by proteins. References [1] Margueritat, J.; Gehan, H.; Grand, J.; Levi, G.; Aubard, J.; Felidj, N.; Bouhelier, A.; Colas-Des-Francs, G.; Markey, L.; De Lucas, C. M.; Dereux, A.; ACS Nano 2011, 5, 1630– 1638. [2] Margueritat, J., Bouhelier, A.; Markey,L; Colas des Francs, G.; Dereux, A.; Lau-Truong, S., Grand, J.; Lévi G, Félidj, N.; Aubard, J.; Finot, E.; The Journal of Physical Chemistry C 2012, 116 (51), 26919-2692 [3] Brulé, T., Yockell-Lelièvre, H.; Bouhélier, A.; Margueritat, J.; Markey, L.; Leray, A.; Dereux, A.; Finot, The Journal of Physical Chemistry C 2014, 118 (31), 17975-17982. [4] Brulé, T., Bouhelier, A., Yockell-Lelievre, H., Clément, J. E., Leray, A., Dereux, A., & Finot, E. (2015) ACS Photonics.

*Poster

Dynamical response and synchronization of beating cells

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Many experiments have shown that cells sense and respond to the mechanical properties of their environment. Such results suggest that cells are not only able to sense mechanical forces applied to them by the matrix in which they are embedded, but are also able to respond by modifying the forces they themselves apply to the matrix. More specifically, recent experiments have shown that isolated cardiac cells mechanically coupled by an underlying substrate, can modify their beating frequency and phase in response to a nearby mechanical probe. It was shown that not only do quiescent cells become contractile due to a periodic, mechanical perturbation of their underlying substrate, but also that these cells synchronize their phase and frequency with that of the oscillating mechanical probe (or another, nearby cell). This response implies that mechanical interaction (and not only electrical pacing) plays a role in the coherent beating of the cardiomyocyte assemblies.

Motivated by these observations, we theoretically analyze how dynamical-mechanical perturbations affect cardiomyocyte beating. We model the cell as a contractile force dipole and generalize the treatment of a static force dipole to a dynamically beating one. The model predicts the time dependent displacements/strains, as a function of the beating frequency ω_0, the friction γ and the substrate effective stiffness $\tilde{E}$. We find that in contrast to static dipoles where the displacements or strains fall off as a power law from the source, that in the dynamic case the displacement or strain decay in space exponentially with a characteristic dynamic inverse length scale $\kappa = \sqrt{\frac{\omega_0 \gamma}{\tilde{E}}}$.

We also predict how the beating phase of two nearby dipoles depends on their relative orientations and their spatial separation. To further predict the synchronization of a beating cell with a mechanical probe that oscillates with an arbitrary frequency, we use a model of a forced non-linear oscillator. When the frequency of the probe is not too different than the internal frequency of the cell, phase-locking is achieved and the cell beats with the same frequency as the probe. These results are supported by the experimental observations, and the fundamental science treated in our theory may have implications for development of tissue, pathological conditions such as arrhythmia and cardiac failure, as well as serving as guidelines in the design of biomedical and bio-mimicking devices.

*Poster

Ising-model description of long-range correlations in DNA sequences

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We model long range correlations of nucleotides in the human DNA sequence using the long range one dimensional Ising model. We show that for distances between 10^3 and 10^6 bp the correlations show a universal behaviour and may be described by the non-mean field limit of the long range 1d Ising model. This allows us to make some testable hypothesis on the nature of the interaction between distant portions of the DNA chain which led to the DNA structure that we observe today in higher eukaryotes. Published on Physical Review E: http://journals.aps.org/pre/abstract/10.1103/PhysRevE.91.052703

*Poster

Signal propagation and dynamical correlation in biological active matter

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Collective phenomena in animal groups have attracted much attention in the last years, becoming one of the most attractive topics in biology. However, while in most of the studies on animal collective behavior it has been tried to understand how a globally ordered state may emerge from simple behavioral rules, less effort has been devoted to the understanding of the way in which information propagates within an animal group. The study of this phenomenon derives its importance from the fact that in order to avoid a loss of cohesion by the group it is crucial that, during the global change of state caused by collective response to an external perturbation, the transfer of information is rapid and robust. The mechanism by which such robustness is achieved, however, is not clear yet. In this work we will focus in understanding the mechanisms underlying the propagation of information about a speed change in a flock of birds. Most of collective motion models consider the modulus of the velocity v0 fixed. However it is well known the existence of density waves that propagates linearly on the flock. The idea of the present work is to consider density waves as a byproduct of speed waves. In particular we present a new inertial model for the speed fluctuations and some tools to determine whether a biological active matter system exhibit propagation of information phenomena or not.

*Poster

Temporal variability in C. elegans

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Physical descriptions of living movement often focus on brownian-like trajectories of the centroid body position. In complex organisms however, these trajectories are encoded in an intricate coordination of postures, which provide a more natural, yet complex, characterization of animal movement. The mathematical framework to extend the physical point-like description into the postural dynamics is still inexistent. Here we address this question in C. elegans, a model organism in fields from neuroscience and genetics to ethology. Recent work has shown that worm postures can be reconstructed using a four dimensional ?eigenworm? representation. Here we use this representation to quantitatively explore the space of behavioral trajectories by means of a local linear model. We develop a novel algorithm in which temporal locality is provided by the system itself by adaptively selecting the window of the local approximation, using statistics. We apply our method to a behavioral setting in which an abrupt heat shock is administered to the worm's head and we find a fine-scale description of the worm behavior which is remarkably more structured than previous, coarse-grained characterizations. This description can be used to sample the variability across behavioral epochs, as well as the transitions between them.

*Poster

Protein accumulation in the endoplasmic reticulum as a non-equilibrium phase transition

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Several neurological disorders are associated with the aggregation of aberrant proteins, often localized in intracellular organelles such as the endoplasmic reticulum. Here we study protein aggregation kinetics by mean-field reactions and three dimensional Monte carlo simulations of diffusion-limited aggregation of linear polymers in a confined space, representing the endoplasmic reticulum. By tuning the rates of protein production and degradation, we show that the system undergoes a non-equilibrium phase transition from a physiological phase with little or no polymer accumulation to a pathological phase characterized by persistent polymerization. A combination of external factors accumulating during the lifetime of a patient can thus slightly modify the phase transition control parameters, tipping the balance from a long symptomless lag phase to an accelerated pathological development. The model can be successfully used to interpret experimental data on amyloid-β clearance from the central nervous system.

*Poster

Stochastic and thermodynamic approaches to understand 12/23 rule involved in RAG-mediated V(D)J DNA cleavage-single molecule analysis

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V(D)J recombination is central to establishing a functional adaptive immune system. The large repertoire of immunoglobulins and T cell receptors is generated in many vertebrates by combinatorial rearrangement of variable (V),diversity (D), and joining (J) gene segments. The recombination signal sequences (RSS) that flank these gene segments are recognized, paired in a synaptic complex, and cleaved by collaboration of the lymphoid-specific proteins RAG1 and RAG2. Rearrangements occur between two gene segments with flanking recombination signal sequences (RSSs) that differ in the length of the spacer (either 12 or 23 bp) between a conserved heptamer and a nonamer elements. The generation of double strand breaks and the overall recombination reaction occur much more efficiently with a 12-23 RSS pair than with 12-12 or 23-23 RSS pairs, a preference known as the 12-23 rule. In this work we would like to explore the 12-23 rule by using thermodynamic and stochastic approaches. We are basically asking if are any thermodynamic constraints that are imposing 12-23 rule or thermodynamically the 12-12 and 23-23 pair complex (PC) are also allowed. We begin by developing a simple kinetic framework for understanding what the measured state lifetimes tell us about the underlying physics of the system. We then use transit state theory to probe the looping reaction pathway and quantify the effects of DNA and protein elasticity in looping kinetics. The work was motivated by Tethered Particle Motion (TPM) experiments performed by group of M. Ciubotaru (results not published) and by D.Schatz and Phillips groups (PNAS 2015 112 (14) E1715-E1723 and PNAS 2014 111 (49) 17396-17401)

*Poster

Generalized run-and-tumble

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Bacteria exhibit a variety of swimming patterns (run-and-tumble, run-stop, run-reverse, run-reverse-flick), in which persistent runs are interrupted by sudden turning events. What are the properties of such random motions? If a complete answer has been given when the turning events follow a Poisson process, it has remained elusive outside this particular case. We present a generic framework for such non-Poissonian run-and-turn random motions. Building on the framework of continuous time random walks (CTRW), we obtain the generating function of moments in terms of non-commutative operators. The approach is applied to a bimodal model of persistent motion that includes as particular cases all swimming patterns observed so far and that is also directly relevant to cell motility. More generally, the method may prove useful in the many domains where CTRWs have found applications.

*Poster

Self healing of holes in the nuclear envelope

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During migration of cells in vivo, both in pathological processes such as cancer metastasis [1] or physiological events such as immune cells migration through tissue [2], the cells must move through narrow interstitial spaces which can be smaller than the nucleus. This can induce extensive deformation of the nucleus which, according to recent experiments, results in hole formation in the nuclear envelope that can lead to cell death [3] if not prevented or healed within an appropriate time. The nuclear envelope, which can be modeled as a viscoelastic gel whose elasticity and viscosity primarily depend on the lamin composition [4] may utilize self-healing mechanisms that allow the hole to be sealed after the stresses that created it are removed. Here, we present a viscoelastic model of the nuclear envelope and quantify the conditions under which the self-healing of existing holes can be related to the viscoelastic properties and to the ratio of lamin A/C and B in the nuclear envelope. [1] Denais, C. M. et al. Nuclear envelope rupture and repair during cancer cell migration. Science, in press, 2016. [2] Raab, M. et al. Escrt iii repairs nuclear envelope ruptures during cell migration to limit DNA damage and cell death. Science, in press, 2016. [3] Harada, T. et al. Nuclear lamin stiffness is a barrier to 3d migration, but softness can limit survival. The Journal of Cell Biology 204, 669–682 (2014). [4] Swift, J. et al. Nuclear lamin-a scales with tissue stiffness and enhances matrix-directed differentiation. Science 341, 1240104 (2013).

*Poster

Low-Reynolds-number predator

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To generalize simple bead-linker model of swimmers to higher dimensions and to demonstrate the chemotaxis ability of such swimmers, here we introduce a low-Reynolds predator, using a two-dimensional triangular bead-spring model. Two-state linkers as mechanochemical enzymes expand as a result of interaction with particular activator substances in the environment, causing the whole body to translate and rotate. The concentration of the chemical stimulator controls expansion versus the contraction rate of each arm and so affects the ability of the body for diffusive movements; also the variation of activator substance's concentration in the environment breaks the symmetry of linkers' preferred state, resulting in the drift of the random walker along the gradient of the density of activators. External food or danger sources may attract or repel the body by producing or consuming the chemical activators of the organism's enzymes, inducing chemotaxis behavior. Generalization of the model to three dimensions is straightforward.

*Poster

How bio-filaments twist membranes

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Interactions between bio-filaments and bio-membranes control many processes such as cell division promoted by actin, or endocytosis promoted by dynamin. Due to their imminent importance for the proper functioning of the biological cell, a lot of research has been already devoted to understand the coupling between the two objects. However, previous works usually did not take into account that bio-filaments can display a more complex behavior than standard semi-flexible chains. In our study, we consider the deformations of a fluid membrane due to the stresses imposed by adhering stiff non-axi-symmetric filaments. This can, for instance, be the case when the filament preferentially interacts with one of its sides, while preferentially curving in an incompatible direction. The frustrated filament then exerts a so-called Darboux-torque on the membrane. Another example of frustration is a twisted filament, which preferentially adsorbs in an untwisted state. We focus on several important cases including closed and super-helical bio-filaments. In particular, we analyze interface-mediated filament/filament interactions and membrane fission when the filaments apply a local torque distribution. Our study reveals that Darboux torques can also shed a new light on the formation of tubes in biological membranes during endocytosis.

*Poster

Computational analysis of tumor oxygenation in vascularized tumors with applications to breast cancer

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Oxygenation of tissue depends strongly on the spatial arrangement of blood vessels. As they supply every part of a living organism, the establishment of a mature organized vascular network is essential for tissue homeostasis. During tumor growth the hierarchically organized arteriovenous blood vessel network of the host tissue is transformed into a chaotic heterogeneously distributed tumor vasculature. In silico modelling can foster our understanding of cancer by augmenting clinical and experimental data with additional information such as blood flow patterns, interstitial fluid flow, nutrient and oxygen distribution, allowing for, for example testing of therapeutic protocols before clinical trial. As first steps in this direction we consider algorithmically constructed blood vessel networks and analyze the resulting intravascular oxygen concentration distribution. The fact that oxygen has a very small diffusion range, caused by tissue consumption, results in a strong dependence of the oxygen distribution on the location of the vessels. Combined with a low vascular density in tumors, this leads to severe hypoxia which plays an important role in cancer invasion and impedes treatment. Our method computes intra-vascular transport, and extravascular diffusion of oxygen self consistently, where vessels are sources and drains of oxygen. Tumor cells are represented by a continuum approach. We were able to handle system sizes of 8 mm diameter where typical features of tumor vascular morphology manifest themselves. We correlate physiological and topological variations with local oxygen availability and quantitatively reproduce IR mammography data showing the oxygen content of breast carcinomas in vivo.

*Poster

Kinetic theory and thermodynamics of living copolymerization

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The kinetic theory of living copolymerization is developed by considering the detachment besides attachment of monomeric units. The kinetic equations can be exactly solved in the regime of steady growth, providing an algorithm that can be a million times faster than Monte Carlo simulations [1]. The inclusion of detachment rates allows us to determine the thermodynamics of copolymerization [2]. The sequence of the growing copolymer is a Markov chain of kth order if the rates depend on k previously incorporated monomeric units. It is shown that this sequence disorder contributes positively to the entropy production and can thus drive the growth against an unfavorable free energy landscape under certain conditions. For copolymerization with a template as in DNA replication, the entropy production also depends on the information transmitted from the template to the copy. Exact results on the effects of sequence heterogeneity can also be obtained with the developed method. References : [1] P. Gaspard and D. Andrieux, Kinetics and thermodynamics of first-order Markov chain copolymerization, J. Chem. Phys. 141, 044908 (2014). [2] D. Andrieux and P. Gaspard, Nonequilibrium generation of information in copolymerization processes, Proc. Natl. Acad. Sci. USA 105, 9516 (2008).

*Poster

Structural Propensities and Entropy Effects in Peptide Helix-Coil Transitions

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The helix-coil transition in peptides is a critical structural transition leading to functioning proteins. Peptide chains have a large number of possible configurations that must be accounted for in statistical mechanical investigations. Using hydrogen bond and local helix propensity interaction terms, we develop a method for obtaining and incorporating the degeneracy factor that allows the exact calculation of the partition function for a peptide as a function of chain length. The partition function is used in calculations for engineered peptide chains of various lengths that allow comparison with a variety of different types of experimentally measured quantities, such as fraction of helicity as a function of both temperature and chain length, heat capacity, and denaturation studies. When experimental sensitivity in helicity measurements is properly accounted for in the calculations, the calculated curves fit well with the experimental curves. We determine values of interaction energies for comparison with known biochemical interactions, as well as quantify the difference in the number of configurations available to an amino acid in a random coil configuration compared to a helical configuration.

*Poster

Highly selective kinetic model of the KcsA potassium ion channel

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Biological ion channels conduct ions through the cell membranes of all biological cells. Paradoxically their charged selectivity filters allow fast conduction (nearly at the rate of free diffusion) and high selectivity. We introduce a kinetic model in the optimal transport regime of the KcsA potassium channel to investigate selectivity and conduction between K^+ and Na^+. Our system is a narrow tube connected at either entrance to bulk reservoirs of mixed ion solution. Total energy is a sum of the electrostatic energy in the filter, plus the electrochemical potential of each ion. Thus in our filter we have quantised energy levels due to ion discreteness of ions and an energy exclusion principle [1,2,3], analogous to discrete electron transport in quantum dots [4]. Selectivity arises due to different excess chemical potentials [5,6]. Solving the kinetic scheme at steady state gives binding probabilities in the filter as a function of the transition rates, which we use to calculate current. Numerically the probabilities give a Coulomb staircase for occupancy and current gives a conduction peak for each individual species. Each peak is shifted in position, differing vastly in order of magnitude and breadth of broadness, indicating strong selectivity. These results also display ionic Coulomb Blockade analogous to its electronic counterpart [2,4]; in agreement with Brownian dynamics simulations of Ca^{++} channels [1] and single-species kinetic theory [3]. To further understand these results we linearise the current [4], and derive expressions for the conductance: $G_i = I_icdote/deltamu_i$ in the limit that we move to equilibrium for each species. Maximising conductance gives energetic conditions of resonant transition, different between species. In summary we have introduced a kinetic model of the KcsA channel in the optimal transport regime, displaying strong selectivity between species. Resonant transition conditions in the near-to-equilibrium regime, display differences between species due to the energetic favouring of K^+. [1] Kaufman, I.K., McClintock, P.V.E., and Eisenberg, R.S., 2015, New J. Phys, 8. ewline [2] Krems, M., and Di Ventra, M., 2013, J. Phys. Condens. Matt. 25. ewline [3] von Kitzing, E., 1992, In Membrane Proteins: Structures, Interactions and Models, Springer, 297-314. ewline [4] Beenakker, C.W.J., 1991, Phys. Rev. B 44, 1646. ewline [5] Noskov, S.Y., and Roux, B., 2007, J Gen Physiol., 129. ewline [6] Eisenman, G., and Horn, R., 1983, J. Membrane Biol.76, 197–225.

*Poster

Viscoelastic properties of Red Blood Cells

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Targeted therapies are one of the most promising advances in the fight against cancer. They require the differentation and characterization of the malignan and healthy cells with hight accuracy. Fluctuation membrane spectroscopy is an extremely reliable technique that allows us to characterize the mechanics of the cells such as the drag coefficient and the membrane stiffness. In order to have a full and precise knowledge of our results we have started studying the mechanics of red blood cells (RBC) whics are one of the simplest cell types. We are able to measure the global and local membrane deformability using two different experimental procedures: (1) Applying a flow to a trapped micron-sized bead attached to the RBC membrane (2) Measuring the force signal fluctuations of the RBC membrane using micron-sized beads coated with fibronectin that bind to the cellular membrane. Once completed this study we will be able to use the gained knowledge to differentiate heterogeneous cellular populations.

*Poster

Complex instability of tubular lipid membrane with nonzero spontaneous curvature under axial tension

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Tubular lipid membranes (TLMs) are soft cylindrical assemblies formed from lipid bilayer that play important role in a whole series of intracellular and cell exchange processes. In the present work we develop a micromechanical theory of the TLM with nonzero spontaneous curvature and analyze its stability with respect to thermal fluctuations and axial tension. We show that such a lipid nanotube can be stable in the absence of external forces. But even small compressive longitudinal force results in the almost simultaneous divergence of thermal fluctuations of two different soft modes. These modes are the TLM buckling and the TLM corrugation with the period close to the TLM circumference. In order to investigate weakly post-critical behavior of the system in the vicinity of this critical point we use the Landau theory of phase transitions formalism. We show that the constraint-induced instability is a sequence of two consecutive second-order phase transitions, resulting in the TLM strain field combining annular corrugation and unconventional chiral helical buckling. Despite the fact that the low-symmetry states of the considered system resemble early stages of the well-known dynamic pearling or varicose instabilities in other tubular membranes, the considered instability is static and physical reasons leading to the corresponding shape distortions predicted by the model developed in our work are quite different. The model accounts for the peculiarities of the TLM pulling experiments and could be used to explain the irregular shape of biological lipid tubes and their interaction with bound and curvature-inducing proteins.

*Poster

Spatially Inhomogeneous Search Strategies for Intracellular Transport: A Random Velocity Model

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Intracellular transport is vital for the proper functioning and survival of a cell. Cargo (proteins, vesicles, organelles, etc.) is transferred from its place of creation to its target locations via molecular motor assisted transport along cytoskeletal filaments. The transport efficiency is strongly affected by the spatial organization of the cytoskeleton, which constitutes an inhomogeneous, complex network. In cells with a centrosome microtubules grow radially from the central microtubule organizing center towards the cell periphery whereas actin filaments form a dense meshwork, the actin cortex, underneath the cell membrane with a broad range of orientations. The emerging ballistic motion along filaments is frequently interrupted due to constricting intersection nodes or cycles of detachment and reattachment processes in the crowded cytoplasm. In order to investigate the efficiency of search strategies established by the cell's specific spatial organization of the cytoskeleton we formulate a random velocity model with intermittent arrest states. With extensive computer simulations we analyze the dependence of the mean first passage times for different search problems on the structural characteristics of the cytoskeleton, the motor properties and the fraction of time spent in each state. We find that cells can optimize the search by convenient alterations of the spatial organization of the cytoskeleton. An inhomogeneous architecture with a thin actin cortex constitutes an efficient stochastic search strategy for diverse tasks of intracellular transport.

*Poster

Cell reprogramming and its relation to gene expression levels.

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Current models of cell reprogramming (e.g. Waddington landscapes) lack some key aspects of cellular biology. Each cell is not a static body, it dynamically evolves according to a cell cycle. Gene regulatory networks do not encode the true hierarchical nature of cell lineages. This work attempts to create a more biologically significant model for the evolution of cell types, with a future aim to be used to predict the required perturbations to reprogram cells (towards a more pluripotent state). Cell types are modelled as a set of hierarchical cell cycles, each of which are fully described by a word of binary gene expression levels. The different stages of the cell cycle would then be represented as variations of the gene expression levels of a given cell state, which are attractors of the network. Each individual cell would transition between the different phases of the cell cycle, in a limit cycle like nature. The techniques used in this work are inspired by models of neural networks.

*Poster

Reciprocity between Robustness of Period and Plasticity of Phase in Biological Oscillators

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Circadian clocks exhibit the robustness of period and plasticity of phase against environmental changes such as temperature and nutrient conditions. Thus far, however, it is unclear how both are simultaneously achieved. By investigating distinct models of circadian clocks, we demonstrate reciprocity between robustness and plasticity: higher robustness in the period implies higher plasticity in the phase, where changes in period and in phase follow a linear relationship with a negative coefficient. The robustness of period is achieved by the adaptation on the limit cycle via a concentration change of a buffer molecule, whose temporal change leads to a phase shift following a shift of the limit-cycle orbit in phase space. Generality of reciprocity in clocks with the adaptation mechanism is confirmed with theoretical analysis of simple models. We will also discuss about biological significance of such reciprocity.

*Poster

Modeling of T-Cell polarization

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The repositioning of the microtubule organizing center is core part of many biological processes. It takes place in T-cell lymphocyte instantly after antigent presenting cell is recognized by the T-Cell. Microtubule dynamics and bending shorter than persistence length have a key role in the repositioning process. Our focus is on development of a model of microtubules and microtubule organizing center and the simulation of cell repositioning. The model is used to elucidate experimental observables. Various mathematical models are used to mimic hydrodynamics of microtubules. Multiple algorithms for Brownian dynamics simulation of microtubules are presented. It is confirmed that these algorithms yield predicted values for equilibrium properties. A model of the microtubule organizing center is introduced. The entire structure of microtubule organizing center and microtubules is submitted to forces simulating action of dynein and it is used for the simulation of cell repositioning. Results from simulation and experiment are compared.

*Poster

Modeling meiotic chromosome in fission yeast - from pinned polymer loop to ASEP and back

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In this contribution, we show that the conformations of a pinned polymer loop embedded in a heat bath with a constant external force field can be modeled by an asymmetric exclusion process (ASEP) with reflecting boundary conditions. This correspondence allows us to find the exact solution for both systems' equilibrium statistics, which is well approximated by the Fermi–Dirac distribution. Moreover, we can quantify not only the behavior of average positions of the particles of the ASEP and the corresponding monomers of the polymer loop, but also their fluctuations. The condition of forming a loop and the corresponding constraint in the ASEP model lead to explicit dependence of the fluctuations on the position of the particles in ASEP and the monomers of the polymer. To close the loop of analogies we show that the kinetic Monte Carlo simulations, which can be performed for the ASEP with a well defined physical time, can be related to the non-equilibrium dynamics of polymer loops.

*Poster

Genotypic complexity of Fisher's geometric model

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Fisher's geometric model (FGM) is a simple fitness landscape model in which an organism is characterized by n phenotypic traits and mutations are random displacements in the trait space. The fitness is given by a smooth and single-peaked function around the optimal combination of phenotypes. Recently, Blanquart extitet al. (2014) introduced an ensemble of genotypic fitness landscapes constructed from FGM by considering an additional genotypic sequence space where each locus represents the presence or absence of a certain mutation. Additionally, they assume that the displacements corresponding to the mutations are vectorially combined. This model is particularly interesting because it presents a natural connection between genotypes and phenotypes, and their interplay produces a nontrivial functional dependence of the structure of the resulting genotypic fitness landscape on phenotypic parameters. To provide a solid understanding of the mechanisms by which ruggedness emerges in such landscapes, we are mainly concerned with calculating various ruggedness measures analytically by establishing a spin glass representation analogous to the Hopfield model, a fundamental model of neural networks. By interpreting the genotypic dimension as the network capacity, these results are compared with the metastability measures of the Hopefield model. Surprisingly, from the results on the different measures, we consistently find that the induced landscapes become less rugged with increasing phenotypic dimension n. Finally, we discuss the biological implications of our analytical results.

*Poster

Wall effects on the dynamics of a self-phoretic swimmer.

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Self-phoretic swimmers are colloid particles endowed with an asymmetric catalytic coating on their surface, able to self-propel in a chemical solution. Here, we study the effects of a planar wall on the self-phoretic swimmer propulsion - taking into account both the hydrodynamic and solute concentration distortion. Tuning the surface reactivity and solute-to-swimmer surface interaction (mobility), it's possible to achieve swimmer-wall bound states. We identified two possible routes to stable propulsion along the wall: First, uniform mobility swimmer with extensile force-dipole flow field (pusher) and second, a swimmer with non-uniform mobility over its surface. However, for the non-uniform mobility scenario, the direction of propulsion relative to the mobility variation polarity determines whether the stable bound state exists. We further rationalise the swimmer dynamics with a simplified cubic polynomial in the swimmer height from the wall.

*Poster

Thermodynamic basis for mechanosensitive kinetics of actin remodeling

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Actin is a ubiquitous, multiple-role protein in eukaryotic cells. The remodeling of actin cytoskeleton is mediated by actin-binding proteins (ABPs), many of which bind to or dissociate from the actin filaments in a mechanosensitive manner. However, the mechanisms of the mechanosensitive kinetics of ABP–actin binding still remain poorly understood. Elucidating these mechanisms is important for understanding how the actin cytoskeletal structure is remodeled by intracellular forces. To gain an insight into these mechanisms, we propose a physical model that explains the force-dependent kinetic preference of actin-binding proteins to actin filaments. Our model is constructed based on the Gibbs-Duhem equation that constrains intensive parameters in the thermodynamic system. We show that this model captures the qualitative responses of ABPs to the forces, as observed experimentally. In addition, our theoretical results demonstrate that depending on the structural parameters of binding region, ABPs can show different kinetic responses even to the same mechanical signal, tension. These findings suggest an evolutionary link between ABPs and the structural parameters that promote ABP binding to or dissociation from actin.

*Poster

A continuum model for tissue dynamics with cell shape change and rearrangement

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Recent progress in tissue mechanics much relies on characterization of cellular behaviors in shape and deformation, as well as in their molecular activities. Numerical schema often employed for simulating the tissue dynamics is 'discrete model', such as cellular Potts (CPM) and cell vertex model (CVM), in which individual cells are explicitly considered. From theoretical point of view, corresponding continuum model is useful, however, most of existing models do not include degrees of freedom for cell shape and deformation by cell rearrangement. Here we propose a continuum scheme for expressing tissue dynamics. By starting from potential function used in CPM/CVM, elastic stress is derived. Then using formula originally developed for form, flow by cell rearrangement is formulated. Self-driven shear flow will be demonstrated. The model will help our understanding in how cellular behaviors are integrated to produce tissue-level dynamics.

*Poster

Evolutionary dynamics of complex phenotypes

Yaroslav Ispolatov * [1], Michael Doebeli

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We study macroevolutionary patterns for a general class of simple competition (logistic) models. We first review our recent results that a gradual evolutionary change in continuous phenotypes (evolutionary dynamics) can be non-stationary and even chaotic when the dimension of the phenotype space in which the evolutionary dynamics unfold is high, and that evolutionary diversification can occur along non-equilibrium trajectories. We combine these lines of thinking by studying long-term coevolutionary dynamics of emerging lineages in multi-dimensional phenotype spaces. We use a statistical approach to investigate the evolutionary dynamics of many different systems, with the following main results: 1) for a given dimension of phenotype space, the coevolutionary dynamics tends to be fast and non-stationary for an intermediate number of coexisting lineages, but tends to stabilize as the evolving communities reach a saturation level of diversity; and 2) the amount of diversity at the saturation level increases rapidly (exponentially) with the dimension of phenotype space. These results have implications for theoretical perspectives on major macroevolutionary patterns such as adaptive radiation, temporal patterns of phenotypic changes, and the evolution of diversity. For adaptive radiation, the results suggest that both the rate of diversification and the rate of evolutionary change should decrease as the radiation unfolds, resulting in stasis once the saturation level is reached. If new phenotype dimensions evolve, e.g. through gene duplication, another bout of accelerating evolutionary dynamics followed by stasis can be expected, thus generating a macroevolutionary pattern of intermittent bursts. Finally, diversity may saturate for a given dimension of phenotype space, but may not saturate over very long time scales as new phenotypic dimensions evolve, essentially resulting in open-ended evolution of diversity.

*Poster

Hamiltonian replica-permutation molecular dynamics simulation studies on the oligomerization of amyloid-beta fragments

Satoru G. Itoh * [1], Satoru G.

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An amyloid-β peptide (Aβ) is composed of 39?43 amino-acid residues. Aβ tends to form amyloid fibrils, which are associated with the Alzheimer's disease. The oligomerization process occurs during the early stage of the amyloid fibril formation process. It is necessary to clarify the oligomerization process in order to find a remedy for Alzheimer's disease. The oligomerization process of Aβ is slow process, and it is difficult to investigate such slow process by conventional canonical molecular dynamics (MD) simulations. In order to study the oligomerization process, the Coulomb replica-permutation method (CRPM) is useful. CRPM is one o the realizations of the Hamiltonian replica-permutation method (HRPM). In HRPM, parameters in the Hamiltonian are permuted among replicas. The Suwa-Todo algorithm is employed for parameter permutations among the replicas to minimize its rejection ratio. We applied CRPM simulations to Aβ fragments, Aβ (29-42) peptides, in explicit water solvent and studied the oligomerization process of the Aβ (29-42) peptides. In our presentation, we will introduce HRPM, briefly. The oligomerization process of the Aβ (29-42) will also be shown.

*Poster

From mode coupling to functionally critical sites in proteins

Alkan Kabakcioglu * [1], B. Kav, M. Ozturk, O. Varol, D. Yuret, B. Erman

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Relevance of mode coupling to energy/information transfer during protein function, particularly in the context of allosteric interactions is widely accepted. However, existing evidence in favor of this hypothesis comes essentially from model systems. We here report a novel formal analysis of the near-native dynamics for proteins, which allows us to explore the impact of the interaction between possibly non-Gaussian vibrational modes of the protein on its dynamical behavior. We show that, an information-theoretic measure based on mode coupling alone yields a ranking of residues with a statistically significant bias favoring the functionally critical locations identified by experiments on Myosin II and AncGR1,2. Reference: O. Varol et al., Proteins: Structure, Function and Bioinformatics, 82(9), 1777 (2014); B. Kav et al., arXiv:1509.05483.

*Poster

Negative scaling relationship between molecular diversity and resource abundances

Atsushi Kamimura * [1], Kunihiko Kaneko

[1] The University of Tokyo – Japan

Understanding how cellular components can be integrated into a reproducing cell is essential to unveil general characteristics of cells and to experimentally synthesize protocells. A catalytic reaction network provides a basic theoretical model in which different molecular species mutually catalyze the replication of each other. Here, I will show relevance of interplay of different timescale in the catalytic reaction network to reproduction, growth-division, tradeoffs and diversity of protocells. In contrast to simple replication system with fewer components, cell reproduction involves replication of diverse molecule species. To address this question of diversity, we theoretically study a cell system with catalytic reaction dynamics that grows by uptake of environmental resources. It is shown that limited resources lead to increased diversity of components within the system, and the number of coexisting species increases with a negative power of the resource uptake. The relationship is explained from the optimum growth speed of the cell, determined by a tradeoff between the utility of diverse resources and the concentration onto fewer components to increase the reaction rate.

*Poster

Two-step relaxation mode analysis with multiple evolution times of an all-atom molecular dynamics simulation of a protein

Naoyuki Karasawa * [1], Ayori Mitsutake, Hiroshi Takano

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Protein dynamics was studied by all-atom molecular dynamics simulation and the newly proposed method, two-step relaxation mode analysis (RMA) with multiple evolution times. RMA investigates the slow dynamics involved in structual fluctuations by estimating the relaxation modes and their relaxtion times. Two-step RMA with multiple evolution times is the improved version of the usual RMA method. It is found that two-step RMA with multiple evolution times extracts structural transitions more effectively.

*Poster

Onset, timing, and exposure therapy of stress disorders: mechanistic insight from a mathematical model of oscillating neuroendocrine dynamics

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The hypothalamic-pituitary-adrenal (HPA) axis is a neuroendocrine system that regulates numerous physiological processes. Disruptions in the activity of the HPA axis are correlated with many stress-related diseases such as post-traumatic stress disorder (PTSD) and major depressive disorder. In this paper, we characterize ?normal? and ?diseased? states of the HPA axis as basins of attraction of a dynamical system describing the inhibition of peptide hormones such as corticotropin-releasing hormone (CRH) and adrenocorticotropic hormone (ACTH) by circulating glucocorticoids such as cortisol (CORT). In addition to including key physiological features such as ultradian oscillations in cortisol levels and self-upregulation of CRH neuron activity, our model distinguishes the relatively slow process of cortisol-mediated CRH biosynthesis from rapid trans-synaptic effects that regulate the CRH secretion process. Crucially, we find that the slow regulation mechanism mediates external stress-driven transitions between the stable states in novel, intensity, duration, and timing-dependent ways. These results indicate that the timing of traumatic events may be an important factor in determining if and how patients will exhibit hallmarks of stress disorders. Our model also suggests a mechanism whereby exposure therapy of stress disorders such as PTSD may act to normalize downstream dysregulation of the HPA axis.

*Poster

Crucial role of the collective displacement modes in the morphological transformation during the maturation of the HK97 bacteriophage

O. V. Konevtsova * [1], V. L. Lorman and S. B. Rochal

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The symmetry and physical origin of collective displacement modes playing a crucial role in the morphological transformation during the maturation of the HK97 bacteriophage and other similar viruses are considered. It is shown that experimentally observed hexamer deformations and pentamer twists in the HK97 procapsid are well described in the continuous approximation as the simplest irreducible shear deformation (normal mode) of a spherical shell which decreases the shell symmetry down to the rotational icosahedral group I. In contrast to the shear field, the simplest radial irreducible displacement field responsible on the icosahedral capsid faceting has the full icosahedral symmetry Ih. We show that the change in the radial field sign results in the dodecahedral faceting observed, for example, in viruses of the Parvovirus family. In the frame of the Landau-Ginzburg formalism we propose a minimal phenomenological model valid for the first reversible steps of the HK97 maturation process [1]. These steps are shown to be associated with two order parameters. The first order parameter describes the isotropic expansion of the protein shell while the second one is responsible for the shape symmetry breaking and the resulting shell faceting. Calculated phase diagram illustrates the discontinuous character of the virus shape transformation. The results of the in vitro and in vivo experiments leading to the virus shell faceting are related to the decrease in capsid shell thickness and the increase of the internal capsid pressure. This work was supported by the Russian Science Foundation (grant number 15-12-10004). [1] O. V. Konevtsova, V. L. Lorman, and S. B. Rochal, Theory of morphological transformation of viral capsid shell during the maturation process in the HK97 bacteriophage and similar viruses, Phys. Rev. E 93, 052412 (2016).

*Poster

Interplay of directed transport and diffusive motion inside cellular protrusions

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Linear cellular protrusions like filopodia, microvilli or stereocilia are characterized by their finger-like structure that is connected to the cell body at one end, the base, and extends into the surroundings at the other end, the tip. A membrane enclosing the protrusion separates the inside of the protrusion from the extracellular and prevents in- and outflux other than at the base. Inside the protrusion bundles of parallel actin-filaments are embedded into cytoplasm so that different types of motion interact with each other: directed transport of cargo towards the tip on the actin-filaments and diffusive motion inside the cytoplasm. Motivated by this biological process we study the steady-state behaviour of a totally asymmetric simple exclusion process (TASEP) that is weakly coupled to different diffusive environments and focus on systems that are closed at the tip of the TASEP. We derive an exact equation that relates the average total occupation on the TASEP to the average total occupation on the diffusive lattice coupled to it. This mass balance equation represents a global detailed balance for the exchange between the two lattices, where detailed balance does not hold locally for any pair of sites but for the two lattices in total. We show that the steady-state profile on the TASEP is given by a localized domain wall whose position can be determined using the mass balance equation. By further exploiting this global detailed balance equation we find an analytic expression for the nearest-neighbour correlations on the TASEP.

*Poster

Self-propulsion of droplets generated by surface tractions and body force densities

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We discuss the flow field and trajectories of active droplets, which are driven either by surface tractions or by body forces with or without chirality. Active stresses can e.g. be generated by myosin contractility or by an active polar medium inside the droplet. The flow fields and the dissipated energy in the inside and outside fluid are calculated analytically for several generic examples and the center of mass and rotation velocities are determined from the force density and the viscosity contrast. Our framework provides a link betweeen hydrodynamic models of active media and models of self-propulsion.

*Poster

Adaptive walks on correlated fitness landscapes

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Adaptive walks are simple evolutionary dynamics defined on a discrete space of genotypes. In one step of the walk, the resident population is replaced by a fitter genotype chosen among the neighbors that can be reached by a single mutation. The walk terminates when no fitter neighbors exist, that is, when the current genotype is a local fitness maximum. Classic results obtained on uncorrelated random fitness landscapes show that adaptive walks are generally quite short. In particular, if the choice among fitter neighbors is uniformly random (*random* adaptive walk) the walk length grows logarithmically with the number of genetic loci L, whereas for *greedy* walks that deterministically pick the largest available fitness increase the length attains a universal finite limit $e - 1 \approx 1.72$ for $L \to \infty$. Here we survey recent exact results for random and greedy adaptive walks on correlated fitness landscapes where the fitness is the sum of an i.i.d. random variable and a deterministically increasing profile [1,2,3]. For the random case the competition between the tail of the distribution of the random fitness components and the deterministic profile can induce a phase transition between short (length $\sim \ln L$) and long (length $\sim L$) walks which is continuous or discontinuous depending on the shape of the tail.

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*Poster

Periodically Driven DNA

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We propose a generic model of driven DNA under the influence of an oscillatory force of amplitude F and frequency ν and show the existence of a dynamical transition for a chain of finite length. We find that the area of the hysteresis loop, $A_{\rm loop}$, scales with the same exponents as observed in a recent study based on a much more detailed model. However, towards the true thermodynamic limit, the high-frequency scaling regime extends to lower frequencies for larger chain length L and the system has only one scaling ($A_{\rm loop} \approx \nu^{-1}F^2$). Expansion of an analytical expression for $A_{\rm loop}$ obtained for the model system in the low-force regime revealed that there is a new scaling exponent associated with force ($A_{\rm loop} \approx \nu^{-1}F^{2.5}$), which has been validated by high-precision numerical calculation. By a combination of analytical and numerical arguments, we also deduce that for large but finite L, the exponents are robust and independent of temperature and friction coefficient. References: 1. Periodically driven DNA: Theory and Simulation Sanjay Kumar, Ravinder Kumar and Wolfhard Janke Phys. Rev. E , 93, 010402 (R)(2016) 2. Statistical mechanics of DNA unzipping under periodic force: Scaling behavior of hysteresis loop Sanjay Kumar and Garima Mishra Phys. Rev. Lett. 110, 258102 (2013)

*Poster

Revealing nonergodic dynamics in living cells from a single particle trajectory

Yann Lanoiselée * [1], Denis S. Grebenkov

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We propose the improved ergodicity and mixing estimators to identify nonergodic dynamics from a single particle trajectory. The estimators are first investigated and validated for several models of anomalous diffusion such as ergodic fractional Brownian motion and diffusion on percolating clusters and nonergodic continuous time random walks and scaled Brownian motion. The estimators are then applied to two sets of earlier published trajectories of mRNA molecules inside live E. coli cells and of Kv2.1 potassium channels in the plasma membrane. These statistical tests suggest that the former set exhibits ergodic behavior while the latter reveals both ergodic and nonergodic features. Having no need in ensemble averages, the nonergodic dynamics can be revealed separately for each trajectory, providing a more flexible and reliable analysis of single-particle tracking experiments in microbiology.

*Poster

Annealed Random Copolymer Model of the B-Z and B-L Transitions in DNA:Torsional Responses

Nam-Kyung Lee * [1]

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Under negative torsion, DNA adopts left-handed helical forms, such as Z-DNA and L-DNA. We represent a single DNA molecule with structural heterogeneity as a helical chain consisting of monomers which can be characterized by different helical senses and pitches. We provide a theoretical description of this transition, based on an annealed random copolymer model. The transition of a switchable sequence is discussed as a function of energetic and geometric parameters of the B- and Z-forms, of the applied boundary conditions, and of the characteristics of the B-Z interface. We address a possible torsional softening upon the B-Z transition. Also by Monte Carlo simulation, where we take into account bending and twist fluctuations explicitly, we study sequence dependence of B-Z transitions under torsional stress and tension focusing on the interaction with B-L transitions. We consider core sequences, (GC)n repeats or (TG)n repeats, which can interconvert between the right-handed B form and the left-handed Z form, imbedded in a random sequence, which can convert to left-handed L form with different (tension dependent) helical pitch. (TG)n repeats are more costly to convert to Z-form but numerous. We show that Z-DNA formation from the (GC)n sequence is always supported by unwinding torsional stress but Z-DNA formation from the (TG)-sequence, can be strongly influenced by the quenched disorder in the surrounding random sequence. Our model can be also applied to other biofilaments with annealed torsional/flexural degrees of freedom.

*Poster

Bridging Filament Dynamics and Reaction Networks in silico

Yao Li * [1], Pieter Rein ten Wolde

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We develop a particle-based simulation method bridging filament dynamics and reaction networks together. Nedelec's method is employed for filament dynamics, and we use Green's function reaction dynamics to treat biomelocular reaction dynamics. The importance of the intricate interplay between membrane pattern formation, transport along cytoskeletal filaments is now increasingly being recognized. Yet, our understanding of these processes is still highly limited, largely because of the complexity of living of a living cell. As a first application of our method, we investigate a feedback-loop through signaling protein transports, activation and microtubule dynamics. It shows that our simulation method can be used, efficiently, to treat the coupling between protein reaction-diffusion and dynamics of filaments. We present systematic investigation of how feedback loop leads microtubule polarization, protein clustering, and centrosome re-positioning. Finally, a short discussion on coupling vesicle dynamics into this model will also be given.

*Poster

sample-dependent first-passage-time distribution in a disordered medium

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Above two dimensions, diffusion of a particle in a medium with quenched random traps is believed to be well described by the annealed continuous-time random walk. We propose an approximate expression for the first-passage-time (FPT) distribution in a given sample that enables detailed comparison of the two problems. For a system of finite size, the number and spatial arrangement of deep traps yield significant sample-to-sample variations in the FPT statistics. Numerical simulations of a quenched trap model with power-law sojourn times confirm the existence of two characteristic time scales and a non-self-averaging FPT distribution, as predicted by our theory.

*Poster

Coordinated and correlated dynamics of human topoisomerase II orchestrating DNA re-ligation

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Topoisomerase II is a crucial enzyme that tightly controls the topology of DNA to facilitate the critical sub-cellular processes involving these genetic materials. It generates transient double-strand breaks (DSB) and transports another DNA duplex through to resolve their topological problems. Although topoisomerase poisons, the drugs arresting the subsequent DNA re-ligation, have been used in anticancer therapy and the recent structural characterization of the enzyme, our understanding of the religation mechanism was still distressingly restricted by the transitory nature of this process. Captivated by the fluent re-ligation following the characteristic DSB by the enzyme, we selected a high-resolution crystal structure of the drug-entrapped intermediate and exploited atomistic molecular dynamics simulations of the very large systems for up to a microsecond to investigate the dynamics of this process. We observed a nearly vectorial transition of the de-poisoned complex toward the resealing-compliant configuration, and the statistical analysis revealed the non-concerted maneuvers of the two different DNA strands mediated by the enzyme. Using a neighborhood-based metric, we captured the important dynamical transitions during the re-ligation from the vast amount of correlated motions and provided the visible links between previously unsettled experimental observations. With the simulations of the drug-bound complexes, we also presented the conformational population shifts of an important residue in response to the binding of different drug molecules. Furthermore, by comparing the coordinated dynamics revealed by different isoforms, we are able to dissect the differential dynamics of the critical DNA re-ligation conducted by the enzymes. We believe these are useful insights for the development of new anticancer drugs with lower cardiotoxicity. (References: Nucleic Acids Res 2015 43:6772-6786; Molecules 2014, 19:7415-7428)

*Poster

Spatiotemporal organization of action potential duration alternans in arrhythmogenesis

Rupamanjari Majumder * [1], M.C. Engels, A.A.F deVries, A.V. Panfilov, D.A. Pijnappels

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Acute injuries to cardiac muscle often lead to a cascade of histopathological and structural changes,i.e., remodeling in the heart, that result in its abnormal functionality. Two key features of such remodeling include (i) fibrosis, i.e., increased numbers and distributions of inexcitable cells called myofibroblasts; and (ii) reduced intercellular coupling. These features are associated with abnormalities in electrical impulse generation and propagation, which predispose to cardiac arrhythmias, leading to sudden death. In the absence of structural remodeling, high-frequency impulse generation can also induce arrhythmias, via the development of dynamic electrical instabilities. However, owing to the complex and stochastic nature of arrhythmias, the combined mechanistic influences of structural and dynamical perturbations on arrhythmogenesis remain incompletely understood. In this study, arrhythmogenesis was investigated using in vitro and in silico monolayer models of neonatal rat ventricular tissue with increased fibrosis and reduced intercellular coupling. Arrhythmia incidence and complexity (i.e., number of phase singularities) increased with decreasing intercellular coupling efficiency. This coincided with the onset of a special type of spatially discordant action potential duration (APD) alternans characterized by island-like spatiotemporal organization of alternans of opposite phase (APIs). The number of APIs correlated positively with the drop in intercellular coupling efficiency and increase in arrhythmia complexity. At higher levels of fibrosis, more APIs were formed and reentrant arrhythmias were more easily induced. This study reveals islands of oppositely phased APD alternans to be important determinants of reentrant tachyarrhythmia initiation and complexity.

*Poster

Single molecule measurement of thermodynamic information in heterogeneous DNA ensembles

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Darwinian theory of biological evolution has two main features: variability and selection. Evolutionary processes occur across all spatial and temporal scales from species and organisms down to the molecular level. Quantifying variability and disorder is, therefore, essential to understand how molecular ensembles of mutants evolve in time. Building on previous work on thermodynamic inference in stochastic thermodynamics citeMarcoFelix we have developed a theoretical framework that allows us to extract the intrinsic thermodynamic information of a disordered ensembled of DNA hairpins using single-molecule force spectroscopy. By combining optical tweezers studies with recent developments in fluctuation theorems and stochastic thermodynamics we characterize an heterogeneous sample of randomized DNA hairpins. A native Watson-Crick 20 base pairs hairpin ending in a tetraloop was randomized by mutating eight nucleotides of four distinct base pairs along the stem to generate a population of $4^8 = 2^{16} = 65536$ different sequences. We show how by averaging the work probability distributions obtained in a experimental set of bidirectional pulling experiments on the molecular ensemble, the Crooks Fluctuation Relation is fulfilled but with an effective temperature which is higher than the bath temperature. We then consider an exactly solvable model to demonstrate how the effective temperature allows us to define a thermodynamic quantity *Upsilon* containing information about the folding free energy spectrum of the heterogeneous ensemble. With the support of numerical simulations we show the feasibility of these experiments tu quantify the heterogeneity of molecular ensembles at the single molecule level. The thermodynamic information quantity *Upsilon* is physically interpreted in terms of missing entropy production that can be inferred (rather than directly measured) from nonequilibrium experiments. Finally we discuss the extension of these studies to genuine mutational ensembles evolved under directed molecular evolution.

*Poster

Criticality in Fertilization

Gustavo Martínez-Mekler * [1], Alejandro Aguado, Alberto Darszon, Jesus Espinal, Daniel Priego

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Fertilization is one of the fundamental processes of living systems. In previous work [1] we introduced a logical regulatory network for the signaling pathway of [Ca2+] concentration oscillations in the flagella of sea urchin sperms, triggered by chemicals surrounding the oocyte. These oscillations modify sperm navigation [2]. Several predictions from the model were subsequently confirmed experimentally leading to a better understanding of the electrophysiology of the flagellum membrane, the action of drugs and chemotaxis [3-4]. Here we show that the network dynamics operates at a critical regime, where robustness and evolvablity coexist. Furthermore, based on criticality as well as non-chaoticity, we reduce the network. Comparison with network reduction based on attractor landscape arguments and correlation calculations is encouraging. Network redundancy is also addressed. The similarity of the reduced discrete network with a system of differential equations model built stepwise is reassuring. Our findings are relevant to the discussion of the role of criticality in essential biological processes and may be of significance to evolution. [1]Espinal, J., Aldana, M., Guerrero, A., Wood, C. D., Darszon, A., and Martínez-Mekler, G. (2011). Discrete dynamics model for the speract-activated Ca2+ signaling network relevant to sperm motility. PloS ONE 6(8): e22619. [2] Guerrero, A., Nishigaki, T., Carneiro, J., Yoshiro Tatsu, Wood, C. D., and Darszon, A. (2010). Tuning sperm chemotaxis by calcium burst timing. Dev Biol, 344(1):52 [3] Guerrero, A., Espinal, J., Wood, C.D., Rendon, J.M., Carneiro, J., Martínez-Mekler, G., Darszon, A., Niflumic acid disrupts marine spermatozoan chemotaxis without impairing the spatiotemporal detection of chemoattractant gradients (2013) Jour- nal of Cell Science 126(6): 1477. [4] Espinal J, Darszon, A., Wood, C., Guerreo A, Martínez- Mekler G, (2014) In silico determination of the effect of multi- target drugs on sea urchin spermatozoa motility. PLoS ONE 9(8): e104451t

*Poster

A stochastic process for anomalous diffusion which combines important characteristics of fBm and CTRW

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Anomalous diffusion has been shown to appear extensively in nature and, consecuently, scientists have developed several and different models that can effectively reproduce it. However, the underlying physics of a plethora of experiments is still not well-understood. This is the case of the motion of mRNA molecules inside living E. coli cells [1], where stochastic processes as the continuous-time random walk (CTRW) can explain non-ergodicity [2] but an alternative like the fractional Brownian motion (fBm) is needed to reproduce p-variation [3]. We found that a family of stochastic processes known as generalised grey Brownian motion (ggBm) [4] can fit correctly that observation. In addition, we include an explicit time-dependent factor to model non-stationarity, usually referred to aging [5] in the specialized literature. In agreement with our computational results, we were able to obtain also analytical expressions for a list of observables, including temporal and ensemble mean square displacements (TAMSD and EAMSD), ergodicity breaking parameter, one-point one-time probability distribution function and p-variation.

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*Poster

Left-right symmetry breaking in C. Elegans

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Left-right (LR) asymmetry in most developed organisms is extremely important for their proper development and survival. However, symmetry breaking along the LR axis is not yet well-understood. Chirality is expected to play an important role and, experimentally it is indeed seen a chiral flow in the cell-cortex prior to the establishment of this asymmetry. We propose that the difference in friction experienced by two of the cells (ABa and ABp) at either sides and asymmetric distribution of cortical constituents during division at the four-cell stage give rise to a net non-zero torque that rotates the cells and breaks the symmetry. I will present the theoretical model and its predictions and how they comprise with the experimental findings carried out through direct imaging of the cell-cortex of C. Elegans during the division at four-cell stage.

*Poster

The effect of twist-bend coupling on the torsional properties of double-stranded DNA

Stefanos K. Nomidis * [1], Stefanos K. Nomidis, Willem Vanderlinden, Jan Lipfert, Enrico Carlon

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Single-molecule experiments of the effective torsional stiffness of DNA have reported a clear deviation from the predictions of the twistable worm-like chain model, i.e. the standard mechanical model of DNA elasticity. Here we show that this discrepancy can be resolved if a coupling term between bending and twisting is introduced. Although the existence of such an interaction was predicted more than two decades ago (Marko and Siggia, 1994), its effect on the static and dynamical properties of DNA has been largely unexplored. Our analysis yields a twist-bend coupling constant of G = 50 nm and we show that its introduction requires a re-tuning of the other elastic parameters of DNA, in particular of the bending stiffness.

*Poster

Asymmetry of Arrangement Induces Phase Synchronization in Mouse Node Cilia

Keiji Okumura * [1], Seiya Nishikawa, Toshihiro Omori, Takuji Ishikawa, Atsuko Takamatsu

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Leftward fluid flow in a mouse node cavity plays an important role to determine the left-right axis at its early developmental stage. The flow is generated by the clockwise rotational movement of the node cilia which are tilted towards the posterior side. Experimental observations revealed that the rotational movements in certain pairs of cilia are phase locked [1]. In this study, to elucidate the effects of near-field hydrodynamic interaction on phase synchronization, we investigate a oscillator model of node cilia on the basis of phase reduction theory. The near-field hydrodynamic interaction between cilia at low Reynolds number is numerically calculated by computational fluid dynamics [2], where a cilium is treated as a rigid cylinder and its trajectory is constrained on the lateral surface of cone. Results show that, while a pair of identical cilia is difficult to synchronize in phase within a certain finite period of observation time, three identical cilia can be easily phase locked as long as symmetry breaking in their arrangement is introduced. [1] A. Takamatsu, K. Shinohara, T. Ishikawa, H. Hamada, extitPhys. Rev. Lett. extbf110, 248107 (2013). [2] T. Ishikawa, M.P. Simmonds, T.J. Pedley, extitJ. Fluid Mech. extbf568, 119 (2006).

*Poster

All-atom molecular dynamics simulations of amyloid beta fibril in explicit water

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Amyloids are insoluble and misfolded fibrous protein aggregates and associated with more than 40 serious human diseases. For example, amyloid-β fibrils ($A\beta$) are known to be associated with the Alzheimer's disease. The $A\beta$ amyloid fibril has a cross-β structure consisting of two β-sheets called β_1 and β_2. It is thought to have a series of the same molecular conformation and translational symmetry along the fibril axis. The amyloid-fibril structure at the fibril end, however, has not yet been revealed by experiments because the end of the one-dimensional fibril has only zero-dimensional small region. To reveal the fibril-end structure, we performed all-atom molecular dynamics simulations of $A\beta$42 and $A\beta$40 fibrils in explicit water. We found that the translational symmetry is broken at the fibril ends. Furthermore, we discovered that molecular structure is different between two ends: The two β-sheets β_1 and β_2 are close to each other, and the $A\beta$ peptide takes a closed form at the even end. On the other hand, at the odd end the $A\beta$ peptide fluctuates more and takes an open form, too, in which the two β-sheets are far from each other. The center region of the $A\beta$ peptide fluctuates even less than the even end and takes the closed form.

*Poster

Interaction between polymer-grafted nanoparticles in chemically identical homopolymer matrix

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In this research, we develop a new numerical scheme of self-consistent field theory (SCFT) to quantify interparticle interaction between two spherical nanoparticles (NPs) coated with polymer grafts in chemically identical homopolymer melts. In our numerical SCFT calculation, two-dimensional finite volume method (FVM) which efficiently conserves the amount of material in curvilinear coordinate is adopted, and the differential equation for partition function is solved in real space with Multicoordinate-system (MCS) scheme which makes use of the mirror symmetry between the two particles. In this research, we investigate how distribution of chain lengths, grafting density and particle curvature interplay roles on stabilization mechanism for dispersion by calculating interaction potentials between two polymer-coated NPs as functions of distance between the two particles. Our results reveal that polydisperse distribution stabilizes dispersions more efficiently than monodisperse counterparts.

*Poster

Modularity enhances the rate of evolution in a rugged fitness landscape

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Biological systems are modular, and this modularity affects the evolution of biological systems over time and in different environments. We here develop a theory for the dynamics of evolution in a rugged, modular fitness landscape.We show analytically how horizontal gene transfer couples to the modularity in the system and leads to more rapid rates of evolution at short times. The model, in general, analytically demonstrates a selective pressure for the prevalence of modularity in biology. We use this model to show how the evolution of the influenza virus is affected by the modularity of the proteins that are recognized by the human immune system. Approximately 25% of the observed rate of fitness increase of the virus could be ascribed to a modular viral landscape.

*Poster

An exactly solvable spatial model of mutation accumulation in cancer

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One of the hallmarks of cancer is the accumulation of driver mutations which increase the net reproductive rate of cancer cells and allows them to spread. This process has been studied in mathematical models of well mixed populations, and in computer simulations of three-dimensional spatial models. But the computational complexity of these more realistic, spatial models makes it difficult to simulate realistically large and clinically detectable solid tumours. Here we describe an exactly solvable mathematical model of a tumour featuring replication, mutation and local migration of cancer cells. The model predicts a quasi-exponential growth of large tumours even if different fragments of the tumour grow sub-exponentially due to nutrient and space limitations. The model reproduces clinically observed tumour growth times using biologically plausible rates for cell birth, death, and migration rates. We also show that the expected number of accumulated driver mutations increases exponentially in time if the average fitness gain per driver is constant, and that it reaches a plateau if the gains decrease over time. We discuss the realism of the underlying assumptions and possible extensions of the model.

*Poster

Onset of chaos and criticality in neural networks with synaptic plasticity

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Models of neural networks are a useful tool to investigate general mechanisms underlying dynamical regimes observed in neuronal systems, such as collective activity oscillations and the presence of critical avalanches in the cortex. We consider a reliable model for cortical neurons, a network of purely excitatory leaky integrate-and-fire neurons connected via the Tsodyks-Uziel-Markram (TUM) dynamical model for synaptic plasticity. We observe a transition to chaos as a function of the coupling strength and of the synaptic time scale, and we investigate this regime through a heterogeneous mean field approach. In the limit of a fully connected network, we are able to reduce the dynamics to a one-dimensional map that clarifies the mechanism underlying the transition. We observe that the onset of chaos in the fully connected model corresponds to a bursty phase on a disordered topology. Moreover, we characterize the bursty phase as strongly correlated and potentially carrying a larger amount of information than quasi-synchronous and asynchronous regimes.

*Poster

Coarse-grained molecular dynamics of the ionic flow through a proteic nanopore

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Coarse-grained models, representing several atoms by one site, are becoming increasingly popular since they can overcome the limitations of all-atom models to simulate molecular dynamics of biological systems for time-lengths closer to experiments. We have performed coarse-grained molecular dynamics simulations, using the MARTINI force-field, of the ionic transport through a proteic nanopore, the alpha-hemolysin channel, inserted into a DPPC lipid membrane bilayer surrounded by solvent and KCl ions, in the presence of different electric fields. We have computed ionic currents through the pore consistent with experiments. In this work we are specially concerned by the so-called "pore rectification? this is, the ionic current asymmetry when positive and negative potentials are applied through the system.

*Poster

Strain-driven phase transition in the nonlinear mechanics of athermal fibre-networks.

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Naturally occurring biopolymers such as collagen and actin form fibrous networks. Disordered fibrous networks are ubiquitous in nature as major structural components of living cells and tissues. The mechanical stability of networks generally depends on the degree of connectivity. The average connectivity of biopolymer-networks found in nature are generally below the isostatic threshold at which central force interactions marginally stabilize the network. In the submarginal regime, such networks are unstable toward small deformations unless stabilized by additional interactions such as bending. We perform numerical studies on the elastic behavior of such networks. We find that branched networks exhibit nonlinear mechanics consistent with athermal critical phenomena controlled by strain. We obtain the critical exponents capturing the nonlinear elastic behavior near the critical point by performing scaling analysis of the stiffening curves. We find that the exponents evolve with the connectivity in the network. We show that the nonlinear mechanics of disordered networks, independent of the detailed microstructure, can be characterized by a strain-driven second-order phase transition, and that the primary quantitative differences among different architectures are in the critical exponents describing the transition.

*Poster

Temperature dependent force spectroscopy in single molecule experiments

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DNA folding/unfolding processes play a key role during replication and transcription of DNA, these processes take place at mesophilic temperatures. Most biomolecular reactions inside the cell are driven by the fine tuning between enthalpy and entropy contributions. Their relative weight is strongly effected by temperature. Therefore, it is crucial to understand what is the effect of temperature in biomolecular reations. In particular it is important to characterize conformational transitions and the elastic properties of biopolymers (e.g. in nucleic acids and protei ns) upon changing properties in the solvent such as the temperature. Here we used an Optical Tweezers (OT) device with a temperature controller to unfold/fold a DNA hairpin using force in single molecule pulling experiments. We studied their conformational transitions to extract thermodynamic quantities such as the free energy, enthalpy and entropy as a function of the temperature.

*Poster

Chiral Separation by Creeping Flows

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Separation of enantiomers by chirality is of great importance in pharmaceutical, agricultural, and environmental industries for their chirality-sensitive biochemical activities.A number of experimental and numerical studies proposed various separation strategies using flow fields. Basic idea is to utilize a certain flow property to induce chirality-dependent drift, yet general conditions are left to be clarified. In this presentation, we introduce a theoretical framework to understand the motion of rigid chiral objects of an arbitrary shape in a linear creeping flow field. From symmetry consideration, we show that the rate-of-strain field should be finite to generate drift of an object in the opposite direction to its chiral pair. Equally crucial condition is drawn from eigenmode analysis: The velocity gradient tensor of the flow fields should be nearly singular for the precise and efficient resolutions of enantiomers. We demonstrate the claims by Langevin dynamic simulation with hydrodynamic interactions implemented by Rotne-Prager tensor.

*Poster

Evolution of Transcription Factor families along the Human Lineage

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We propose a new way to organize Transcription Factors (TFs) into families, based on the network of co-occurence of the same Position Weight Matrix among different TFs. This network has a very simple structure, being composed of several disconnected components of high density, which we identify as "motif" families. Based on this TF organization we then propose a simple one parameter model of the Birth Death Innovation type which describes remarkably well the empirical distribution of these families. We used this model as a null model to identify the relevant evolutionary forces which shaped the TF repertoire in the vertebrate lineage and devised two main patterns: three over-expanded families corresponding to HOX and FOX type genes and a set of "singleton" Transcription Factors of probable Prokaryotic origin which seem to be selected against duplication.

*Poster

Ultrasensitivity in the 3-State Barkai-Leibler Model

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Chemotaxis receptors in *E.coli* are subject to successive methylation and demethylation reactions by the enzymes CheR and CheB, in addition to binding of attractant or repellant molecules. These processes modulate receptor activity and contribute to adaptation and response. Here, we study the mean and fluctuations in receptor activity in a simplified version of the Barkai-Leibler [1] model of receptor modification kinetics with three methylation levels per receptor, $m = 0, 1$ and 2. In this model, inactive/active receptor-CheA complexes are successively methylated/demethylated by CheR/CheB enzymes respectively, while the activity of a single receptor is enhanced by methylation and suppressed by attractant binding. Starting from the complete master equation of this model, we first develop a set of non-linear Fokker-Planck equations in the large N (N=total number of chemotaxis receptors) limit, from which the mean fractions of receptors populating each methylation state are first determined as "fixed points" of the corresponding macroscopic ("mean-field") equations. The fluctuations are then obtained systematically under the Linear Noise Approximation (LNA), which leads to a set of linear Fokker-Planck Equations (LFPE). We show rigorously that in the limit of large receptor concentration, the mean activity per receptor shows ultrasensitive response as $\nu = [CheR]/[CheB]$ is varied, and undergoes a sharp switch from near-zero to near-unity at a "critical" value $\nu = \nu_c$. This behaviour is identical to Zero order ultrasensitivity (ZOU) in two-state covalent modification systems predicted by Goldbeter and Koshland in 1981 [2]. While the (ultrasensitive) mean is independent of the attractant concentration $[L]$, the variance of activity peaks at ν_c; at fixed ν, the variance is an increasing function of $[L]$ and decreasing function of N. We also determined the mean populations of receptors at each methylation levels, as well as the correlation coefficients between them. For low $[L]$ the average fraction $\overline{\xi_2}$ of substrate molecules at the highest methylation level $m = 2$ is vanishingly small, while at large $[L]$, the lowest level $m = 0$ is poorly populated. For fixed $[L]$, $\overline{\xi_2}$ is an ultrasensitive, increasing function of ν, while $\overline{\xi_0}$ is a similar decreasing function of ν. The mean population $\overline{\xi_1}$ of the middle level $m = 1$, on the other hand, is a non-monotonic function of ν, with a peak at ν_c. We carried out Gillespie simulations for the system, the results being in tandem with the corresponding theoretical predictions from LFPE. Extending the above formalism to time-dependent $[L]$, we also compute the linear response function for mean activity and use it to make predictions for the chemotactic drift velocity [3] of a population in a spatial gradient of attractant, as a function of ν, $[L]$ and N.

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*Poster

Collective motion switches directionality of molecular motor along filament

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Regulations of cellular process are highly complex: it requires several conflicting tasks to be used properly in a context-dependent manner. Specifically, mitotic spindle formation requires two different kinds of motors: motor with plus-end directionality (i.e. motor that walks along microtubule toward its plus-end) and motor with minus-end directionality. Could it then be possible to embed such two conflicting directionality into a single type of motor so that it functions context-dependently? In this talk, from theoretical perspective, we show a design principle of a dual-directional motor that switches its directionality depending on the number of motors that bind to the same microtubule. Such motors can function as both plus- and minus-end directional motors depending on the configuration between microtubule and motors. Indeed, in a quite recent experiment, a kinesin was found to show such dual-directionality, however the mechanism for it has not been clarified. Our theoretical framework provides the mechanism of the dual-directional kinesin. Suggestions to confirm the proposed mechanism experimentally and biological relevance of such motors in the formation of mitotic spindle are also discussed.

*Poster

Hydrodynamic theory of epithelial flows

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How processes inside the cell result in tissue reorganisation at the scale of the organism is a crucial question to understand embryonic development. Epithelial tissues in particular are dynamically remodelled due to forces generated in the cells, cellular rearrangements, and cell division and apoptosis. In this work, we introduce a physical description of the slow timescale behavior of an epithelium. We obtain hydrodynamic constitutive equations describing the continuum mechanics of an epithelium on spatial scales larger than a cell. Within this framework, topological rearrangements relax elastic stresses in the tissue and can be actively triggered by internal cell processes. Using segmentation of the development of the Drosophila fly wing, we analyze experimental patterns of flow field and tissue shear. We show that topological transitions respond to cell elongation with a delay, are autonomously polarised in the tissue, and can robustly control cell shape during morphogenesis.

*Poster

Mechanics and dynamics of a thick cell layer with fluid transport

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We study the dynamics of a thick epithelial which pumps an interstitial fluid. We consider a tissue with average cell polarity normal to the tissue layer. The cell pump fluid against a pressure difference. Using a two-component hydrodynamic continuum theory, we study the dependence of tissue stress, cell velocity and fluid flow on the the external fluid pressure difference and the cell pumping activity. We find that the existence of steady states depends strongly on the external pressure difference, the pumping activity and the properties of the interface separating the tissue from the surrounding fluid.

*Poster

Fluctuations in the sliding motion of filaments driven by molecular motors

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Motor proteins generate force to contract muscles, transport cargos in cells, assemble cytoskeletal filaments during cell division, and so on. Motors work individually or in a small group in some cases (e.g., in transport of cargos), and they work in a large group in other cases (e.g., in muscle contraction). A natural question to be asked would be whether motors generate force independently or cooperatively when they operate in a group. It was pointed out [1] that this question may be answered by examining fluctuations in the motion of cytoskeletal filaments propelled by motors fixed on a surface: if the motors generate force independently, the diffusion coefficient will be inversely proportional to the filament length. Noda extitet al. [2] measured the diffusion coefficient of actin filaments sliding over myosin filaments driven by myosin motors in the latter filaments. They found that the diffusion coefficient is almost independent of the actin length, and suggested that the force generation by myosin motors is cooperative. However, this experimental result has not seem to be successfully explained by theory [3]. In this work, we analyze the diffusion coefficient of sliding filaments by using simple models such as the one proposed by Duke [4] for motor proteins. It is found that there is a range of filament length over which the diffusion coefficient does not vary much with the filament length and that this range tends to be larger if motors work cooperatively. If the experimental condition in Ref. [2] happened to lie in this range, our theory predicts that experiments with longer actin filaments or lower ATP concentrations will reveal a clear dependence of the diffusion coefficient on the actin length. [1] K. Sekimoto and K. Tawada, Biophys. Chem. extbf89, 95 (2001). [2] N. Noda extitet al., Biophysics extbf1, 45 (2005). [3] Y. Imafuku extitet al., J. Phys. Chem. B extbf112, 1487 (2008). [4] T. A. J. Duke, Proc. Natl. Acad. Sci. USA, extbf96, 2770 (1999).

*Poster

Information and power stroke in molecular motors

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Molecular motors convert chemical energy directly into mechanical work and impress with high efficiencies in an environment that is dominated by strong fluctuations. We address the question if the usage of information can be the basis for these high efficiencies. Two main mechanisms for translational motors are commonly being discussed: first, the power stroke mechanism, where the ATP consumption is thought to lead to a strong conformational change of the protein, pushing the motor actively forward [1]. Second, a rectification process of thermal fluctuations through feedback, which can extract energy from the thermal bath at the expense of information processing. The latter is sometimes referred to as a ?Feedback Brownian ratchet? [2]. We have developed a generic theoretical model that can describe both mechanisms and their interaction. We include Shannon entropy estimators in our definition of efficiency and we find that for certain step lengths the highest efficiency can be achieved by a combination of power stroke and rectification process. The model consists of a particle diffusing freely in a piecewise linear potential coupled to a feedback control system. Depending on the particles position, potential barriers are set up at specific predetermined positions. Both the positions and shape of the barriers can be varied. Thus the model allows to gradually explore the interplay of power stroke and of work extracted from the heat bath using information about the particles position. The system is investigated both analytically and with dynamical Langevin simulations. We conclude that the interplay of power stroke and information leads to maximum efficiency and moreover increases the robustness of the process. [1] J. Howard, Protein power strokes, Curr. Biol. 16 (2006), 517?9 [2] U. Seifert, Stochastic thermodynamics, fluctuation theorems and molecular machines. Reports Prog. Phys. 75 (2012) 126001

*Poster

Enhanced Diffusion of F_1-ATPase in the Presence of ATP and External Torque

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Diffusion coefficient D of a particle subject to a periodic potential V can be enhanced if an external torque N of appropriate magnitude is applied. In other words, function $D(N)$ has a peak at a certain value of N [1]. Recently this phenomenon was observed experimentally in a biomolecule "F_1-ATPase (F_1)" [2]. F_1 consists of a stator and a rotor, which rotates by consuming adenosine triphosphate (ATP). The experiment was performed in the absence of ATP. In this situation, the rotor-stator interaction provides a periodic potential for the rotor. When an external torque was applied to the rotor, the enhancement of the rotational diffusion coefficient $D(N)$ was observed, from which the barrier height of the potential was inferred. The purpose of the present work is to see whether the diffusion enhancement occurs when F_1 rotates spontaneously in the presence of ATP. The hydrolysis of ATP takes place at catalytic sites on the stator, and the structure of the stator changes upon the hydrolysis, which results in a switching of the interaction between the rotor and the stator. This switching causes the rotation of the rotor. We construct a model similar to the previous one [3], in which the potential of the rotor is switched stochastically by the ATP hydrolysis or synthesis. We have solved numerically the Fokker-Planck equation to calculate the rotational diffusion coefficient D as a function of external torque N for various ATP concentrations. It has turned out that the diffusion enhancement occurs even in the presence of ATP and that the peak position of $D(N)$ shifts as the ATP concentration is varied. We have found that the mechanism of the diffusion enhancement in the presence of potential switching differs from the one in the case of a single static potential [4].

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*Poster

Minimal Perceptrons for Memorizing Complex Patterns

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Feedforward neural networks have been investigated to understand learning and memory, as well as applied to numerous practical problems in pattern classification. It is a rule of thumb that more complex tasks require larger networks. However, the design of optimal network architectures for specific tasks is still an unsolved fundamental problem. In this study, we consider three-layered neural networks for memorizing binary patterns. We developed a new complexity measure of binary patterns, and estimated the minimal network size for memorizing them as a function of their complexity. We formulated the minimal network size for regular, random, and complex patterns. In particular, the minimal size for complex patterns, which are neither ordered nor disordered, was predicted by measuring their Hamming distances from known ordered patterns. Our predictions agreed with simulations based on the back-propagation algorithm.

*Poster

Steady State Thermodynamics in Population Dynamics

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Prediction and control of a population of growing cells are relevant for understanding evolution of microorganisms and for designing effective drug treatment to pathogenic and cancer cells. Methods of statistical physics can contribute to resolving these problems because of a mathematical similarity between statistical physics and population dynamics. The long term expansion rate of population size (population growth) is an important observable in the population dynamics. In a fixed environment, the population growth converges to a stationary growth rate, and can be evaluated mathematically by the largest eigenvalue of the time-evolution operator of the population dynamics by using the Perron-Frobenius theorem. In contrast, in a changing environment, the evaluation of the population growth is a more difficult problem because the higher eigenvalues non-negligibly contribute to the population growth due to disturbance of the convergence by the changing environment. In this study, we extract the contribution of the higher eigenvalues from the population growth and attempt to evaluate it. To be more precise, we decompose the population growth into two parts, the sum of the stationary growth rate for each condition during the environmental change (i.e. the contribution of the largest eigenvalues) and the excess growth generated by the switching of environmental condition (i.e. the contribution of the higher eigenvalues). To evaluate the latter growth (excess growth), we employ the framework of steady state thermodynamics (SST), which is used in nonequilibrium statistical physics. SST was established for understanding a "thermodynamics" of transitions between nonequilibrium steady states (NESS). The core of this theory is a decomposition of total heat during environmental change into housekeeping and excess parts. The housekeeping heat represents the sum of the stationary heat dissipations in each NESS, and the excess heat is the heat generated due to the change of environment. By using this decomposition, Clausius inequality is formulated for the excess heat. Taking into account a mathematical similarity between the SST framework and the calculation of population growth, we can obtain a Clausius inequality for population dynamics, which gives the upper bound of the excess growth. The equality is shown to be achieved in quasistatic environmental changes. We also clarify that this bound can be evaluated by "lineage fitness", which is an experimentally observable quantity. Reference [1] Y. Sughiyama and T. J. Kobayashi, arXiv:1509.06448 (2015). [2] Y. Sughiyama, T. J. Kobayashi, K. Tsumura and K. Aihara, Phys. Rev. E 91, 032120 (2015).

*Poster

Coarse-grained modelling of RNA

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We present a new nucleotide-level coarse-grained model of RNA, oxRNA. The model is designed to reproduce basic structural, mechanical and thermodynamic properties of RNA, and the coarse-graining level aims to retain the relevant physics for duplex formation from single-stranded RNA. The model can be used for efficient simulations of systems with up to thousands of base pairs (on GPU), and for the assembly of systems of up to hundreds of base pairs. We first describe the parametrization of the model a then give examples of its versatility by comparing it to a range of experiments in nanotechnological and biological settings, such as the folding thermodynamics of a pseudoknot, the formation of a kissing loop complex, the unzipping of a hairpin motif, and RNA plectoneme formation at 0.1M salt. We further use the model to study the thermodynamics and kinetics of an RNA toehold- mediated strand displacement reaction, a process during which an invading strand replaces an incumbent strand that was previously bound in a duplex with a complementary strand. Strand displacement is an essential part of nanotechnological applications and is speculated to occur in vivo as well. The source code implementing oxRNA both on CPU and GPU is freely available for public use at dna.physics.ox.ac.uk.

*Poster

How a short double-stranded DNA bends and loops

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The short double-stranded DNA (dsDNA) bending on nanometer scales plays a key role in many cellular processes, as packing on nucleosome, transcription control step and viral genome packing. In a recent experiment using fluorescence microscopy, the dsDNA fragments shorter than 100 base pairs(bp) exhibited the loop probabilities higher than predicted by the worm-like chain (WLC) model[1]. Using an analytical model, we showed that a bending above a critical level initiates nucleation of a thermally induced bubble, which is none other than the previously hypothesized kink[2]. It leads to tremendous enhancement of the cyclization probabilities, in a reasonable agreement with experiment. Related to this, our FRET experiments have shown that a short dsDNA fragment bent to D-geometry has two types of conformations induced by local melting, namely, a kink in the middle and forks at the ends [3]. This phenomenon is corroborated by our Breathing DNA model simulation, which allows us to evaluate the bi-stable free energy landscape for the two conformational states that can thermally interconvert to each other. [1] R. Vafabakhsh and T. Ha, Science 337, 1101(2012). [2] J. Shin, O. Lee and W. Sung, J. Chem. Phys. 142, 155101 (2015). [3] C. Kim, O. Lee, J.-Y. Kim, W. Sung, and N. K. Lee, Angewandte Chemie 127, 1-6 (2015)

*Poster

Cell Motility: Active Gel Coupled To Adhesion Sites.

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The crawling motion is a coordinated action of the cytoskeleton and the adhesion between the cell and the substrate. Most of the theoretical models emphasized the roles played by the cytoskeleton, while experimental probes reported force exerted on the substrate through the adhesion sites. In this model we use a simple one-dimensional active gel coupled to adhesion sites to model the basic physics of cell crawling dynamics. Through the force distribution of the adhesion sites, a multipole analysis is performed and compared to experimental observations.

*Poster

Sequence Hypercycles by Competitive Ligation

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The first life form has presumably developed in the soup of information polymers such as peptides, RNA, DNA, and their analogues. For developing into a highly complex life form, the emergence of molecular species sustaining genetic information is a crucial step. However, no scenario has clearly addressed how information polymers can self-organize into a stable self-replicating species without lapsing into an error catastrophe lacking any order nor a frozen state dominated by the most stable species. Here, we experimentally and numerically explore the templated ligation of DNA strands, which is the simplest and most primitive reaction of information polymers. We find that, by repeated templated ligations, DNA strands inevitably form a precursor of species, a stable and complex nonequilibrium structure replicating its genetic information, under nonequilibrium driving force of temperature cycling, feeding, and diluting. The key concept behind is the cooperative hyper-exponential growth of sequence information caused by the general property of templated ligation that longer strands hybridize more stably than shorter strands. The resultant frequency-dependent selection suppresses the error catastrophe while provides a rich complexity to the sequences by preventing the most stable sequence from dominating the sequence space. As the direct consequences of the frequency-dependent selection, we demonstrate the spontaneous symmetry breaking of sequence information and the coexistence of different species in spatially resolved systems.

*Poster

Signature of Efimov physics in triplex DNA melting properties

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In the quantum Efimov effect, identical bosons form infinitely many bound trimer states at the bound dimer dissociation threshold, with their energy spectrum obeying a universal geometrical scaling law. Inspired by the formal correspondence between the possible trajectories of a quantum particle and the possible conformations of a polymer chain, the existence of a triple-stranded DNA bound state when a double-stranded DNA is not stable can be predicted by means of a scaling argument. Evidence for the latter Efimov-like behavior will be provided by modeling three directed polymer chains both in low-dimensional lattices, by using either renormalization group methods in fractal lattices ($d < 1$) and the transfer matrix technique in euclidean $d = 1$ lattice, and in $d = 3$ euclidean lattice, by means of Monte Carlo simulations. A finite melting temperature for double-stranded DNA requires in d
$le2$ the introduction of a weighting factor penalizing the formation of denaturation bubbles. The details of how bubble weighting is defined for a three-chain system will be shown to crucially affect the presence of Efimov-like behaviour, even in a very narrow temperature range. When Efimov-like behaviour is absent, on the other hand, we discover the presence of a different thermodynamic phase, that we call a mixed state, where the strands are pairwise bound but without three chain contacts. In the presence of Efimov-like behaviour, however, no evidence is found for triple-stranded bound states other than the ground state at the 2-chain melting temperature. Monte-Carlo simulations in $d = 3$ will be shown to hint that Efimov-like DNA behaviour indeed belongs to a novel universality class, different from the quantum Efimov one. The possibility of detecting Efimov-like behaviour for real triple chain DNA will be finally discussed.

*Poster

Exploring Gliding Motility: Model of Helical Transport of Cell Surface Proteins in Flavobacterium Johnsoniae

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Powered by the migration of surface adhesive proteins SprB along a left-handed helical loop on cell surfaces, a Flavobacterium johnsoniae exhibits rapid gliding on a solid surface. In this study we develop a model of rigidly coupled adhesins on a helical loop to study the mechanism of this gliding motility. The model takes into account the helical geometry of the loop and the stochastic binding/unbinding dynamics of SprB. Numerical calculations of our model reproduce the main features of Flavobacterium johnsoniae motion observed in the experiments. Cell body translation along its long axis displays a bidirectional motion via spontaneous symmetry breaking as predicted in a previous simple one-dimensional model. However, this linear movement has a characteristic switching length comparable to cell length due to end effect. As a cell undergoes translation, the cell body rotates counterclockwise about its principle axis when viewed from its rear. Furthermore, SprBs with strong binding at a cell pole naturally introduce an asymmetric force distribution that uplifts the cell body and leads to end-over-end flipping.

*Poster

Tug-of-war between elastically coupled molecular motors

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Intracellular transport is based on molecular motors that pull cargos along cytoskeletal filaments. Many cellular cargos are observed to move bidirectionally, with fast transport in both directions. This behaviour can be understood as a stochastic tug-of-war (ToW) between two teams of antagonistic motors. The original ToW model introduced in [1] was based on two simplifying assumptions: (i) both motors move with the same velocity in the direction of the stronger motor, and (ii) this velocity matching and the associated force balance arise immediately after the rebinding of an unbound motor to the filament. In this study, [2] we extend the ToW model by including an elastic coupling between the antagonistic motors, and by allowing the motors to perform discrete motor steps. Each motor step changes the elastic coupling and generates a force that acts on all motors. Depending on the strength and stability of the motors (characterised by their stall and detachment forces), as well as on the stiffness of the elastic coupling, the motors can perform multiple steps before they reach a state of force balance. In general, the ToW model with elastic coupling is found to generate a lower average force between the motors compared to the original model. The behaviour of the latter model is recovered in the limit of small unbinding rates of the motors. In all cases, we determine the time needed to reach a state of force balance. This time scale becomes larger when the elastic coupling becomes weaker. [1] M. I. J. Müller, S. Klumpp, and R. Lipowsky, PNAS 105, 4609 - 4614 (2008). [2] M. C. Ucar and R. Lipowsky (in preparation).

*Poster

Length-dependence study of the elastic response and secondary structure of single-stranded DNA

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Single-stranded DNA (ssDNA) plays a major role in several biological processes, such as replication or transcription. Therefore, it is of fundamental interest to understand how the elastic response and the formation of secondary structures are modulated by non specific base pairing and the electrostatic interactions. In general,these are non-specific interactions that make the elastic properties of ssDNA more complex than those of double-stranded DNA (dsDNA). Furthermore, its properties have been less well studied than those of dsDNA. Here we study the elastic properties and secondary structure that arise at a low mechanical forces of four ssDNA with different lengths using Optical Tweezers.

*Poster

Mechanical stability of cellular blebs

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Blebs are round protrusions of the plasma membrane used by cells to explore the environment. We present a thorough analysis of a one-dimensional model of a cell as an elastic membrane coupled to a contracting cortex. Our model shows that cellular blebs are not an equilibrium solution of the model. We then simulate a discretized version of the model and present evidence that blebs only arise as a result of non-equilibrium processes, or as unstable mechanical configurations of the membrane.

*Poster

Disorder profile of nebulin encodes a vernier–like position sensor for the sliding thin and thick filaments of the skeletal muscle sarcomere

Ming-Chya Wu * [1], Jeffrey G. Forbes, Kuan Wan

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Nebulin is an about 1μm long intrinsically disordered scaffold for the thin filaments of skeletal muscle sarcomere. It is a multifunctional elastic protein that wraps around actin filament, stabilizes thin filaments and regulates Ca-dependent actomyosin interactions. This study investigates whether the disorder profile of nebulin might encode guidelines for thin and thick filament interactions in the sarcomere of the skeletal muscle. The question was addressed computationally by analyzing the predicted disorder probability of human nebulin (6669 residues, 200 actin-binding repeats) by PONDR and the periodicity of the A-band stripes (reflecting the locations of myosin-associated proteins) in the electron micrographs of the sarcomere. Using the detrended fluctuation analysis, a scale factor for the A-band stripe image data with respect to the nebulin disorder probability was determined to make the thin and thick filaments aligned to have maximum correlation. The empirical mode decomposition method was then applied to identify hidden periodicities in both the nebulin disorder profile and the rescaled A-band data. The decomposition reveals three characteristic length scales (45nm, 100nm and 200nm) that are relevant for correlational analysis. The dynamical cross-correlation analyses with moving windows at various sarcomere lengths depict a vernier-like design for both periodicities, thus enabling nebulin to sense position and fine tune sarcomere overlap. This shows that the disorder profile of scaffolding proteins may encode a guideline for cellular architecture.

*Poster

Accumulation of microswimmers near a surface

Kuan-Ting Wu * [1], Yi-Teng Hsiao, Chia-Chun Chan, Wei-Yen Woon

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Microbial processes including biofilm formation or bio-fouling are ubiquitous and influence human extensively from daily life to various industrial systems. For decades, researchers have been study on the processes and strategies of bacteria accumulation on surfaces. Considering the initial stage of biofilm formation, before the cell adhesion, swimming cells were reported swim along the surface for prolong times. To describe the phenomenon, models of different perspectives of physics had been established, including far and near field hydrodynamic, steric, sedimentation and diffusion effects. To reach a more complete picture of the cell-surface interaction, we manipulated the swimming speed of single polar-flagellated bacteria with strains of pusher, puller and bimodal swimming characteristic. Observing the steady-state bacteria distribution in a microchannel and the distinct bacteria circulating trajectories at a surface among different bacteria strain and speed, contributions of each mechanism can be evaluated. Our results show that the surface entrapment of bacteria is mainly dominated by steric and near-field hydrodynamic effects at low swimming speed and would be wiped out by diffusion effect at high swimming speed.

*Poster

Stem cell self-renewal and lineage aging explains clone size fluctuations in rhesus macaques

Song Xu * [1], Tom Chou

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Virally-tagged hematopoietic stem cells (HSCs) were autologously transplanted in 4 rhesus macaques. The peripheral blood cells were sampled over 14 years and the abundances of tagged clones were measured. Previous analysis of the sampled clone data using a neutral growth model indicated fast establishment of equilibrium of the cumulative clone-size distributions after transplantation. In this work, we explore the highly dynamic fluctuations of the sizes of individual clones. The noisy populations of individual clones, including their apparent extinction and resurrection, can be explained by a refined neutral model with HSC self-renewal and lineage aging. Our model tracks the multi-stage stochastic dynamics of HSCs to mature peripheral blood and provides estimates for the HSC self-renewal patterns and differentiation rates.

*Poster

Dynamical Crossover of Clone Size Statistics in a Stochastic Model of Cell Fate Decision

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Recently, experimental and theoretical studies have revealed the universal behavior of the asymptotic statistics in cell fate decision in biological tissues [1]. We here perform a statistical-mechanical study of the asymptotic behaviors of stochastic cell fate decision between proliferation and differentiation [2]. We propose a model based on a self-replicating Langevin system, where cells choose their fate (i.e., proliferation or differentiation) depending on the local cell density. A crucial point of our model is the self-organized criticality, which ensures the tissue homeostasis as a consequence of cell-cell interaction. Furthermore, we numerically demonstrate that the asymptotic clonal analysis exhibits the dynamical crossover of clone size statistics. Our results bridge the missing link between previous models, and provide a unified view on the roles of the spatial and time scales of interaction between cells in general tissue homeostasis. Previously, tissue homeostasis has been theoretically studied by two simple nonequilibrium stochastic models, which are known as the critical birth-death process (CBD) and the voter model (VM). These models have successfully explained the observed behavior of the asymptotic clone size statistics [2]. However, these simple models require the fine-tuning of parameters, which is crucial to explain the experimental results. In addition, the relation between CBD and VM has been unclear, because VM is defined on a lattice, while CBD does not have any spatial structure. In order to overcome these problems, we propose a novel model of cell fate decision, where the local cell density affects cell fate decision. The attractive fixed point of the local growth rate gives rise to self-organized criticality, which ensures the tissue homeostasis. Our numerical results have revealed that the CBD/VM statistics is reproduced when the length scale of cell-cell interaction range is sufficiently large/small, respectively. In other words, the previous models are unified in terms of the interaction range. The dynamical crossover suggests that the interaction range in actual biological tissues is possibly estimated by the experimental data. [1] E. Clayton et. al., Nature 446, 185 (2007); A. M. Klein et. al., Cell Stem Cell 7, 214 (2010); A. M. Klein and B. D. Simons, Development 138, 3103 (2011). [2] H. Yamaguchi, K. Kawaguchi, and T. Sagawa, in preparation (2016).

*Poster

Impact of Cell Motility and Cell-Cell Junction Penetration on Trans-endothelial Migration of Cancer Cells

Hsiao Yi-Teng * [1], Hsiang-Ying Chen, Shu-Chen Liu, Wei-Yen Woon, Lin I

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Trans-endothelial migration of cancer cells is a vital process in cancer metastasis. Previous studies revealed that immune cells tend to be navigated by mechanical stiffness on endothelium layer, moving from cell centers toward cell edges, before penetrating through the endothelium layer by breaking the cell-cell junctions. It is therefore intriguing to study whether the cancer cell exhibit the similar process, and the respective roles played by cell navigation, junction penetration, and junction breaking-healing, in trans-endothelial migration process. In this work, we report in-situ observation on the spatio-temporal dynamics of trans-endothelial migration of two types of cancer cells, wild type BM1, and mutant BM1. Comparing with the former, the latter has lower 2D cell motility but higher penetration ability. It is found that, similar to immune cells, both types of cancer cells tend to move toward the junction of the endothelium cells before trans-endothelium migration. Although the wild type cancer cell is able to more quickly move to the cell-cell junctions than the mutant cancer cell, the trans-endothelial rate is fluctuating due to competition between junction breaking and reconstruction during the penetration processes. On the other hand, the mutant cancer cell shows a higher averaged trans-endothelial rate with lower fluctuation despite its lower 2D cell mobility.

*Poster

Kinetic Transition Network Based on Trajectory Mapping

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[1] University of Chinese Academy of Sciences – China

The understanding of biomolecular systems can be greatly improved by constructing conformational transition networks. Trajectory mapping (TM) method could naturally detect metastable states of biomolecules and construct the hierarchical kinetic transition networks. In TM, multiple simulation trajectories are mapped to high-dimensional vectors, and the interrelation between these trajectory-mapped vectors is analyzed to locate metastable states. Meanwhile, we can get a set of slow variables. Kinetic information can be quantitatively extracted through simple algebraic manipulations of the identified metastable states. The slow variables could be used for enhance sampling methods, such as Metadynamics, to improve sampling speed. We apply TM method to two peptides in implicit solvent - 6-residue -hairpin peptide, 35-residue-fragment (HP-35) villin headpiece - to assess its ability to generate physically meaningful states and faithful kinetic models.

*Poster

Topic 6: Soft matter-Posters

Electrostatic Attraction between Overall Neutral Surfaces

Ram Adar * [1], David Andelman, Haim Diamant

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When solid surfaces are immersed in aqueous solutions, some of their charges can dissociate, and in numerous experimental set-ups, they leave behind charged patches. When the surfaces are overall neutral, the nature of the surface charge distribution is crucial in determining the inter-surface interaction. Experiments have been conducted on such systems, where the surface charge was quenched and distributed in the form of patches. A long range attraction was observed, but it remains unexplained by van der Waals interactions between the two surfaces or by Debye-Hückel theory for ionic solutions. In the present work, we calculate the osmotic pressure in such systems within the Poisson-Boltzmann framework. The osmotic pressure changes with the charge density and the inter-surface separation, but a new important quantity emerges – the charged-patch size. We show that even for relatively weakly charged and finite-size patches, the pressure profile as function of inter-plate separation has a complex behavior. In particular, we derive an expression for the crossover between repulsion and attraction.

*Poster

Dynamics of Camphoric Acid Boat at the Air-Water Interface

V Sathish Akella * [1], Dhiraj K Singh, Mahesh M. Bandi, Ravi K Singh, Shreyas Mandre

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We experimentally study the dynamics of camphoric acid loaded agarose gel tablets (cboats) at the air-water interface. When placed at the air-water interface and let go, a cboat is spontaneously set in motion by the interfacial tension gradients. We explain the cboat dynamics in terms of a dimensionless quantity $\xi = \frac{\Delta\sigma\ a}{\rho\ u^2\ a^2}$, where $\Delta\sigma\ a$ is the interfacial tension force acting along a characteristic length a of cboat; $\rho\ u^2\ a^2$ is the drag force experienced by the cboat. By definition, $\xi = 1$ when the interfacial tension force and drag force are equal and the cboat moves with terminal velocity. We show three distinct modes, viz. harmonic, steady, and periodic cboat motion arise for $\xi > 1$, $\xi \sim 1$ and $\xi < 1$ respectively by varying the air-water interfacial tension.

*Poster

Crack propagation in two-dimensional viscoelastic networks

Yuko Aoyanagi * [1], Ko Okumura

[1] Ochanomizu University – Japan

We study the speed of crack propagation in a simple two-dimensional viscoelastic network model by numerical calculations. In the simulation, we prepare a stretched network with an initial strain and introduce a line crack. As a result we confirm that the crack propagation proceeds with a constant speed in the network model. We find a scaling regime in the relation between the crack propagation speed and energy release rate, where the rate is revealed to possess lower and upper bounds in a clear manner. Near the lower bound, the propagation speed is slow and the crack shape looks parabolic. Near the upper bound, the propagation speed is high and the crack shape becomes sharp. The lower bound is suggested to be governed by the internal structure of the material and this fact may be useful as a guiding principle for toughening the material.

*Poster

Cooperative strings and glassy interface

Maxence Arutkin * [1], M. Arutkin, J. Salez, K. Dalnoki-Veress, E. Raphaël, J. A. Forrest, T. Salez

[1] ESPCI ParisTech – France

We introduce a minimal theory of glass formation based on the ideas of molecular crowding and resultant string-like cooperative rearrangement, and address the effects of interfaces in various geometries. In the bulk case, we obtain a scaling expression for the number of particles taking part in cooperative strings, and we recover the Adam-Gibbs description of glassy dynamics. Then, by including thermal dilatation, the Vogel-Fulcher-Tammann relation is derived. Moreover, the random and string-like characters of the cooperative rearrangement allow us to predict a temperature-dependent expression for the cooperative length of bulk relaxation. Finally, we explore the influence of sample boundaries in various geometries where the system size becomes comparable to the bulk cooperative length. The theory is in agreement with measurements of the glass-transition temperature Tg in confined polymeric systems, and allows to quantify the temperature- dependent thickness of the interfacial mobile layer.

*Poster

Shocks and turbulence in active and chiral fluids with odd viscosity

Debarghya Banerjee * [1], Anton Souslov, Benjamin C. Van Zuiden, Vincenzo Vitelli

[1] Lorentz Institute for theoretical physics – Netherlands

In this talk we investigate the compressible hydrodynamics of active fluids composed of active rotors or chiral particles at finite temperature. The hydrodynamics of these systems contains an odd viscosity generated by breaking time reversal or parity. We illustrate the consequences of the odd viscosity, originally observed in quantum Hall fluids, on the formation of shocks and turbulence in a simplified model based on Burgers equation.

*Poster

Electro-Osmotic And Droplet Electrophoresis Phenomena In Bicomponent Fluid

Andrei Bazarenko * [1], Marcello Sega

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The electro-osmotic flow and the Droplet Electrophoresis are two phenomena relying on the action of an external electric field on solvated counter ions, which are used to transport fluids in microfluidic devices. Interestingly, both phenomena can be seen as two extreme cases of the same physical model, where the solvation free energy of the counter ions is the control parameter of a continuous transition between the electro-osmotic and the electrophoretic cases. In this study we investigate numerically, how several physical properties change during this transition, by solving the coupled equations of motion of the counter ions in interaction with a continuous model of the flow. The system is modelled by coupling the Langevin equation of motion of off-lattice, point-like counter ions (interacting through the full, long range electrostatics) with an on-lattice description of a bicomponent fluid, simulated using the Shan-Chen model. The presence of explicit ions allows us to go beyond the simple Poisson-Boltzmann approximations, and investigate a variety of flow regimes.

*Poster

Bundle formation in parallel aligned polymers with competing interactions

Panayotis Benetatos * [1], Sandipan Dutta, YongSeok Jho

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Supramolecular assemblies of polymers are commonly observed in soft and biological matter. The main elements of these assemblies in the latter are charged semiflexible polymers (polyelectrolytes) generally interacting via a long(er)-range repulsion and a short(er)-range attraction. The most common supramolecular structure formed by these polymers is the bundle. In this talk, we present a general mechanism of bundle formation as the breaking of the translational invariance in parallel aligned polymers with competing interactions. We derive a criterion for finite-size bundle formation as well as for macroscopic phase separation (formation of infinite bundles).

PB and Y. S. Jho, Bundling in semiflexible polymers: A theoretical overview, Advances in Colloid and Interface Science, (2016), in press

S. Dutta, PB and Y. S. Jho, Bundle formation in parallel aligned polymers with competing interactions, submitted to EPL (arXiv:1511.03795)

*Poster

Liquid-solid-like phase transition in a 2D granular gas with magnetic dipolar interactions.

Michael Berhanu * [1], Gustavo Castillo, Eric Falcon, Simon Merminod

[1] MSC, CNRS, University Paris Diderot – France

We consider a quasi-2D system of macroscopic particles with tunable repulsive dipolar interactions controlled by an external magnetic field. In this out-equilibrium system, kinetic energy is provided by a continuous mechanical shaking. By increasing the magnetic field, the repulsive interaction strength between particles is increased. For sufficiently high ratio between magnetic interaction potential energy of particles and their kinetic energy, the system transits from a dissipative granular gas to a hexagonal crystal [Merminod2014]. Similarly to the method evidencing a critical solid-liquid-like phase transition in a dense vibrated granular layer [Castillo2012,Castillo2015], we analyze the transition from a disordered granular gas to a solid-like hexagonal phase by studying in the spatial Fourier space, first the static structure factor and the 6-fold bond-orientational order parameter. Results are compared with the insights of the KTNHY theory describing the 2D-melting of a hexagonal crystal. Then, by extracting the longitudinal and transverse current correlations in dynamical regime, the spectrum of excitations can be measured. Dispersion relations are obtained, showing longitudinal wave propagation in the two phase and transverse wave propagation in the solid-like phase only. The corresponding " sound " velocity is found to increase with the applied magnetic field, as system rigidity augments. [Merminod2014] Simon Merminod, Michael Berhanu, and Eric Falcon. Transition from a dissipative to a quasi-elastic system of particles with tunable repulsive interactions. EPL, 106, 44005 (2014) [Castillo2012] Gustavo Castillo, Nicolás Mujica, and Rodrigo Soto. Fluctuations and Criticality of a Granular Solid-Liquid-Like Phase Transition. Physical Review Letters, 109(9), (2012) [Castillo2015] Gustavo Castillo, Nicolás Mujica, and Rodrigo Soto. Universality and criticality of a second-order granular solid-liquid-like phase transition. Physical Review E, 91, (2015)

*Poster

Molecular Dynamics characterization of line tension through intrusion in hydrophobic nanopores

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Fluid dynamics at the nanoscale involves physical phenomena that are usually neglected at the micro and macro scales. Many studies have focused on the solid-liquid boundary conditions that may diverge from the classical no-slip assumption. Our work is dedicated to the understanding and measurement of the triple line, limiting solid liquid and vapour phases. Its physics partly governed by line tension, a parameter that measures the triple line contribution to the free energy. A great discrepancy exists between experimental results. Measured line tension values diverge by six orders of magnitude and its sign may be positive or negative. Molecular dynamics may provide a precise insight to help understanding the possible mechanisms at stake in the triple line region. Some simulations have already measured the line tension coefficient. We propose a new simulation method that makes it possible to measure the line tension without using the usual shape regression method. To do so we control the intrusion of a non-wetting fluid in an ideal conical geometry using a piston. The pressure with respect to volume curve is a direct consequence of the various contributions to the free energy, including line tension. Knowing precisely the volume and surface parameters of our system, we can deduce the mechanical properties of the triple line.

*Poster

Kinetics of Fluid Demixing in Complex Plasmas: Domain Growth Analysis using Minkowski Tensors

Alexander Boebel * [1], Christoph Raeth

[1] DLR (German Aerospace Center) – Germany

The demixing process of a binary complex plasma, in particular its onset, is analysed and the role of distinct interaction potentials is discussed by using morphological Minkowski tensor analysis of the minority phase domain growth in a demixing simulated binary complex plasma. These Minkowski tensor methods are compared with previous results that utilized a power spectrum method based on the time-dependent average structure factor. It is shown that the Minkowski tensor methods are superior to the previously used power spectrum method in the sense of higher sensitivity to changes in domain size. It is found that increasing the tensor rank of the Minkowski methods from rank one to rank two and four results in ever decreasing sensitivity. However even the rank 4 Minkowski tensor method performs better in terms of sensitivity compared to the previously used power spectrum methods. By analysis of the slope of the temporal evolution of Minkowski tensor measures qualitative differences between the case of particle interaction with a single length scale compared to particle interactions with two different length scales (dominating long range interaction) are revealed: In the case of different length scales the slope grows fast until it reaches its maximal value and then decays whereas for a single length scale no decay is observed. After proper scaling the graphs for the two length scale scenario coincide, pointing towards universal behaviour. These differences are evidenced by distinct demixing behaviour: In the long range dominated cases demixing occurs in two stages. At first neighbouring particles agglomerate then domains start to merge in cascades. However in the case of only one interaction length scale only agglomeration but no merging of domains can be observed. Thus, Minkowski Tensor analysis are likely to become a useful tool for further investigation of this (and other) demixing processes. It is capable to reveal (nonlinear) local topological properties, probing deeper than (linear) global power spectrum analysis, however stillproviding easily interpretable results founded on a solid mathematical framework.

*Poster

Crystallization of self-propelled discs : a new scenario

Guillaume Briand * [1], Michael Schindler, Olivier Dauchot

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We experimentally study the crystallization of a monolayer of vibrated disks with a built-in polar asymmetry, a model system of active liquids, and contrast it with that of vibrated isotropic disks. Increasing the packing fraction, the quasi-continuous crystallization reported for isotropic discs is replaced by a new scenario, where domains of close-packed discs coexist with liquid regions. In the coexistence regime, the dynamics is highly intermittent and heterogeneous : crystalline domains advected by the active liquid, spontaneously break, merge and melt leading to a full decoupling of the dynamics from the static structure. The relaxation time of the crystalline structure being longer than the characteristic lifetime of the crystalline domains, it is not even clear that the concept of crystalline phase remains valid. This state of affair remains up to the highest possible packing fraction questioning the stability of the crystal for active discs, unless at ordered close packing.

*Poster

Modeling of Droplet Evaporation on Superhydrophobic Surfaces

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[1] Universidade Federal do Rio Grande do Sul – Brazil

When a drop of water is placed on a rough surface, there are two possible extreme regimes of wetting: the one called Cassie Baxter (CB) with air pockets trapped underneath the droplet and the one called the Wenzel (W) state characterized by the homogeneous wetting of the surface. A way to investigate the transition between these two states is by means of evaporation experiments, in which the droplet starts in a CB state and, as its volume decreases, penetrates the surface's grooves, reaching a W state. Here we present a theoretical model based on the global interfacial energies for CB and W states that allows us to predict the thermodynamic wetting state of the droplet for a given volume and surface texture. We first analyze the influence of the surface geometric parameters on the droplet's final wetting state with constant volume and show that it depends strongly on the surface texture. We then vary the volume of the droplet, keeping the geometric surface parameters fixed to mimic evaporation and show that the drop experiences a transition from the CB to the W state when its volume reduces, as observed in experiments. To investigate the dependency of the wetting state on the initial state of the droplet, we implement a cellular Potts model in three dimensions. Simulations show very good agreement with theory when the initial state is W, but it disagrees when the droplet is initialized in a CB state, in accordance with previous observations which show that the CB state is metastable in many cases. Both simulations and the theoretical model can be modified to study other types of surfaces.

*Poster

Determination of Anharmonic Free Energy Contributions: Low Temperature Phases of the Lennard-Jones System

Carles Calero * [1], H. Eugene Stanley, Giancarlo Franzese

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The knowledge of the free energy is fundamental to determine the relative stability of the different phases in thermodynamic equilibrium. In particular, a versatile method to calculate the free energies is needed to ascertain the equilibrium phases of colloidal crystals, which can exhibit different interaction potentials. In this contribution, we investigate a general method to calculate the free energy of crystalline solids by considering the harmonic approximation and quasistatically switching the anharmonic contribution. The advantage of this method is that the harmonic approximation provides an already very accurate estimate of the free energy, and therefore the anharmonic term is numerically small and can be determined to high accuracy. Additionally, we show that the anharmonic contribution to the free energy satisfies a number of exact inequalities that place constraints on its magnitude and allows approximate but fast and accurate estimates. We use the method to calculate the low temperature phase diagram for Lennard-Jones particles. We demonstrate that hcp is the equilibrium phase at low temperature and pressure and obtain the coexistence curve with the fcc phase, which exhibits reentrant behavior.

*Poster

Dynamic self-assembly of non-Brownian spheres studied by molecular dynamics simulations

Osvaldo Carvente * [1], M. Salazar-Cruz, F. Peñuñuri, J.C. Ruiz-Suárez

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Granular self-assembly of confined non-Brownian spheres under gravity is studied by molecular dynamics simulations. Starting from a disordered phase, dry or cohesive spheres organize, by vibrational annealing, into body-centered-tetragonal or face-centered-cubic structures, respectively. During the self-assembling process, isothermal and isodense points are observed. The existence of such points indicates that both granular temperature and packing fraction undergo an inversion process that may be in the core of crystal nucleation. Around the isothermal point, a sudden growth of granular clusters having the maximum coordination number takes place, indicating the outcome of a first-order phase transition. We propose a heuristic equation that successfully describes the dynamic evolution of the local packing fraction in terms of the local granular temperature, along the entire crystallization process.

*Poster

The Manning Transition Revisited

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A system of a charged cylinder in the presence of oppositely charged counterions shows binding-unbinding transition of counterions to the charged cylinder. This critical phenomenon, known as the Manning condensation transition, demonstrates different properties depending on the strength of electrostatic interaction. As the system becomes charged more highly, the coupling between counterions and the charged cylinder becomes strong and the correlation of counterions becomes significant. For an extensive range of the strength of electrostatic interaction, we examine its equilibrium states, performing Monte Carlo simulation and analytic calculation. Using various thermodynamic quantities, we determine the phase boundaries between states and also discuss underlying mechanism and criticality.

*Poster

Packing and Self-Assembly of Hard Spheres in Cylinders

Patrick Charbonneau * [1], Lin Fu, William Steinhardt, Joshua E. S. Socolar

[1] Duke University – United States

Hard spheres in a cylinder capture the essence of soft matter systems as varied as fullerenes in nanotubes and colloidal-wire formation. Here, we consider both the packing and self-assembly of this model. Finding the densest configurations of hard spheres of diameter σ in a cylinder of diameter D is a geometric problem that grows increasingly complex with D/σ. By adapting the Torquato-Jiao sequential-linear-programming approach, we have identified 17 new structures– almost all of them chiral–between $D \approx 2.85$ and $D = 4.00\sigma$. This regime is especially challenging to study because most of the structures have an outer shell and an inner core that compete for close packing. In some cases the shell adopts its own maximum density configuration and the core spheres stack one another independently, resulting in quasiperiodic packings; in other cases interplay between the two shells gives rise to the formation of relatively simple periodic packings. Interestingly, only some of these structures can be easily assembled by compression. Although the system formally does not display long-range order at finite pressures, compressing the system to its densest packing is not always smooth. Comparing the growing static order with the system self-assembly reveals the complex process through order here develops.

*Poster

Phase ordering kinetics in two- and three-dimensional disordered XY model.

Swarnajit Chatterjee * [1]

[1] Indian Association for the Cultivation of Science – India

Effect of immobile random impurities on a system with continuous order parameter is non-monotonous and is of practical significance. In magnetic systems, long-range or quasi long-range order (QLRO) of the magnetic spins gets affected due to the torques applied to individual spins by randomly distributed static local fields. XY model exhibit quasi-long range ordering that arises due to the presence of stable topological defects (vortices and anti-vortices). Transition from a QLRO to a disordered state, is characterized by vortex-antivortex pair unbinding occurring Berezinskii-Kosterlitz-Thouless (KT) temperature. In this work, we present comprehensive Monte Carlo (MC) simulation study of the BKT transition temperatures and the coarsening dynamics with non-conserved Glauber kinetics of the two- and three dimensional classical random bond XY model (RBXY). We characterize the ordering kinetics of these systems by studying the evolution of the domain lengths R(t) extracted from equal time spatial correlation function C(r;t) and structure factor S(k;t). The nature of two-time autocorrelation function C (t;tw) has also been investigated. We find that the critical temperatures as well as the growth exponents of the respective models gradually decrease with the increase of disorder amplitude. Dynamical scaling is maintained for both the models. Growth exponents (n) in two-dimension show evidence of a crossover from a 'power-law growth with disorder-dependent exponent' to an asymptotic regime with 'logarithmic growth'. Scaling arguments, accounting the energy barrier due to quenched disorder, supports logarithmic exponent and predict behavior as functions of temperature and disorder amplitude. References: [1] Y. Imry and S. K. Ma, Phys. Rev. Lett. 35, 1399 (1975). [2] J. M. Kosterlitz and D. J. Thouless, J. Phys. C: Solid State Phys. 6, 1181 (1973). [3] A. J. Bray, Advances in Physics 43, 357 (1994). [4] A. J. Bray and A. D. Rutenberg, Phys. Rev. E 49, R27 (1994). [5] R. Paul, S. Puri, and H. Rieger, Europhys. Lett. 68, 881 (2004).

*Poster

Enhanced Transport of DNA in More Crowded Environment

Yeng-Long Chen * [1], Fan-Tso Chien Po-Keng Lin Wei Chien

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We observed enhanced transport of DNA molecules in more crowded nanoslit micropost arrays, contrary to the expectation of slower diffusion in more crowded environments. The nanofabricated post arrays are weakly attractive and emulate crowded interactive environments, resulting in weak DNA adsorption. The coupling between DNA diffusion with adsorption to the microposts results in increased mobility with increasing post density, in contrast to studies of decreased DNA/protein mobility in dense gels. Hidden Markov analysis was employed to identify the apparent free energy barriers, which is in agreement with theoretical estimates of based on polymer conformation fluctuations between posts. We also performed Langevin dynamics simulations of macromolecular transport in micropost arrays to verify the enhanced diffusion in denser arrays. Faster DNA diffusion and hopping in crowded systems have important implications for biological systems and for technological applications such as macromolecule purification, and targeted drug delivery.

*Poster

The computer simulations of state-rate dependence of granular materials under shear

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We have performed computer simulations of three-dimensional granular system under shear condi- tions with zero gravity. The granular materials are conned by two plates, the top plate is subjected to a stable normal force and driven by a constant velocity. The results show that there are dramatic changes for the friction force at transition points. At the same time, the top plate will vibrate in z direction. To understand the mesoscopic structural and dynamical properties of state-rate depen- dence behavior of granular materials, we treat the granular system as a weighted network in which the granular particles are nodes and the contact forces are weighted edges. We nd that the time dependence of the friction force and the vibration of top plate are highly correlated with communitystructures of granular system by community detection.

*Poster

Fluctuating clouds of counter-ions around polyelectrolytes

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Significant progress have been made to understand the ubiquitous tendency of charged biological macromolecules, such as DNA and proteins, but an accepted theoretical framework has been slow to develop due to the complex coupling between the conformation of the polyelectrolyte chain and the association of the ionic species in solution. Specifically, the existence of a diffuse ?polarizable? cloud of counter-ions around polyelectrolytes, in addition to the condensed counter-ions, is an effect with significant potential implications for polyelectrolyte self-assembly, as argued by Kirkwood and coworkers, as well as, later researchers. To probe this old and complex problem, we use molecular dynamics simulations that include both salt and an explicit solvent. We focus on the influence of counter-ion valency on the flexibility of highly charged flexible polymer chains and on the variation of molecular topology (e.g., spheres, linear chains, stars, and unknotted and trefoil rings) since molecular topology influence the average molecular shape and segmental density and chain topology should then affect the coupling between chain conformation and the counter-ion distribution. In particular, we find that the counter-ions are distributed in a non-uniform fashion on the polyelectrolyte backbone, forming dynamic clusters whose form and average size is sensitive to molecular architecture. In addition, we find that the residual bound counter-ions, not located in either the interfacial layer or bulk solution, form a diffuse ionic cloud around the polyelectrolyte due to the residual unscreened polyelectrolyte charge along the backbone. The diffuse counter-ion spatial extent is strongly influenced by charge valence, but in the case of monovalent counter-ions we find that the size of the diffuse counter-ion cloud nearly coincides with the polyelectrolyte radius of gyration, independent of molecular topology. Finally, we demonstrate that the charge fluctuations strongly correlate with the molecular fluctuations at short distances, but at larger distances (around the size of radius of gyration) the charge fluctuations strongly anti-correlate. These findings provide a foundation for understanding the general trends of polyelectrolyte self-assembly in solution.

*Poster

Membrane-mediated interactions between nano-objects

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The interaction induced by lipid membranes between included molecules and other nano-objects is of fundamental interest (from the point of view of soft matter physics) and relevant to understanding the activity of important biological molecules, but it has only recently been measured quantitatively. In order to model it, we revisited the standard continuum elastic model, showing that new terms must be added, and we calculated by means of a multipolar expansion the resulting pairwise interaction between two membrane inclusions with hydrophobic mismatch. Fitting the experimental results yields precise values for some material parameters, including the elusive and much debated angular anchoring term. Systematic experiments on several membrane systems in various conditions are in progress.

*Poster

Relaxation process of a sandpile shape caused by vibration

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It is known well that a sandpile loses its shape when an external perturbation is applied. Although this sandpile-relaxation phenomenon is a very fundamental feature of granular matter, the mechanism has been poorly understood. In order to explain the relaxation process of a sandpile due to vibration, Jaeger et al. (1989) have proposed the model based on the idea of electrical conduction. However, its applicability has not been investigated well by systematic experiments. Thus, with the aim of understanding the sandpile-relaxation process, systematic experiments are performed and corresponding models are considered accordingly. As an approach to this issue, we follow the report that surface terrain of a rocky planet covered with a granular layer is relaxed by strong vibration induced by meteorite impacts, the process of which follows the diffusion equation (Richardson et al, 2004). In this study, to clarify whether the relaxation of a sandpile can be described by the diffusion process as well, the following experiment and analysis have been conducted: - A sandpile with the angle of repose is built, then vertical vibration is applied to it. - During the vibration, the surface profile is taken by the high-speed laser profiler. - Obtained data are compared to the numerical solution of the diffusion equation. - The parameter dependences of the diffusion coefficient are revealed. As a result, we found that the relaxation of a sandpile is consistent with the diffusion process, and the diffusion coefficient is proportional to the hopping velocity, which is defined as the velocity at the moment that the acceleration level of the vibration exceeds the gravitational acceleration. It should be noted that the vibration strength might determine which model is applicable, Jaeger et al. (1989) or Richardson et al. (2004). In the presentation, we only focus on the vibration range in which the diffusion model of Richardson et al. (2004) can be applied. Reference Jaeger, H. M., Liu, C., and Nagel, S. R., Phys. Rev. Lett 62, 40 (1989) Richardson, J. M., Melosh, H. J., and Greenberg, R., Science 306, 1526 (2004)

*Poster

Nonlocal constitutive equations for shear flow of strongly inhomogeneous fluids

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We present new theoretical expressions for the density, strain rate and shear pressure profiles in strongly inhomogeneous fluids undergoing steady shear flow with periodic boundary conditions. The expressions that we obtain take the form of truncated functional expansions, where the independent variables are the spatially varying longitudinal and transverse forces that we apply in non-equilibrium molecular dynamics simulations. We conduct non-equilibrium molecular dynamics simulations to calculate all of the response functions needed to describe the response of the system for weak shear flow in the presence of strong density inhomogeneity up to the third order in the functional expansion. These response functions are then substituted directly into the truncated functional expansions and used to predict the density, velocity and shear pressure profiles. The results are compared to the directly evaluated profiles from molecular dynamics simulations and we find that the predicted profiles from the functional expansions give excellent agreement with the directly computed density, velocity and shear pressure profiles.

*Poster

Density Induced Phases in Active Nematic

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We introduce a lattice model for two-dimensional active nematic, composed of a large number of self-propelled apolar active particles, and study the order-disorder transition with the variation in density. Each particle, depending on its orientation, moves anisotropically to unoccupied nearest neighbour lattice sites. They interact with their nearest neighbours within the framework of the Lebwohl- Lasher model. At a density lower than the equilibrium isotropic-nematic transition density, the active nematic shows a first order transition from a disordered isotropic state to a banded state, where particles get clustered and aligned. The banded state extends over a range of density, and the scalar order parameter shows a plateau like behaviour, similar to the frustrated magnetic systems. In the large density limit, the active nematic shows a bistable behaviour between a homogeneous globally ordered state and an inhomogeneous state with local ordering. Reference: R. Das, M. Kumar and S. Mishra, arXiv:1509.05166 (2015)

*Poster

Arrested Phase Separation in Biphasic Active Fluids

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Coarse grained models for active fluids have become increasingly popular over recent years due to their ability to reproduce many features of dense suspensions of motile organisms, or other biological material (e.g. actomyosin). These models usually combine the dynamical equations for an orientational order parameter of its components - drawing from nematodynamics theory - coupled to the hydrodynamics of the fluid in which they are suspended. Activity is introduced as a non-thermal stress contribution in the equations for momentum. In recent works[1], extensile/contractile activity has been shown to cause an effective alignment of the orientational order along/perpendicular to fluid interfaces in biphasic systems. In our work, we quantitatively characterise the effect of this 'active anchoring', and find striking evidence that the aligning effect influences the coarsening of domains in mixtures of passive and active fluids: the competition between the surface tension and the 'active anchoring' W leads to either complete phase separation when the former prevails, or to a bicontinuous phase characterised by a finite length scale when the active anchoring is stronger. We characterised this transition with an "active capillary number" defined as the ratio between interfacial tension and aligning forces. We believe that this phenomenon is a general feature of active biphasic fluids, as its existence relies principally the presence of activity and surface tension. [1] Biphasic, Lyotropic, Active Nematics. Matthew L. Blow, Sumesh P. Thampi, and Julia M. Yeomans. Phys. Rev. Lett. 113, 248303

*Poster

Multiscale Stick-Slip instability during adhesive tape peeling

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We present an experimental study of the peeling of an adhesive tape at a constant velocity. In a given range of imposed peeling velocity, the detachment front displays a jerky dynamic, alternating periodically fast and slow phases, characteristic of a Stick-Slip instability. Recent studies have evidenced the crucial role of the peeling angle [1] and the ribbon inertia [2] on such unstable motion, as well as its multi-scale nature [3,4]. Indeed, during the fast phase ("Slip") of the stick-slip cycles, a secondary stick-slip instability has been observed involving significantly smaller temporal and spatial scales. We pursue those recent studies in the present experimental work. Using an high speed camera, we follow the unstable propagation of the detachment front of an adhesive tape, peeled from a flat surface at a constant velocity. On one hand, we provide a detailed characterization of the multi-scale stick slip instability - amplitudes and durations of the slow and fast phases - as a function of the peeling velocity, peeling angle and peeled tape length. On the other hand, we focus on the onset of the instability. We could indeed observe a quasi-periodic oscillatory peeling front motion occurring at the transition between the regular and the Stick-Slip peeling dynamics. Such oscillatory peeling front motion can be explained by considering inertial effects modeled recently [2].

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*Poster

Bayesian Optimization of Dissipative Coarse-Grained Models for Molecular Simulations

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Simulations of the molecular dynamics (MD) with atomic resolution can yield relatively accurate results. However, when dynamics is slow (polymers, ionic liquids,...) or for big systems (micelles), the computational cost rapidly becomes prohibitive. Coarse-grained (CG) models are an appealing alternative because they allow for both reducing the number of degrees of freedom and increasing the simulation time step. The challenge is thus to develop as faithful coarse grained representations of the atomic systems as possible. The eliminated degrees of freedom can be taken into account using random and dissipative interactions. We introduce a new method [1] for parameterizing dissipative CG models by maximizing the likelihood to reproduce a high resolution reference MD trajectory. The method yields both conservative and dissipative model parameters. A practical, analytical expression of the optimal parameters can be obtained for simple CG models. Single-bead pentane was used as a test case. Simulations of the optimized CG model show a very good agreement with the reference regarding structure (RDFs) and dynamics (self-diffusion). Extensions of the method allow for including box dimensions and/or tilt as dynamical degrees of freedom (NPT ensemble) and for combining reference trajectories at multiple temperatures/pressures. Liquid vapor equilibria of pentane could be simulated with good agreement regarding liquid density, vapor pressure and surface tension over more than 200 K up to the critical point [2]. [1] A. Dequidt and J. G. Solano Canchaya. "Bayesian Parametrization of Coarse-Grain Dissipative Dynamics Models." J. Chem. Phys. 143 (2015) 084122 [2] J. G. Solano Canchaya, †A. Dequidt, F. Goujon and P. Malfreyt. "Development of DPD Coarse-Grained Models: from Bulk to Interfacial Properties.", in preparation

*Poster

Studying the interplay between optical and elastic forces acting on an optically trapped Brownian probe immersed in a viscoelastic fluid.

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We analyze thermal noise statistics for the distribution of positions of probe microbeads immersed in different viscoelastic fluids in optical trapping interferometry. We discuss the influence of the surrounding viscoelastic media in the linear approximation which assumes a harmonic potential exerted by the optical tweezers on the micro-spheres. We conclude that the harmonic potential is valid for viscoelastic fluids in a range where their elastic modulus at low frequency is small enough compared with the trap stiffness and where the optical force does not modify the local fluid's polymeric structure. In that range, the harmonic potential approximation is valid and we propose an alternative methodology to calibrate this kind of experimental set-up when non-Newtonian fluids are used. Understanding the reach of the linear approximation on the optical potential is essential for a correct interpretation of the mechanical properties of biomaterials and living matter obtained by optically-trapped probe-based studies.

*Poster

Leidenfrost impact on a single micrometric defect

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As a water drop erodes a rock, bounces on a leaf or hits the refrigerant part of a condensor, its dynamic is governed not only by inertial and capillary effects but also by the surface nature. The surface chemistry (and in particular its hydrophobicity) has been widely studied and shows different spreading regime. However, it has been also shown that one can break the circular symmetry of the spreading drop with a well defined textured surface. To better understand the influence of this texture, we consider the impact near a single micrometric defect on a plane surface. The surface is also superheated, to reach a Leidenfrost regime in order to avoid the effect of friction. The apparent simplicity of the situation leads however to many different spreading regimes, whose frontiers seem to be independent of the impact velocity and only correlated to the thickness of the fluid lamella of the expanding drop. In each case, the circular symmetry of the spreading is broken and leads to emergence of singularities at the periphery of the drop in the wake of the single defect. The dynamic of such singularities is also shown to be driven by an interial-capillary recoil.

*Poster

Wetting effect on Torricelli's law

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This work reports the effect of wetting on the draining of a tank through a hole the size of which is of the order of magnitude of the capillary length. The obtained results show that although the flow follows a Torricelli's like behavior, wetting strongly aects the speed of drainage that goes through a minimum as the outside surface of the tank bottom plate changes from hydrophilic to hydrophobic. The wetting seems to have a maximum effect in slowing down the flow for a static wetting angle of about 60°. We propose that this non-monotonic effect of wetting originates from the meniscus that forms at the hole outlet, and a simple model that calculates the variation of kinetic energy within the meniscus captures the key points of this phenomenon.

*Poster

Rheology of deformable droplet suspensions: a lattice Boltzmann study

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We study the response of a two-dimensional suspension of deformable droplets of variable area fraction to a pressure-driven flow by means of computer simulations (via the Lattice Boltzmann method). Our method allows us to study a system where droplet coalescence is disallowed, which corresponds to a model foam. We find that the viscosity of the system increases with the droplet volume fraction, and diverges for a density corresponding to jamming of the droplets: at this point, there is a yield stress to be overcome before our foam can be made to flow. Intriguingly, just before jamming, our system displays oscillations in the velocity of either the underlying fluid or of the droplets, and we discuss the mechanism leading to this phenomenon. Finally, we find that our model foam is strongly shear thinning.

*Poster

Characteristics of a 2D system of hard ellipses by event oriented molecular dynamics

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We have simulated the dynamics of a two dimensional system of hard ellipses by event-oriented molecular dynamics in NEV ensemble. Various quantities namely longitudinal and transverse velocity auto-correlation functions, translational and rotational diffusion mean squared displacements, pressure, intermediate self scattering function, radial distribution function and angular spatial correlation have been obtained and their dependence on packing fraction is characterised. Despite absence of prominent positional ordering, the orientational degree of freedom behaves nontrivially and exhibits interesting features. Slowing down is observed in the angular part of the motion near isotropic-nematic phase transition. It is shown that above a certain packing fraction the rotational mean squared displacement exhibits a three stage temporal regime including a plateau. Comparison to 2D system of hard needles is made and it is shown that from positional viewpoint, the ellipse system is more ordered. Analogous to our previous findings in a 2D needle system, many of the temporal autocorrelation functions, both translational and rotational, exhibit a sort of slow dynamics and multi step relaxation. The most interesting feature of the system which has not been explored earlier is the existence of three regimes in the temporal behaviour of the angular mean square displacement. This can be attributed to slow dynamics and possibly the angular glassy dynamics in the system. From the spatial viewpoint, the ellipse system is much more organised than the needle system which seems almost structureless. Our findings show that relaxation of the translational degrees of freedom does not smear out angular slow dynamics. The dependence of translational and rotational diffusion coefficients on the packing fraction have been computed and compared to existing results obtained by Monte Carlo simulations.

*Poster

Lattice Model for water-solute mixtures

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A lattice model for the study of mixtures of associating liquids is proposed. Solvent and solute are modeled by adapting the associating lattice gas (ALG) model. The nature of interaction so- lute/solvent is controlled by tuning the energy interactions between the patches of ALG model. We have studied three set of parameters, resulting on, hydrophilic, inert and hydrophobic interactions. Extensive Monte Carlo simulations were carried out and the behavior of pure components and the excess properties of the mixtures have been studied. The pure components: water (solvent) and so- lute, have quite similar phase diagrams, presenting: gas, low density liquid, and high density liquid phases. In the case of solute the regions of coexistence are substantially reduced when compared with both the water and the standard ALG models. A numerical procedure has been developed in order to attain series of results at constant pressure from simulations of the lattice gas model in the grand canonical ensemble. The excess properties of the mixtures: volume and enthalpy as function of the solute fraction have been studied for different interaction parameters of the model. Our model is able to reproduce qualitatively well the excess volume and enthalpy for different aqueous solutions. For the hydrophilic case we show that the model is able to reproduce the excess volume and enthalpy of mixtures of small alcohols and amines. The inert case reproduces the behavior of large alcohols such as, propanol, butanol and pentanol. For last case (hydrophobic), the excess properties reproduce the behavior of ionic liquids in aqueous solution.

*Poster

Stability analysis of the homogeneous hydrodynamics of a model for a confined granular gas

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The linear hydrodynamic stability of a model for confined quasi-two-dimensional granular gases is analyzed. The system exhibits homogeneous hydrodynamics, i.e. there are macroscopic evolution equations for homogeneous states. The stability analysis is carried out around all these states and not only the homogeneous steady state reached eventually by the system. It is shown that in some cases the linear analysis is not enough to reach a definite conclusion on the stability, and Molecular Dynamics simulation results are presented to elucidate these cases. The analysis shows the relevance of nonlinear hydrodynamic contributions to describe the behavior of spontaneous fluctuations occurring in the system, that lead even to the transitory formation of clusters of particles. The conclusion is that the system is always stable. The relevance of the results for describing the instabilities of confined granular gases observed experimentally is discussed.

*Poster

Phase diagram of the ground states of DNA condensate

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Phase diagram of the ground states of DNA in a bad solvent is studied for a semi-flexible polymer model with a local elastic bending potential and effective self-attraction promoting compaction. Using an analytical theory supported by Monte Carlo simulations, we derive the full phase diagram in the stiffness-length plane, and find a transition between rod-like and toroidal condensate for increasing stiffness at a fixed length L. Strikingly, the transition is found to have a L1/3 dependence, irrespective of the details of the interactions between neighboring molecules [1]. A generalization of the usual worm-like chain model is proposed [2] to account for the results of prior experimental and computational studies and to make predictions for the specific geometries of the ground states. The results underscore the impact of the form of the microscopic bending energy at macroscopic observable scales. [1] T.X. Hoang et al, Phys. Rev. E 92, 060701(R) (2015) [2] T.X. Hoang et al, J. Chem. Phys. 140, 064902 (2014)

*Poster

Torque free polarization of active colloids under sedimentation

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A lot of studies have been made in active matter these last years, with objective to define a framework for out of equilibrium systems. If the concept of effective temperature in a dilute phase of active particles is now widely used, recent work have highlighted that the notion of pressure is not trivial in such systems. In this work we study experimentally the sedimentation of active particles under high gravity field. We observe a torque free polarization against the field and get a very good agreement with theoretical predictions. We also measure the pressure and compare it with the pressure expected for systems at equilibrium under the same gravity field. For high sedimentation angles, we observe a net difference between these two quantities as predicted in recent theory.

*Poster

Grafted polymer under shear flow

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A self-attracting-self-avoiding walk model of polymer chain on a square lattice has been used to gain an insight into the behaviour of a polymer chain under shear flow in a slit of width L. Using exact enumeration technique, we show that at high temperature, the polymer acquires the extended state continuously increasing with shear stress. However, at low temperature the polymer exhibits two transitions: a transition from the coiled to the globule state and a transition to a stem-flower like state. For a chain of finite length, we obtained the exact monomer density distributions across the layers at different temperatures. The change in density profile with shear stress suggests that the polymer under shear flow can be used as a molecular gate with potential application as a sensor. Reference: Sanjiv Kumar, Damien P Foster, Debaprasad Giri, and Sanjay Kumar, J. Stat. Mech.:Theo & Expt., (Accepted, 2016)

*Poster

Island Size Distribution with Hindered Aggregation

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We study the effect of hindered aggregation on the island size distribution (ISD) in a one-dimensional model for epitaxial growth with arbitrary critical nucleus size i. In our model, the attachment of monomers to pre-existing islands is hindered by an additional attachment barrier. Due to the barrier, one finds a crossover between two different regimes: diffusion-limited aggregation (DLA) and reaction-limited aggregation (RLA). We use a self-consistent (SC) approach [1,2] to describe analytically the time evolution of the ISD. We test the SC approach with extensive numerical simulations for different values of i. The aggregation barrier modifies the ISD, allowing us to use the model to improve the analysis of experimental data where the standard DLA approach is not enough to describe the results [3,4]. Acknowledgements: This work was carried out with financial support from "Fondo Nacional de Financiamiento para la Ciencia, la Tecnología y la Innovación" (Colciencias, Agreement FP44842-014-2015). [1] J. G. Amar, M. N. Popescu, and F. Family, Surf. Sci. **491**, 239, (2001). [2] M. N. Popescu, F. Family, J. G. Amar, Atomistic Aspects of Epitaxial Growth, Vol. **65** of the series NATO Science Series, 99-109 (2002). [3] J. R. Morales-Cifuentes, T. L. Einstein, and A. Pimpinelli, Phys. Rev. Lett. **113**, 246101 (2014). [4] P. Gambardella, H. Brune, K. Kern, and V. I. Marchenko, Phys. Rev. B **73**, 245425 (2006).

*Poster

Magnetocapillary self-assemblies : micromanipulation and low Reynolds number locomotion.

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Magnetic particles floating on a liquid can self-assemble into cristal-like structures, by a combination of magnetic dipole-dipole interactions and attractions due to the interfacial deformations. These structures are periodically deformed in a non reciprocal way using magnetic fields, which leads to controllable low Reynolds number locomotion. Such microswimmers provide a basis for micromanipulation applications such as transport of micro-objects, laminar fluid mixing or surface cleaning.

*Poster

Nucleation and growth of the ZIF-8 metal organic framework

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Metal-organic frameworks (MOFs) are highly porous crystalline materials with applications ranging from gas storage to catalysis and drug delivery. MOFs form spontaneously in solution, through the self-assembly of metal ions and organic linker molecules. Despite the growing number of MOF topologies synthesized in experiments, the microscopic mechanism of MOF formation is largely unknown; rational design of new MOFs therefore remains challenging. Here, we report on our efforts to develop a pseudo-atomistic model for ZIF-8, a prototypical metal-organic framework. This model reproduces well the lattice parameters and elastic properties of bulk ZIF-8 and is able to grow ZIF-8 crystals spontaneously from dilute solution in molecular dynamics computer simulations. We reveal the nucleation mechanism of ZIF-8 and discuss the crucial role of the shape of linker molecules in determining network topology.

*Poster

Particle dynamics in dense colloidal suspensions with varying interparticle attraction

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We study the structure and dynamics of dense colloidal suspensions by using depletion forces as a way of controlling the interparticle attraction. Confocal microscopy and particle tracking techniques allow us to determine particle trajectories in systems with varying interparticle attraction strengths. For a fixed volume fraction of colloidal particles we observe three qualitatively different states when varying the inter particle attraction strength. We observe changes in the mean square displacement and long time diffusion constant as the system is brought from a repulsive glass at low attraction strength, through ergodic liquids at moderate attraction strengths, to attractive arrested glasses at highest interparticle attraction studied. We use the non-Gaussian parameter and a self overlap function to probe for heterogeneities in particle dynamics. Results indicate that the most heterogeneous dynamics occur at longer lag times in the arrested states than in the fluid state. Variance in the self overlap and in the spatial positions of mobile particles show that heterogeneous rearrangement events in attractive arrested systems are less frequently distributed spatially but occur over a larger range of length scales than the repulsive glassy states. The length scale that maximizes four point susceptibility across a range of attraction strengths exhibits a reentrant glass behavior similar to that of the long time diffusion constant.

*Poster

Dynamical Symmetry Breaking of Relaxation Rates of a Single Star Polymer with 6 Arms due to Excluded Volume Effects at the Center

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Relaxation modes and rates of a single star polymer with 6 arms are examined for various topologies of center connection by coarse-grained molecular dynamics (cgMD) simulations. We considered an excluded volume polymer chain of the Kremer-Grest model and the same length of arms. As topologies of center connection, point center, ring connection, octahedron connection, and full connection are considered. From viewpoint of topological symmetry, for the point center and the full connection, we expected degeneration of the f - 1 slowest relaxation rates, where f denotes the number of arms. For the ring and octahedron connection, degeneration of the 2 and 3 slowest relaxation rates is expected, respectively. We confirmed that these expectations agree with results of cgMD simulations for the cases except for the full connection. For the case of the full connection, we observed dynamical symmetry breaking of relaxation rates. This breaking is originated from excluded volume of beads at the center. We found that the 3 slowest relaxation rates are degenerated. By reducing excluded volume among 6 beads at the center, we confirmed that the dynamical symmetry breaking is vanished. We hope that this can be confirmed by some experiments such as the dielectric relaxation measurements for synthesized polymer chains.

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*Poster

Molecular dynamics calculations of intermediate scattering functions for a model colloidal fluid with explicit solvent

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Colloidal suspensions are extremely useful model systems for the study of nucleation and vitrification. They show a phase behavior which can be mapped onto a hard-sphere (HS) system, but also exhibits a glass transition. [1,2] The common method used to study these systems experimentally are dynamic light scattering (DLS) and x-ray photon correlation spectroscopy (XPCS). As a compliment to light scattering experimental results, Molecular Dynamics (MD) simulation was used to study a model colloidal suspension. Using an model which has been shown to reproduce structural and dynamical properties of a real colloidal suspension [3] we study the intermediate scattering function over a wide range of concentrations leading up to the freezing point. A multiexponential analysis of the results was done and found that the data was fit well by the sum of two exponentials, which is in line with previous analysis of experimental colloidal suspensions. The amplitudes and decay coefficients of the two modes are studied over a large range of wavevectors at concentrations leading up to the freezing point. [1] P. N. Pusey and W. van Megen, Nature London 320, 340 (1986). [2] W. van Megen and S. M. Underwood, Nature London 362, 616 (1993). [3] S. D. W. Hannam, P. J. Daivis and G. Bryant, Molecular Simulation (2015). DOI: 10.1080/08927022.2015.1066505

*Poster

Critical three-body Casimir interaction

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It was shown by Burkhardt and Eisenriegler that the critical Casimir interaction between two colloids at $T = T_c$ can be calculated exactly by a conformal mapping in arbritary dimension d [1]. For the two-dimensional case $d = 2$ Bimonte et al. extended this calculation to arbritary shaped objects [2], where the form of the interaction potential between two disks is known exactly. Utilizing those concepts we present a calculation which maps the case of two separated two-dimensional disks onto a limiting case of a three-body system, where two particles are in contact and one is free to move. We compare the results of this calculation to Monte Carlo simulations, using a highly efficient cluster algorithm [3]. [1] T. W. Burkhardt and E. Eisenriegler, Phys. Rev. Lett. 74, 3189 (1995). [2] G. Bimonte et al., Europhys. Lett. 104, 21001 (2013). [3] H. Hobrecht and A. Hucht, Phys. Rev. E 92, 042315 (2015)

*Poster

Viscosity of supercooled water and two-state interpretation of water anomalies

Bruno Issenmann * [1], Lokendra Pratap Singh Amine Dehaoui Frédéric Caupin

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Water is a familiar liquid but also exhibits many anomalies. In most liquids far from the glass transition, viscosity and self-diffusion coefficient are coupled by the Stokes-Einstein relation. In water, viscosity starts decoupling from translational diffusion near 20°C. Molecular dynamic simulations relate this behaviour with a putative phase transition between two distinct liquid forms of supercooled water [1]. Whereas extensive experimental values for the self-diffusion coefficient are available for supercooled water [2], viscosity data are scarce [3]. We report two new viscosity experiments: one based on Brownian motion and performed at atmospheric pressure down to -34°C [4]; the other based on Poiseuille flow performed up to 300 MPa and down to 20°C below the melting line. An extension of a quantitative two-state model [5] allows us to consistently describe dynamic properties of supercooled water. [1] P. Kumar, S. V. Buldyrev, S. R. Becker, P. H. Poole, F. W. Starr, H. E. Stanley, Relation between the Widom line and the breakdown of the Stokes-Einstein relation in supercooled water, Proc. Natl. Acad. Sci. U.S.A. 104 9575 (2007) [2] W. S. Price, H. Ide, Y. Arata, Self-Diffusion of Supercooled Water to 238K Using PGSE NMR Diffusion Measurements, J. Phys. Chem. A 103 448-450 (1999) [3] J. Hallett, The temperature dependence of the viscosity of supercooled water, Proc. Phys. Soc. 82 1046 (1963) [4] A. Dehaoui, B. Issenmann, F. Caupin, Viscosity of deeply supercooled water and its coupling to molecular diffusion, Proc. Natl. Acad. Sci. USA 112 12020 (2015) [5] V. Holten and M.A. Anisimov, Entropy-driven liquid–liquid separation in supercooled water, Sci. Rep. 2, 713 (2012).

*Poster

Telechelic star polymers under shear: a multiscale simulational approach

Diego Jaramillo * [1], Manuel Camargo, Christos N. Likos

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Telechelic star polymers (TPSs) are macromolecules formed by a number of diblock copolymers (arms) anchored to a common central core, being the internal monomers solvophilic (A-type) and the end monomers solvophobic (B-type). Very recent studies [1-3] have demonstrated that TPS constitute self-assembling building blocks with specific softness, functionalisation, shape and flexibility: depending on different physical and chemical parameters, e.g. number of arms f, solvophobic-to-solvophilic ratio Alpha, temperature T, and solvent quality Lambda, the geometrical conformation of TSPs features a well defined number of attractive spot on the surface. In this way, they can be considered as very tunable soft-patchy colloids and therefore can lead to the formation of well-controlled ordered and disordered phases in soft condensed matter systems. In this work, we systematically study the conformation of TSPs under shear by means of a combination of multiparticle-collision dynamics (MPCD) for the solvent and standard molecular dynamics (MD) for the monomers. By employing the Lees-Edwards boundary condition that allows to impose a uniform shear on the simulated system, we systematically evaluate the gyration tensor of low functionality TPSs (f ¡ 20), as well as the number, monomer population and size of the attractive patches that each star forms as a function of the solvophobic-to-solvophilic ratio, the temperature and the share rate. Since the conformation of single stars is expected to be preserved in low-density bulk phases, the presented results are a first step in understanding the rheological properties of suspensions of this kind of polymers. [1] B. Capone et al. Phys. Rev. Lett. 109: 238301 (2012) [2] E. Bianchi et al. Faraday Discuss., 181: 123 (2015) [3] L. Rovigatti et al. Nanoscale (2015) DOI: 10.1039/C5NR04661K

*Poster

Adhesion force hysteresis with a capillary bridge of yield-stress fluid

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We present experiments where a capillary bridge of yield-stress fluid (carbopol microgel) is stretched or compressed by steps between two parallel surfaces. The force perpendicular to the plates is measured via the deflection of a cantilever, and plotted versus a quantity L (scaling like a length) quantifying the surface curvature of the bridge. With a simple fluid the force is shown to be proportional to L, the slope being equal to the surface tension of the fluid, providing a precise surface tension measurement. However with the yield stress fluid, the force-L curve exhibits a hysteresis whose amplitude increases as yield stress increases. A simple model allows us to reproduce qualitatively this behavior, by taking into account the residual internal stress after the flow arrest. We also show that under some conditions it is nevertheless possible to extract a reliable surface tension value from this experiment, even if the yield stress is not known. This work highlights that yield-stress fluids cannot reach a thermodynamical equilibrium, and for this reason equilibrium laws such as Laplace's law or Young's law cannot be used as is.

*Poster

Molecular crowding and bacterial chromosome organization

Youngkyun Jung * [1], C. Jeon, J. Kim, B.-Y. Ha

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Bacterial chromosomes are macroscopically long but still reside in a micron-sized intracellular subspace. What controls their spatial organization in harmony with other biological processes such as transcription? A number of recent studies highlight molecular crowding as a key determinant of biomolecular organization. Here we present a detailed account of molecular crowding in organizing chain molecules. In a crowded medium, a chain molecule can be entropically phase-separated into a collapsed state, similarly to what has been seen with bacterial chromosomes in cellular environments. Similar entropic effects are responsible for the clustering of transcription-active sites into the so-called 'transcription foci' in a bacterial cell.

*Poster

Electronic structure of walls influences ionic transport in nano-channels

Vojtech Kaiser * [1], Lyderic Bocquet

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We present a model for transport in a nano-channel with conducting walls. The channel's ionic conductivity is regulated by the applied potential, electron properties of the walls, and the ionic strength of the confined electrolyte. Our main result concerns the influence of the density of states at the Fermi level on the degree of screening of the external potential, leading to a tell-tale crossover in ionic conductivity between limiting laws at high and low concentrations.

*Poster

Zero modes in sticky sphere clusters

Yoav Kallus * [1], Miranda Holmes-Cerfon

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Low energy geometries of finite clusters are are known in many cases to be incompatible with global order, and this incompatibility leads to geometric frustration in the bulk. For sticky spheres, hard-core spheres with short-range surface adhesion, many cluster geometries achieve the same minimum energy, and their relative stability is determined by entropic effects. In particular, clusters with zero modes in the vibration spectrum are strongly favored, and we give a tractable method to calculate their anharmonic vibration entropy. Our analytic results are supported by simulations and experiments. In the zero-range limit, we show that every two zero modes in the vibration spectrum contribute to the stability of the cluster as much as an extra bond. Using comprehensive enumerations of sticky sphere rigid cluster geometries, we explore how bulk behavior is approached as the number of spheres increases.

*Poster

Nonlinear fractional waves in biological membranes

Julian Kappler * [1], Shamit Shrivastava, Matthias F. Schneider, Roland R. Netz

[1] Freie Universität Berlin – Germany

Recently, there has been experimental interest in nonlinear sound waves in two dimensional systems. However, a deep theoretical understanding of their behavior is still unknown. In our talk, we will provide this analytical description, starting from standard hydrodynamics, and deriving a nonlinear fractional wave equation for 2D sound waves in a membrane on water. We compare numerical solutions of our theory with experimental data and show that our model reproduces several key experimental features, such as an abrupt increase in both range and velocity as a function of excitation amplitude.

*Poster

Fragmentation arrested viscous coarsening in glasses

Yuliya Karanouskaya * [1], David Bouttes, Emmanuelle Gouillart, Elodie Boller, Davy Dalmas, Damien Vandembroucq

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Viscous coarsening of a phase-separated high-temperature silicate melt is studied by X-ray tomography. This 3D imaging technique allows us to give a fine geometrical and topological characterization of the domain growth and to test the dynamical scaling behaviour usually expected in coarsening phenomena. Viscosity contrast between the two liquid phases is shown to induce an original fragmentation process. In particular, a power law distribution of droplets is observed. The gradual fragmentation process is shown to eventually arrest viscous coarsening. Ref: D. Bouttes et al., Fragmentation and Limits to Dynamical Scaling in Viscous Coarsening: An Interrupted in situ X-Ray Tomographic Study, Phys. Rev. Lett. 112, 245701 (2014)

*Poster

Collective effects with camphor boats

Ronan Kervil * [1], Cécile Cottin-Bizonne, Florence Raynal, Mickael Bourgouin, Romain Volk, Christophe Ybert.

[1] Ilm, équipe Liquides et Interfaces – France

Active matter exhibits fascinating collective effects at different scales from birds'flocks, school of fish or bacteria's swarms.To mimic these many particles systems we study assemblies of self-propelled camphor boats (agar gel matrices filled with camphor, a hydrophobic molecule that sublimates easily) floating on free water surface. We highlight the different swimming behaviours from low to high swimmers density. When a small number of particles is considered, the motion is continuous and ballistic like for an individual swimmer. When a larger number of particles is considered, a transition from continuous to intermittent swimming appears: particles speeds decrease until the system reaches a motionless meta-stable state; then one particle starts to swim again and unsettles its motionless neighbours that destabilize their other neighbours as a domino effect. Interestingly, at high density of swimmers, the velocity distributions become highly non Gaussian, with algebraic tails, like in highly turbulent flows. Similarly, the velocity spectrum exhibits both a -2 and a -4 slope, as found in Sawford's work (PoF 1991) that considers Lagrangian stochastic models of turbulent dispersion. With these observations we conclude that such a simple 2D system as camphor boats collectively behaves like passive particles in a 3D highly turbulent flow.

*Poster

Dielectric elastomers based on carbon blacks functionalized with organic molecules: Experiment and simulation

Heesuk Kim * [1], Youngpyo Ko, Seulki Kwon, Sang-Soo Lee, Jongho Kim, Bong June Sung

[1] Korea Institute of Science and Technology – South Korea

The dielectric properties of elastomer-based composites with high dielectric fillers have been intensively examined for a variety of potential applications, including dielectric elastomer actuators, capacitive touch sensor, and embedded capacitor materials. In this study, we functionalize carbon blacks (CB) with organic molecules such as alkylsilanes in order to improve their dispersibility in solvent and elastomer matrix. We confirm that the dispersibility and dielectric properties of elastomer/CB composites depend on the amount of organic molecules. The elastomer composites including 3wt% CB functionalized with alkylsilane exhibit much higher dielectric constant of 900 and dielectric loss of 0.12 (at 100 Hz) than the elastomer/CB composites without alkylsilane treatment (dielectric constant of 7.5 and dielectric loss of 0.02 at 100 Hz at the same amount of CB). We also perform extensive molecule simulations to elucidate how one can obtain such a good dielectric property by treatment of CB with organic molecules.

*Poster

Lattice modeling of nonconcatenated ring melts

Max Kolb * [1], Elham Ghobadpour, Ralf Everaers

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Melts of long, unknotted and nonconcatenated ring polymers serve as a model for biological polymer systems under topological constraints and in particular for the organisation of chromatin fibers. They also shed light on the structure and relaxation dynamics of crumpled polymer globules. Due to the topological constraints the static and dynamic properties of rings differ significantly from those of linear polymers. Here we use a coarse-grained lattice polymer model to study the static and dynamic properties of such melts. The aim is not to model the melts in detail but rather to calculate the scaling behaviour for long chain lengths. Monte Carlo (MC) simulations of lattice rings and double folded lattice rings (tree model) are compared with reference Molecular Dynamics (MD) simulations. Both ideal gaussian and excluded volume interactions are considered. For the ideal systems the expected static and dynamic scaling results are reproduced. For excluded volume interactions the experimentally observed structure, a compact crumpled state and its organisation in terms of territories, is recovered for all models. Dynamically, there is only qualitative agreement in monomer and center of mass displacements. The data is not accurate enough to decide if the observed discrepancies are due to a conceptual difference between the ring and the tree model. Numerically both the full and the simplified MC lattice models perform by orders of magnitude better than the more detailed reference MD model.

*Poster

Rheology of a Sheared Dissipative Fluid: Bagnold Scaling and Integration through Transients

Till Kranz * [1], Fabian Frahsa, Annette Zippelius, Matthias Fuchs, Matthias Sperl

[1] DLR Cologne – Germany

We generalize the Integration through Transients (ITT) formalism to the non-equilibrium stationary state of randomly driven inelastic hard spheres. ITT was first developed for Brownian suspensions and has been successfully employed to explain phenomena beyond weak shear. As a result we obtain generalized Green-Kubo-relations and an equation of motion for the transient scattering function. Since the seminal work of Bagnold it has been recognized that dissipative hard spheres (i.e. granular particles) have an unusual rheology. In particular, the shear stress σ varies with the square of the shear rate γ, i.e., Bagnold scaling, $\sigma = \eta\gamma^2$, holds. We will discuss the response to shear and the dependence on the degree of inelasticity and packing fraction. This includes the transient density correlator and the prefactor, η, of the Bagnold scaling relation. We will comment on the relation to the elastic and the unsheared case, clarifying how Bagnold scaling emerges.

*Poster

Simulations of the dynamics of a foam-fibre dispersion

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In paper manufacturing, wet foams can be used instead of water as a carrier for the fibre network [Skelton, 1987; Lehmonen et al., 2013]. It has been showed experimentally [Al-Qararah et al., 2013] that the presence of cellulose (wood) fibres dispersed within a foam modifies its properties (e.g. bubble size distribution). In this study, we investigate numerically the flow behaviour of a two-dimensional foam-fibre dispersion. The foam dynamics is computed using the bubble or soft-disk model [Durian, 1995], which has been shown to reproduce correctly the nonlinear rheology of a 2D flowing foam (whether it is a bubble raft or confined in a Hele-Shaw cell) [Langlois et al., 2008]. We first present the dynamics of an individual fibre (tethered or entrained by the bubble flow) as a function of its mechanical properties (length and flexibility) and then analyze the effect of enriching the foam with a given density of fibres on its rheological properties, under conditions of both simple shear and Poiseuillle flow.

*Poster

Washboard road instability

Charles-Edouard Lecomte * [1], Nicolas Taberlet

[1] Laboratoire de physique de l'ENS de Lyon – France

When a sand track is subjected to repeated passages of vehicles, under certain conditions, a regular pattern of ripples appear : this is known as washboard road, which is common on dry unpaved roads. We reproduced this instability with a experimental apparatus and also thanks to soft sphere molecular dynamics simulations. Previous experimental work and numerical simulations have shown that ripples appear above a critical speed. Then this phenomenon was studied when a simple inclined blade was used as vehicle, to exhibit the role of grain transportation in the instability. A linear stability analysis was built, which predicts quantitatively the characteristics of the ripples formation. We will present the latest experimental and numerical work on the washboard road, when the sand track is wet and therefore cohesive. We studied the dependence of the main characteristics of the instability : critical speed, growth rate, amplitude as function of the cohesion of the wet granular media. The investigation of a wide range of rheological properties aims at understanding the fundamental processes which causes the washboard road instability.

*Poster

A Bethe-lattice-like mean-field model for plastic deformation of amorphous solids

Edward D. Lee * [1], Archisman Raju, Danilo Liarte, Karin Dahmen, James P. Sethna

[1] Cornell University – United States

We propose a Bethe-lattice inspired mean-field theory of the pseudogap found in avalanche systems with long-range anisotropic interactions using analytical and numerical tools. The pseudogap in the density of spins near the threshold of instability emerges from the competition between stabilizing interactions between spins in an avalanche and the destabilizing random movement towards the threshold caused by anisotropic couplings. Many experiments show that the distribution of avalanche sizes decays with a power law with an exponent consistent with $\tau = 3/2$ as predicted by the random-field Ising model (RFIM). But a number of theoretical and numerical arguments show that tau depends on the distribution of couplings and the dynamics of the model (Pazmandi and Zimanyi, Lin and Wyart, Jagla). On the other hand, realistic simulations suggest that a consistent value of $\tau \approx 1.3$ (Budrikis et al., Salerno and Robbins), not far from the RFIM prediction. We propose a model similar to Lin and Wyart's where any given spin has anisotropic, long-range couplings with a finite fraction of the system like in a Bethe lattice. Our initial numerical results suggest that in our model the pseudogap scales with a consistent exponent at the critical point regardless of the range of the distribution of couplings but depends on the applied stress. Correspondingly, τ does not seem to depend on the distribution of couplings; however, it does depend on the dynamical details of our simulation.

*Poster

Out-of-equilibrium dynamics and effective temperatures in dense active matter

Demian Levis * [1]

[1] Universitat de Barcelona – Spain

Active matter systems are made of interacting units (active particles) which can convert energy from their environment into mechanical work and, in the situations we consider here, locally produce motion. As a result, these self-propelled particles are intrinsically out-of-equilibrium, giving rise to interesting collective behavior. Artificial active suspensions made of Janus colloids can now be realized in the lab using state of the art techniques, opening the possibility of creating new soft materials with novel functionalities. The systematic characterization of these non-equilibrium systems clearly needs further theoretical work. Here I will present the recent attempts to establish an effective thermodynamic framework to describe these non-equilibrium systems and discuss its main advantages and limitations. In order to study how the equilibrium dynamics of colloidal matter is affected by the competition between self-propulsion and steric effects, I introduce a model of self-propelled disks where particles perform a persistent random walk. We further investigate which equilibrium thermodynamic quantities, like temperature, can be extended to characterize the dynamics of active matter. To do that, we extract an effective temperature from the violations of the fluctuation-dissipation theorem. I will discuss the evolution of the effective temperature over a broad range of densities and activities, as the system approaches a non-equilibrium glass transition at high densities. We then discuss whether the effective temperature we focus on is a meaningful (and relevant) thermodynamic concept in the context of active matter. We compare our predictions with the experimental results obtained in suspensions of Janus colloids.

*Poster

Earthquakes in the lab

Sébastien Lherminier * [1], Ramon Planet, Gilles Simon, Loïc Vanel, Osvanny Ramos, Knut Jorgen Maloy

[1] Institut Lumière-Matière – France

In order to analyze different questions related to earthquakes and scale-invariant phenomena in general, we present an original experimental setup that mimics the dynamics of a tectonic fault by studying a two-dimensional granular layer that is sheared continuously while submitted to a controlled confining pressure. As the '(tectonic) plates' move in relation to each other at a controlled and very low speed, shear stresses build up on the packed grains, and eventually they are liberated through sudden avalanches (reorganization of the pack), with sizes distributed following a power law $P(s) \sim s^{-b}$ (similar to the Gutenberg-Richter law for earthquakes magnitudes). Acoustic measurements are the main and more precise source of information. However, a mechanical monitoring is also realized and we will show the non-trivial correlation between the two monitorings. Finally, the position of all the grains and the force networks in the structure can be obtained thanks to photoelasticity. We will present the first results obtained in this experiment, which show a very good resemblance with real earthquakes, both in terms of amplitude of events and temporal occurences.

*Poster

Weirdest Martensite: Smectic Liquid Crystal Microstructure and Weyl-Poincaré Invariance

Danilo Liarte * [1], Matt Bierbaum, Ricardo Mosna, Randall Kamien, James Sethna

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Smectic liquid crystals are remarkable, beautiful examples of materials microstructure, with ordered patterns of geometrically perfect ellipses and hyperbolas. The solution of the complex problem of filling three-dimensional space with domains of focal conics under constraining boundary conditions yields a set of strict rules, which are similar to the compatibility conditions in a martensitic crystal. Here we present the rules giving compatible conditions for the concentric circle domains found at two-dimensional smectic interfaces with planar boundary conditions. Using configurations generated by numerical simulations, we develop a clustering algorithm to decompose the planar boundaries into domains. The interfaces between different domains agree well with the smectic compatibility conditions. We also discuss generalizations of our approach to describe the full three-dimensional smectic domains, where the variant symmetry group is the Weyl-Poincaré group of Lorentz boosts, translations, rotations, and dilatations.

*Poster

Aspect Ratio Effect of Cold Liquids with Densely Packed 2D Rod-like Particles

Jyun-Ting Lin * [1], Jyun-Ting Lin, Wen Wang, Lin

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For the cold liquid with densely packed rod like particles, rod aspect ratio plays an important role for determining micro-structure and motion. At the large aspect ratio limit, the system enters the smectic or tetratic phase under cooling. The anisotropic interaction and topological constraint of long rods cause symmetry breaking which leads to higher translational diffusivity than rotational diffusivity. However, the micro-structure and dynamics as the aspect ratio approaching one still remain elusive. In this work, these issues are numerically explored using densely packed short spheroids with modified Lennard Jones potential. The micro-structure and motion under the competition between the ordered domains of triangular lattice structure and tetratic structure, how the rotational and translational motions are correlated and decoupled, and their spatiotemporal scales, by gradually tuning the aspect ratio away from one, will be presented and discussed.

*Poster

Tension control of domain nucleation in lipid bilayers

Michael A. Lomholt * [1], Allan G. Hansen, Jonas C. Jeppesen, John H. Ipsen, Adam C. Simonsen

[1] MEMPHYS, University of Southern Denmark – Denmark

When lipid molecules in a bilayer freeze they tend to lower the area that they occupy in the membrane. Thus during the nucleation process of a solid domain of lipids the nucleating domain will have to pull against the local tension in the bilayer, an effect that will lower the rate at which these domains nucleate. I will present a model of domain nucleation and growth, which explains how the dynamics of the tension via this effect can determine the distribution of nucleation points observed in experiments on supported lipid bilayers. The friction between the bilayer and the support plays an important role in this model, by slowing down the relaxation of locally increased tension.

*Poster

Direct calculation of the critical Casimir force by simulation of a binary fluid

David Lopes Cardozo * [1], Francesco Puosi, Sergio Ciliberto, Peter C W Holdsworth

[1] Laboratoire de Physique - ENS de Lyon – France

I will discuss how critical Casimir effects can be accessed through direct numerical simulation of a model binary fluid as it passes through the demixing transition in the high density phase. Simulations were performed in the semi grand canonical ensemble, in which the fluid composition fluctuates at fixed density. In slab geometry, a critical pressure anisotropy is observed in which the force per unit area parallel and perpendicular to the confinement direction are different. The measured anisotropy collapses into a universal scaling form closely related to that for the critical Casimir force. The critical Casimir force itself can be defined as the critical excess contribution to the generalized pressure function, $P_\perp - n\mu$, conjugate variable to volume changes at fixed density n, with $P_\perp$ the pressure perpendicular to confinement and μ the chemical potential. In the context of existing experimental and numerical studies of the critical Casimir force, such an approach could open the way to dynamical and non-equilibrium studies.

*Poster

Structural and thermodynamic properties of hard-core fluids in fractal dimension

Mariano López De Haro * [1], Andres Santos

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Analytic approximations for the radial distribution function and the equation of state of hard-core fluids in fractal dimension $d(1 \leq d \leq 3)$ are developped. They rely on a heuristic approach similar to the one used [1] to derive the radial distribution function of a hard-disk fluid from the knowledge of the exact and Percus-Yevick results for the hard-rod fluid and the hard-sphere fluid, respectively. In order to asess their value, such approximate results are compared with those of recent MonteCarlo simulations [2]. [1] S. B. Yuste and A. Santos, J. Chem. Phys. 99, 2020 (1993). [2] Marco Heinen, Simon K. Schnyder, J. F. Brady, and H. Löwen, Phys. Rev. Lett. 115, 097801 (2015).

*Poster

Can active fluids be stable?

Ananyo Maitra * [1], Martin Lenz

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"Active hydrodynamics", which augments standard descriptions of equilibrium fluids with non-equilibrium stresses and currents, is the standard paradigm for describing the long-distance, large-time physics of internally driven systems, such as those encountered in biology. A well-known property of orientable active fluids, which has been implicated in cellular flows and bacterial turbulence, is the threshold-free hydrodynamic instability of the (polar or nematic) oriented state irrespective of the sign of the non-equilibrium stress. In this work, we examine general (p-fold) orientationally-ordered active systems and ask whether they are generically unstable. We discover a novel non-equilibrium effect which is distinct from the active current and stress hitherto discussed in the context of polar and nematic ordering. We demonstrate that it leads to a wavevector-independent stabilisation or destabilisation of the orientationally-ordered phase depending on its sign. This new non-equilibrium effect is present in all p-fold orientationally-ordered systems in contrast to the popular active current and stress which is present only for p=1 or 2 i.e. polar or nematic ordering. In systems with polar or nematic symmetry, it competes with the mechanism that renders them unstable, and can lead to hydrodynamically stable phases. Our examination of the orientationally-ordered phases of active systems shows that the currently popular active nematic theory is a one-activity-constant approximation of a more complete description. We expect that our theory will have implications for experiments on both biological systems and their artificial analogs.

*Poster

Simple model for the mechanical response of biological tissues

D.A. Matoz-Fernandez * [1], Kirsten Martens, Jean-Louis Barrat

[1] Univ. Grenoble Alpes, LIPHY, F-38000 Grenoble, France; CNRS, LIPHY, F-38000 Grenoble, France – France

We study a simple model of biological tissue where the cells can organize collectively by cell division and apoptosis. As is well known the cell division introduces a new time scale in the cell dynamics. In this talk I will discuss how to characterize the athermal noise created through the cell activity. Further I will address the interplay between this noise and its mechanical counterpart created through the elastic response to cell rearrangements when driven by an external force.

*Poster

Kinectic theory and hydrodynamics of a model for a confined granular gas

Pablo Maynar * [1], J. J. Brey, M. I. García de Soria, V. Buzón

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The non-equilibrium statistical mechanics and kinetic theory for a model of a confined quasi-two-dimensional gas of inelastic hard spheres is presented. The dynamics of the particles includes an effective mechanism to transfer the energy injected in the vertical direction to the horizontal degrees of freedom. The Boltzmann equation is formulated and used to study the dynamics of the distribution function. For homogeneous states, a hydrodynamic solution is found, i.e. a solution in which all the time dependence goes through the instantaneous granular temperature. For inhomogeneous situations, hydrodynamic equations are derived via the Chapman-Enskog expansion. The theoretical predictions are compared with numerical simulations finding a very good agreement. J. J. Brey, M. I. García de Soria, P. Maynar, and V. Buzón, Phys. Rev. E, **88**, 062205 (2013). J. J. Brey, P. Maynar, M. I. García de Soria, and V. Buzón, Phys. Rev. E, **89**, 052209 (2014).

*Poster

The polymorphic behavior of Wigner bilayers.

Martial Mazars * [1], Moritz Antlanger, Ladislav Samaj, Gerhard Kahl, Emmanuel Trizac

[1] Laboratoire de Physique Théorique, Univ. Paris-Sud, Université Paris-Saclay – France

Self-assembly into target structures is an efficient material design strategy. Combining analytical calculations and computational techniques of evolutionary and Monte Carlo types, we report about a remarkable structural variability of Wigner bilayer ground states, when charges are confined between parallel charged plates. Changing the inter-layer separation, or the plate charge asymmetry, a cascade of ordered patterns emerges. At variance with the symmetric case phenomenology, the competition between commensurability features and charge neutralization leads to long range attraction, appearance of macroscopic charges, exotic phases, and non conventional phase transitions with distinct critical indices, offering the possibility of a subtle, but precise and convenient control over patterns. In this contribution, we discuss the phase diagram found for asymmetric Wigner bilayer and the thermal stability of the ordered phases found with the evolutionary algorithm, analytical computations and Monte Carlo simulations.

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*Poster

On the aggragation of discotic particles. A computer simulation study.

Juan Neftali Morillo Garcia * [1], Bruno Martinez Haya, Alejandro Cuetos Menendez

[1] Universidad Pablo de Olavide – Spain

The aggregation of discotic particles at low density is relevant in some technological fields. An example of this is the aggregation of asphaltenes in oil pipes, or the precipitation of amyloid particles. We have studied this problem by means of Monte Carlo and Brownian Dynamic simulation. For this we have used different interactions potentials between the particles such Kihara and Gay-Berne-Kihara potentials, modeling situations where the face-to-face interaction is favored, or those where the interaction between the edge of the particles are more relevant, besides the situations where the interaction has the same symmetry than the shape of the particles. We have found than the kinetic of aggregation of the particles and the shape of the aggregates is highly influenced by the potential considered. Thus, the geometry of the cluster varies from columnar to planar clusters. The condition, temperature and density, at what the formation of cluster is more relevant is also very dependent on the geometry of the interaction.

*Poster

Flocking through disorder

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For more than two decades physicists have contemplated the idea of describing flocks, herds, shoals and swarms as spontaneously flowing material. Inspired by this appealing idea, experimentalists have recently devised new synthetic materials out of autonomous motile units: active materials. Appart from very rare exceptions our understanding of active matter has been hitherto restrained to self-propelled particles collectively moving in homogeneous media. However, none of the potential applications of active materials, or collective robotics, would occur in homogeneous environments and in the wild, most animal groups propel in strongly heterogeneous settings. Here, we combine experiments and theory, to elucidate the emergence and the suppression of collective motion in disordered media. We first report on the flocking dynamics of colloidal rollers cruising though random repelling obstacles. Upon increasing the obstacle density, collective motion is restrained to increasingly sparse channel networks akin those found at the onset of plastic depinning in driven condensed matter. Further increasing disorder, macroscopic flocks are abruptly destroyed. We theoretically demonstrate the robustness of all our experimental findings. We show that the emergent channel networks originate from the competition between orientational elasticity and obstacle repulsion, and quantitatively evidence that the sharp suppression of orientational order is a genuine first order phase transition generic to all polar active materials.

*Poster

Nonperturbative renormalization group approach to polymerized membranes

Dominique Mouhanna * [1], O. Coquand, K. Essafi, J.-P. Kownacki

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The physics of polymerized membranes has known a renewed interest due to the discovery of single layer carbon structures, like graphene, that are very well described, as for their elastic properties, by polymerized membranes. For practical reasons - notably the design of materials with optimized optical and electronic properties - or from a more fundamental perspective, a qualitative and quantitative description of these systems is highly needed. However polymerized membranes are, from the statistical point of view, non-trivial interacting and strongly fluctuating systems whose precise description calls for efficient tools. The renormalization group, as conceived by Kadanoff and Wilson is a universal framework designed to investigate such kind of situations. Unfortunately while it is nonperturbative in its conception, its use has been, for a long time, confined to the perturbative domain: in a vicinity of the upper or lower critical dimension, at weak coupling constant, at low temperatures, etc. In the 90's Wetterich has introduced a new formulation of this technique that turns out to be extremely suitable to tackle with truly nonperturbative issues: physics far from the upper or lower critical dimensions, at strong coupling constant, with topological excitations, bound states, etc In my talk I present this technique and illustrate its efficiency in the context of two dimensional polymerized membranes and show that it leads to qualitatively and quantitatively precise predictions for the behaviour of both for these systems and for materials like graphene.

*Poster

Folding of small knotted proteins: Insights from a mean field coarse-grained model

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A small but relevant number of proteins whose native structure is known features nontrivial topology, i.e., they are knotted. Understanding the process of folding from a swollen unknotted state to the biologically relevant native conformation is, for these proteins, particularly difficult, due to their rate-limiting topological entanglement. To shed some light into this conundrum, we introduced a structure-based coarse-grained model of the protein, where the information about the folded conformation is encoded in bonded angular interactions only, which do not favor the formation of native contacts. A stochastic search scheme in parameter space is employed to identify a set of interactions that maximizes the probability to attain the knotted state. The optimal knotting pathways of the two smallest knotted proteins, obtained through this approach, are consistent with the results derived by means of coarse-grained as well as full atomistic simulations.

*Poster

Design Principles for Self-Assembling Polyomino Tilings

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The self-assembly of simple molecular units into regular 2d (monolayer) lattice patterns continues to provide an exciting intersection between experiment, theory and computational simulation. We study a simple model of polyominoes with edge specific interactions and introduce a visualisation of the configuration space that allows us to identify all possible ground states and the interactions which stabilise them. By considering temperature induced phase transitions away from ground states, we demonstrate kinetic robustness of particular configurations with respect to local rearrangements. We also present a rigorous sampling algorithm for larger lattices where complete enumeration is computationally intractable and discuss common features of the configuration space across different polyomino shapes.

*Poster

Generalized nematics and lattice gauge theory

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We discuss exotic nematics that break the rotational symmetries of isotropic space to a general three-dimensional point group. We show how a lattice gauge theory can incorporate the coarse-grained order parameter theory of such generalized nematics and allows them to be studied on a general footing. The lattice gauge theory consists of a nematic nearest-neighbor interaction of gauged $O(3)$-rotors and a term for the gauge fields that encodes for the nematic defects. The phase diagrams of the model can be obtained efficiently by simulations and these show the generalized nematic phases at low temperatures. In this common framework, we quantify the fluctuations of the orientational order parameters of generalized nematics by comparing the lattice model with different point-group symmetries. For highly symmetric nematics, a chiral liquid phase is found in between the nematic and the isotropic liquid via an order-out-of-disorder mechanism. The gauge theory also allows us to list the minimal order parameter tensors allowed by the symmetries for all point groups. Finally, we show how many phase transitions between different nematics can be accessed by tuning the parameters of the theory.

*Poster

Generalized Drift Velocity of a Cholesteric Texture in a Temperature Gradient

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Cholesteric liquid crystals (LC) are chiral nematics. Under the action of a temperature gradient, their texture can drift in a permanent way. This drift can be rotational or translational. The most simple example of a rotational drift is the continuous rotation of translationally invariant configurations (TICs) [1]. In the TICs (photo 1), the director field is only twisted along the normal to the glass plates limiting the sample and the temperature gradient is parallel to the helical axis. Another example of rotational drift is the rotation of the texture of cholesteric droplets (photo 2), when they coexist with their isotropic liquid at the melting temperature of the LC. This is the Lehmann effect discovered in 1900 and re-observed recently [2]. (1) (2) (3) An example of translational drift is the transverse drift of the cholesteric fingers (CFs) leading to the formation of spirals (photo 3). Isolated CFs form in homeotropic samples when the equilibrium helical pitch is close to the sample thickness. Their drift is induced by a temperature gradient perpendicular to the plates. This phenomenon was first observed close to the compensation temperature of a compensated cholesteric LC [3] and more recently in dilute cholesteric mixtures close to the transition to the smectic phase [4]. All these drifts can be explained by invoking a chiral coupling called the Leslie torque. We propose a general formalism to calculate the generalized drift velocity of these textures [5] and we show that other mechanisms can lead to a similar drift. In particular, the role of the temperature variations of the elastic constants and of the "nematic like" thermomechanical coefficients of Akopyan and Zel'dovich is analyzed in each of the experiments cited above. [1] P. Oswald and A. Dequidt, "Direct measurement of the thermomechanical Lehmann coefficient in a compensated cholesteric liquid crystal," Europhys. Lett. 83, 16005 (2008). [2] P. Oswald and A. Dequidt, "Measurement of the continuous Lehmann rotation of cholesteric droplets subjected to a temperature gradient," Phys. Rev. Lett. 100, 217802 (2008). [3] P. Oswald and A. Dequidt, "Thermomechanically driven spirals in a cholesteric liquid crystal," Phys. Rev. E 77, 051706 (2008). [4] P. Oswald, "Experimental study of the growth of cholesteric fingers subjected to an AC electric field and a temperature gradient," Liq. Cryst. 36, 967–975 (2009). [5] A. Dequidt and P. Oswald, "Generalized drift velocity of a cholesteric texture in a temperature gradient," in preparation.

*Poster

Interaction between polymer-grafted nanoparticles in chemically identical homopolymer matrix

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In this research, we develop a new numerical scheme of self-consistent field theory (SCFT) to quantify interparticle interaction between two spherical nanoparticles (NPs) coated with polymer grafts in chemically identical homopolymer melts. In our numerical SCFT calculation, two-dimensional finite volume method (FVM) which efficiently conserves the amount of material in curvilinear coordinate is adopted, and the differential equation for partition function is solved in real space with Multicoordinate-system (MCS) scheme which makes use of the mirror symmetry between the two particles. In this research, we investigate how distribution of chain lengths, grafting density and particle curvature interplay roles on stabilization mechanism for dispersion by calculating interaction potentials between two polymer-coated NPs as functions of distance between the two particles. Our results reveal that polydisperse distribution stabilizes dispersions more efficiently than monodisperse counterparts.

*Poster

Molecular emulsions: bridging the gap between liquids and emulsions

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By using the universality of micro-heterogeneity in aqueous and non-aqueous mixtures, we propose to unify liquids with soft matter through the concept of molecular emulsions. This proposition encompass the micro-segregation -typically observed in aqueous mixtures, and the micelles -observed in emulsions in a single microscopic description. The statistical mechanical basis for such unified description are proposed, and the pivotal conceptual foundation is the distinction between concentration fluctuations and the pre-peak in the structure factor. The former control the mechanical stability of the mixtures (as witnessed by the k=0 part of the structure factor) and correspond to macroscopic thermodynamical response. The latter is a typical microscopic response, universally witnessing the appearance of stable microscopic equilibrium heterogeneity. This second feature poses several problems that we review, such as i) the existence or not of the pre-peak as an observable in the scattered intensity (Xray, neutron or light) in relation to molecular conformations; ii) the problems posed in computer simulations of systems exhibiting micro-heterogeneity at different scales; iii) problems posed in statistical liquid state theories. The existence of such problems turns out be be at the heart of our description of matter from a wider point of view.

*Poster

Mechanics of a knitted fabric

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Knitting is a thousand year old technology, though considered by most as a mere art and craft hobby. Unlike weaving, it can produce loose yet extremely stretchable fabric with almost vanishing rigidity, a desirable property exhibited by hardly any bulk material. It also enables the engineering of arbitrarily shaped two- and three-dimensionnal mechanical objects with tunable response. As such, it is a promising venue to achieve four-dimensional functionality and mechanical metamaterials. In contrast with the extensive body of related popular knowledge, and despite a growing industrial interest, the physical ingredients underlying these intriguing mechanical properties remain poorly understood. As a matter of fact, the interplay between the constitutive yarn properties and local topological features - the stitches - cannot be easily described by standard continuum mechanics. In order to make some progress in this direction, we study a model tricot made of a single elastic thread knitted into the common pattern called stockinette. On the one hand, we experimentally investigate its tensile response and measure local stitch displacements during deformation. On the other, we derive a first-principle mechanical model for this displacement field based on the yarn bending energy and the conservation of its length. Quantitative agreement is found between our predictions and measurements for the shape and mechanical response of this system. This work thus provides a fundamental framework for the understanding of knitted systems, paving the way to thread based smart materials.

*Poster

Kinetic models of chemically reactive dense fluids

Jacek Polewczak * [1]

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I consider various simple reacting spheres (SRS) kinetic models of dense fluids. In the SRS models, the molecules behave as if they were single mass points with two internal states. Collisions may alter the internal states of the molecules, and this occurs when the kinetic energy associated with the reactive motion exceeds the activation energy. Reactive and non-reactive collision events are considered to be hard spheres-like. A four component mixture A, B, A^* is considered in which the chemical reactions are of the type $A + Bightleftharpoons A^* + B^*$, with A^* and B^* being distinct species from A and B. Fundamental physical and mathematical properties of the SRS models are provided.

*Poster

Determining the Inter-Particle Force-Law in "Static" Colloids and Amorphous Solids from a Simple Visual Image

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We propose a new algorithm to determine the inter-particle normal force-laws for colloidal or other amorphous system which are static (up to vibrations) within the observation time-scale. A visual providing the particle positions in addition to a measurement of the pressure is all that is required. Having n different types of constituents we determine the coefficients in the Laurent expansions for the $n(n+1)/2$ different normal force-laws. The derived force-law and per-particle net forces are employed in a novel process that not only improves the prediction of the force-law but also allows us to correct the unavoidable experimental measurement errors in the positions.

*Poster

Experimental study of rising bubbles in a confined polymer solution: Morphology, dynamics and interactions

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This study focuses on the rising of air bubbles in a viscoelastic, shear-thinning fluid confined in a vertical quasi bidimensional system (vertical Hele-Shaw cell). The fluid is a concentrated polymer solution of polyethylene oxide (PEO) in water. First, we report the shape of a single rising bubble as a function of its volume, and check the appearance of a singularity at its rear (cusp). Second, we follow the bubble dynamics and evidence that, when the bubble is large enough, an instability develops. The front of the bubble flattens at a given angle, and the bubble does not follow a vertical trajectory anymore. Depending on the flattening angle of the front, the bubble either deviates from its trajectory or develops a downward finger, recalling the Saffman-Taylor instability, which leads to its fragmentation. Finally, when a constant air flow-rate is injected at the cell bottom, bubbles rise continuously and interact to form clusters or coalescing bubbles. Preliminary results on the evolution of their shape and dynamics due to these interactions will be presented.

*Poster

Lehmann effect: the end of the Leslie paradigm

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In 1968, Leslie developed nematohydrodynamics. In generalizing the theory to the cholesteric phase, he showed the existence of new thermomechanical terms in the constitutive equations of the phase leading to a torque on the director of expression $\mathbf{\Gamma_{Leslie}} = \nu\mathbf{n} \times (\mathbf{n} \times \mathbf{G})$ with $\mathbf{G}$ the temperature gradient, ν the Leslie coefficient, and $\mathbf{n}$ the director. Leslie immediately proposed that this torque was responsible for the rotation of the cholesteric droplets observed by Lehmann in 1900 when they are subjected to a temperature gradient. Up to recently this explanation was adopted by the majority of researchers. In this report, we present two sets of experiments to demonstrate that this explanation must be revised. First, ν was directly measured by observing the rotation of the helix in cholesteric samples treated for planar sliding anchoring. The main result is that ν is independent of the equilibrium twist of the phase, q. In particular, ν and q are not always of the same sign [1] and ν is different from 0 at the compensation temperature of the phase, when $q = 0$ [2]. This result shows that ν is of microscopic origin, i.e. related to the molecular chirality, and it is not due to the twist of the director field. Second, the Lehmann effect was reproduced [3]. Measurements with cholesteric phases evidenced that the rotation velocity of droplets such as the banded one shown above is directly connected to q. More precisely, it was shown that the sense of rotation is always given by the sign of q, independently of the sign of ν. In addition, the order of magnitude of the droplet rotation velocities is incompatible with the value of ν [4]. These results cannot be explained by Leslie's model, since the macrocopic twist of the phase determines the Lehmann rotation. To definitively prove the macroscopic origin of the Lehmann rotation [5], we prepared twisted bipolar droplets of a lyotropic chromonic nematic phase, such as the one shown above. Because the phase is not chiral, the director field inside the droplets can be right- or left-handed. By subjecting these droplets to a temperature gradient, we observed their rotation, half of them rotating clockwise and the other half counterclockwise. This experiment provides evidence that the Lehmann effect also exists in achiral nematics and that it is only due to the macroscopic chirality of the director field. This definitely proves that the Leslie thermomechanical coupling cannot explain the Lehmann effect. [1] P. Oswald, *Europhys. Lett.*, 2014, **108**, 36001 and 59901 (Erratum).
[2] P. Oswald and A. Dequidt, *Europhys. Lett.*, 2008, **83**, 16005.
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[4] P. Oswald, *Eur. Phys. J. E*, 2012, **35**, 10.
[5] J. Ignés-Mullol, G. Poy and P. Oswald, in preparation.

*Poster

Polymer models with competing collapse interactions on Husimi and Bethe lattices

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In the framework of Husimi and Bethe lattices, we investigate a generalized polymer model that incorporates as special cases different models previously studied in the literature, namely, the standard *interacting self-avoiding walk*, the *interacting self-avoiding trail*, and the *vertex-interacting self-avoiding walk*. These models are characterized by different microscopic interactions, giving rise, in the two-dimensional case, to collapse transitions of an apparently different nature. We expect that our results, even though of a mean-field type, could provide some useful information to elucidate the role of such different *theta points* in the polymer phase diagram. These issues are at the core of a long-standing unresolved debate.

*Poster

Shear banding and the soft sphere model

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This paper studies shear banding and shear localization phenomena in foams using the 2-dimensional Durian bubble model. The shear is induced in a planar Couette configuration, using moving boundaries in the y-direction, and periodic boundaries in the x-direction. Depending on the interparticle potentials and drag velocities used, we find four possible scenarios: 1) Linear flow profile, 2) Total wall slip at the moving wall, 3) Transient shear banding during the start-up phase, or 4) Shear localization. Based on the parameters, each scenario corresponds to a unique system as follows. Linear flow profile is obtained for repulsively interacting soft spheres with drag induced by the background, corresponding to a Bragg raft[1]. Total wall slip is observed for repulsively interacting soft spheres, with zero drag, the case of a bubble raft confined between two plates [2]. Transient shear banding [3] could be found in the case of short-range attractive soft spheres, i.e. a bulk foam, or a microgel [3]. Shear localization appears in a system of short-range attractive soft spheres at small shear rates. Furthermore, the evolution of the pair correlation functions are analyzed during the start-up flows to shed light on the transition between flowing and stationary state. [1] J. Lauridsen, G. Chanan, M. Dennin, Phy Rev Lett 93, 18303 (2004). [2] G. Debregeas, H. Tabuteau, J.M. di Meglio, Phys Rev Lett 87, 17–8305 (2001). [3] T. Divoux, D. Tamarii, C. Barentin, S. Manneville Phys. Rev. Lett. 104, 208301 (2010).

*Poster

Pumping aqueous electrolytes in submicron tubes, using a beam of light

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We consider a focused laser beam which passes through an aqueous electrolyte. The beam is partially absorbed by electrolyte; consequently electrolyte's temperature locally rises, in and around focal area. The positive/negative ions then move in the spatially varying temperature field. For a 1:1 electrolyte, say NaCl + water, both types of ions show some tendency to move toward the colder parts of the electrolyte. But this tendency is not equal for positive and negative ions. Consequently, when the steady state is reached, there would be a net charge accumulated in the heat absorbing area. We put forward the idea of using a focused beam to heat up a small region in a submicron tube; the tube is filled with aqueous electrolyte. We calculate the net charge which gathers in the heat absorbing area. Moreover, we find an oppositely charged diffusive layer which is formed in the vicinity of tube's lateral boundary. We also calculate how the net accumulated charge decreases, as the focal area approaches – close enough to – the tube's lateral boundary. Now, an external electric field, applied parallel to tube's axis, will exert forces on both the net charge in the focal area, and on the oppositely charged diffusive layer, in the vicinity of tube's boundary. The boundary imposes a significant hydrodynamics friction on the fluid, and ions, in its vicinity and inhibits their motion. Therefore, the dominant part of fluid flow comes from the force exerted on the accumulated charge in the focal area, and not from the electric force exerted on the diffusive layer. This results in a net flow, which is adjustable by changing the distance between focal area and tube's lateral boundary. To best of our knowledge, this is the first suggested method for inducing and controlling fluid flow inside submicron tubes, using a beam of light. We appreciate another existing method, suggested by Dieter Braun and his colleagues, which uses an advancing focal area to induce fluid flow [Weinert, Franz M., et al. "Microscale fluid flow induced by thermoviscous expansion along a traveling wave" Physical review letters 100 164501 (2008)]. Their method, however, does require a backward flow (i.e. loops of fluid motion) to function. It functions in 2D geometry, like a fluid film, but not in the semi-1D geometry of thin tube. Thus, we are suggesting the first light induced/controlled pumping method which is capable of generating fluid flow inside a thin submicron – or even nano – tube. • Note: The corresponding manuscript is under preparation for resubmission to PRL. I will inform statphys2016 organizing committee if it happens to be accepted for publication there.

*Poster

Modeling the active motion of vesicles in the oocyte

Nitzan Razin * [1], Nir Gov

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We study how the active motion of particles can cause a pressure gradient on a large passive object, that moves it to a target position. This is motivated by recent experiments, which showed that the nucleus of a mouse oocyte (immature egg cell) moves from the cortex to the center due to a pressure gradient exerted by the active motion of vesicles. Assuming an active Brownian particle model, we explore what are the possible density, velocity and pressure profiles. Specifically, we suggest two possibilities for reproducing the experimentally observed profiles for the vesicles.

*Poster

Structure and dynamics of binary liquid mixtures near their demixing transitions

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The critical behaviour of five binary Lennard-Jones liquid mixtures, close to their demixing points (model H'), are studied computationally with a combination of semi-grand canonical Monte Carlo simulations and graphic processing units (GPU) based large-scale molecular dynamics (MD) simulations. The symmetric binary liquid mixtures considered cover a variety of densities, a wide range of compressibilities, and different interactions between the unlike particles. The static quantities studied here encompass the bulk phase diagram (including both the binodal and the λ-line), the correlation length, the concentration susceptibility, the compressibility of the finite-sized systems at the bulk critical temperature T_c and the pressure. Concerning the collective transport properties, the focus is on the interdiffusion coefficient and the shear viscosity. The critical power-law singularities of these quantities are analysed in the mixed phase (above T_c) and non-universal critical amplitudes are extracted. In this context, two universal amplitude ratios are also calculated. Our results are compared to the theoretical predictions of mode-coupling and dynamics renormalization group theories for dynamics and for statics, with the expectations for three dimensional Ising universality class. Evidence is reported for an inverse proportionality of the pressure and the isothermal compressibility at the demixing transition.

*Poster

The Voronoi Liquid

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In soft matter physics Voronoi tessellations are widely used to probe the local environment of particles. For instance, by considering analytical properties of these tessellations, two new conserved fields have been proposed recently as new tools to probe phenomenology arising in the supercooled regime of glass-forming polymer melts [1]. In contrast with this "passive" role of observable on a given system, we present here a new way of dealing with the Voronoi tessellations, by defining a new type of liquid, for which the force field is directly expressed through a polarisation field of the Voronoi tessellations [1] [2]. Beyond the fact that the interactions are intrinsically many-body this so-called "Voronoi liquid" has very unusual properties : unique thermodynamic scaling properties, a zero-separation theorem reminiscent of what is known in the context of hard spheres or an apparent violation of the hydrodynamic scaling for the sound attenuation. Through numerical simulations we studied the Voronoi liquid at constant density for a wide range of temperatures. We demonstrated the thermodynamic stability of the fluid, the existence of a bcc crystalline phase with a high mobility and marked pretransitional effects. The model studied is actually one example of a whole family of models which could be devised using similar concepts. In particular, a binary generalization of the Voronoi liquid is possible, for which the crystallisation is prevented. We showed that the outcoming glass-forming liquid has a marked degree of fragility, as well as a strong heterogeneity of the dynamics. We will discuss the possible link of these characteristics with an observed well developped pre-hydrodynamic power law regime. [1] J.Farago et al. Eur. Phys. J. E (2014) 37, 46 [2] C.Ruscher et al. EPL, 112 (2015) 66003

*Poster

Local insight of ultrasound echography in shear-thickening fluids

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We study shear-thickening in two concentrated suspensions of density-matched micronized particles : PMMA (6 μm) particles suspended in a NaI aqueous solution and cornstarch suspensions in a CsCl aqueous solution. By combining ultrafast ultrasonic imaging and macroscopic rheometry in small-gap Couette geometries, we show that the flow of these suspensions remains spatially homogeneous through both continuous and discontinuous shear-thickening transitions. We also find evidence for finite-size effects in the flow behaviour and for the absence of an intrinsic local flow rule. We further characterize temporal fluctuations that may occur during discontinuous shear-thickening and discuss our results in light of recent experimental and theoretical work.

*Poster

Solid-liquid like phase transition in a model confined granular suspension

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We present an experimental study of a liquid-solid like phase transition in a two-dimensional dynamically suspended granular media. Particles are placed in a vertical Hele-Show cell filled with a denser solution of cesium-chloride. Thus, when the cell is rotated around its axis, hydrostatic pressure exerts a centripetal force on the particles which confines them towards the center. This force is in competition with gravity, and by modifying the rotation rate, it is possible to transform continuously and reversibly the sample from a disordered loose state to an ordered packed state. The transition is characterized by the appearance of instable locally crystallized clusters in the liquid state which grows in size, until they percolate to form a unique stable crystallized phase, and two scaling exponents are extracted from the cluster size distributions. We discuss the possibility to extend the grand-canonical formalism to out-of equilibrium systems, in order to uncover a state equation between the density and the pressure in the medium.

*Poster

An exactly solvable model for discontinuous transitions in the velocity of crack propagation in viscoelastic solids

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In viscoelastic solids, discontinuous transitions in the velocity of crack propagation have experimentally been observed in a narrow range of the energy release rate by using elastomers filled with carbon black particles [1-3]. Although various theoretical studies have been performed on the crack propagation in viscoelastic solids [4-7], the physical mechanism of the transition has yet to be clarified. In this study, we propose a simple model for the crack propagation in viscoelastic solids for which an exact analytic solution exhibiting the velocity transition is available for the energy release rate as a function of the crack propagation velocity. On the basis of the exact expression, we provide an existence condition of the velocity transition and simple relationships useful as guiding principles to develop tough polymer materials, elucidating the physical mechanism of the transition. Our result implies that the discontinuous transition in the crack propagation velocity is a universal phenomenon that should be observed in a broad class of viscoelastic solids. An analogy between the velocity transition of our model and conventional discontinuous phase transitions are also discussed. The healing length of the stress and strain distributions plays a role of an order parameter in the context of conventional discontinuous phase transitions. [1] A. Kadir and A. G. Thomas, Rubber Chem. Technol. 54, 15 (1981). [2] K. Tsunoda, et al., J. Mater. Sci. 35, 5187 (2000). [3] Y. Morishita, K. Tsunoda, and K. Urayama, Phys. Rev. E, in press (2016). [4] J. A. Greenwood and K. L. Johnson, Philos. Mag. A 43, 697 (1981). [5] M. Barber, J. Donley, and J. S. Langer, Phys. Rev. A 40, 366 (1989). [6] B. N. J. Persson and E. A. Brener, Phys. Rev. E 71, 036123 (2005). [7] G. Carbone and B. N. J. Persson, Phys. Rev. Lett. 95, 114301 (2005).

*Poster

Exact Energy Computation on the 2d Dyson gas for Even Values of the Coupling Parameter

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Using the approach of Vandermonde determinant to the power $\Gamma = q^2/(k_B T)$ expansion on the monomial functions, it is provided a way to find the energy of the excess energy U_{exc} of two dimensional one component plasma 2dOCP on the hard and soft disk for even values of Γ. The excess energy is fitted to the anzats of the form $U_{exc} = K_\Gamma^1 N + K_\Gamma^2 \sqrt{N} + K_\Gamma^3 + K_\Gamma^4/N + O(1/N^2)$ to study the finite-size correction with K_Γ^i coefficients for several values of the coupling parameter $\Gamma = 2, 4, 6 \ldots$. At the special coupling $\Gamma = 2$ the K_2^i coefficients are computed explicitly finding that the excess energy per particle K_2^1 is in agreement with the well known result of Jancovici for the hard disk.

Key words: Coulomb gas, one-component plasma

*Poster

Equilibrium configurations of flexible magnetic filaments: effects of static external magnetic fields

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We study, by means of Langevin dynamics computer simulations, how the presence of a static external magnetic field modifies the conformational phase diagram of magnetic filaments in the limit of infinite dilution. The knowledge and control of the different types of structures that magnetic filaments may adopt is a key factor for the tuning of the properties of finite concentrations and, consequently, determinant for the potential applications of these systems, like nanoactuators or magnetoresponsive coatings. Here, we consider the filament immersed in either a good or a poor solvent (non-sticky filaments and Stockmayer polymer-like filaments, respectively). We found that, under the influence of an applied field, filaments are much more susceptible to background parameters such as temperature and solvent quality. This increased susceptibility of the filaments is due to the fact that the external magnetic field tends to flatten the configurational free energy landscape, favoring the coexistence of conformational states that were separated by large differences in the zero-field case. In this new scenario, conformational multistability arises, manifesting itself in the existence of broad regions in the phase diagram where two or more equilibrium configurations coexist.

*Poster

Dynamics of auto-motile filament propelled by self-generated solute gradient

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Self-propulsion of objects by utilizing the chemical energy is commonly observed phenomena in bi- ological as well as non-biological systems.In the biological context, molecular motors such as kinesin, swimming bacteria such as E. coli are such kind of examples. In nature, these kind of active motors can be distributed along the length of a line like filament. Microtubule is such an example where molecular motors seating on them convert chemical energy into mechanical energy and moves along the length of the microtubule. With this movement, the microtubule shows conformational change and exhibits fascinating cilia-like beating phenomenon. In recent past, people have fabricated biocompatible active polymeric motors in the lab which show highly efficient mode of transportation and drug release. Till date, the underlying mechanism behind the dynamics of these kinds of active polymer still not understood very well. Motivated by those examples, we propose a model of a semi-flexible polymer having "active" elements distributed along its length, which is responsible for its directed motion when introduced in a solution with the fuel for energy conversion. The activity in the filament is incorporated by inserting chemically active dimers at regular intervals along the chain. The chemical reactions at the catalytic bead of the dimer produce a self-generated concentration gradient and gives sufficient fuel to exhibit self-propulsion for the filament. We show that this active filament displays the variety of dynamical states like rotational(R), snaking(S) and transnational (T), depending upon the rigidity and configuration of the chain. We investigate the various dynamics obtained during the spontaneous motion of the filament and elucidate the consequences of principal factors that control the filament directed movement. We employ the hybrid MD-MPCD model to study the polymer dynamics. References [1] R. D. Vale and R. A. Milligan, Science 288, 88 (2000). [2] T. Sanchez, D. Welch, D. Nicastrro and Z. Dogic, Science 333, 456(2011). [3] Z. Wu et al., Angew. Chem. Int. Ed 52, 7000 (2013). [4] Coarse-grained simulations of an active filament propelled by self-generated solute gradient. Debarati Sarkar and Snigdha Thakur. (Accepted in Phys. Rev. E).

*Poster

Two-Step Relaxation Mode Analysis with Multiple Evolution Times: Application to a Single [n]Polycatenane

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A method of two-step relaxation mode analysis (RMA) with multiple evolution times is proposed. In this method, usual RMA with single evolution time is first applied to relevant physical quantities. Then, RMA is applied again to a part of the slowest relaxation modes obtained by the first RMA, where the evolution time for each mode is determined from its relaxation rate. The first step gives rough estimation of the relaxation modes and rates, while the second step corresponds to the reduction of the degrees of freedom and the refinement of the estimation. The effectiveness of the method is demonstrated by its application to a Brownian dynamics simulation of a single [n]polycatenane in the free-draining limit.

*Poster

Crystallization of a confined monolayer of magnetized beads

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We present experimental results obtained with a model experimental system dedicated to the study of 2D phase transitions and structures. The system is composed of a set of millimetric soft ferromagnetic beads confined in a 2D horizontal cell. The beads are immersed in a vertical magnetic field inducing magnetic dipole-dipole interactions. Due to the confinement, produced by the repulsive edges of the cell, the interactions tends to order the system. In addition, the system is submitted to a mechanical agitation which produce an erratic motion of the beads and thus creates disorder. Controlling the competition between interaction energy and entropy, allows us to explore different structures of 2D system. With such an experimental set-up, the melting of a two dimensional crystal has been studied (see results in Phys. Rev. E.87, 062201 (2013)). The influence of the shape of the repulsive cell on the crystal state of the system is also discussed. Indeed, the repulsive edges of the cell represent geometrical constraints forcing the local orientation of the crystal and thus frustrations when the symmetry of the cell is far from the natural symmetry of the lattice (hexagonal). The frustration leads to the observation of grain boundaries delimiting multiple domaines in the crystal.

*Poster

Simulation of polymer melts with GPU acceleration

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We implemented the elastic lattice polymer model on the GPU (Graphics Processing Unit), and showed that the GPU is very efficient in these calculations. A speedup of a factor 35 is reported over a very well optimized CPU implementation. The new GPU implementation allows us to study the static and dynamic properties of polymer melts in more detail than before. A prime example is the system of non-concatenated ring polymers in a melt, which could give important clues towards our understanding of large scale chromosome organization.

*Poster

Topology-induced quantisation of density levels in fluids confined to nanometric pores

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The confinement of simple fluids to narrow pore spaces changes the phase behaviour of the fluid, leading to phenomena such as capillary condensation or adsorption. A central open question in this context is the dependence of thermodynamic properties on the shape of the pore geometry. The morphometric approach for simple fluids is derived by assuming that the grand potential $\omega(K, \mu, T)$ of a fluid is an additive functional of the pore geometry K. In this case, Hadwiger's theorem states that $\omega(K, \mu, T)$ can only depend on K as a linear combination of the so-called Minkowski functional, $\Omega = -p(\mu, T)V[K] + \sigma(\mu, T)A[K] + \kappa(\mu, T)C[K] + \overline{\kappa}(\mu, T)X(K)$ where V and A are the volume and interface area of the pore and $C[K]$ the integrated mean curvature. $X[K]$ is the Euler number that characterises the pore connectivity and is a topological constant. We here use density functional theory using the fundamental measure theory functionals to demonstrate that this theory is consistent with numeric DFT results, for the important case of triply-periodic network-like pore geometries defined by cubic minimal surfaces. For these, the formula $\langle N \rangle(K, \mu, T) = -\partial\Omega/\partial\mu$ can be inverted to give an estimate of X deduced from the simulated densities – the Euler number 'felt' by the fluid. We show that for the Primitive, Gyroid and Diamond minimal surfaces the obtained values are close to the morphological Euler number, confirming a posteriori the assumptions of the theory. Counter-intuitively, this result suggests that hard sphere fluids can 'feel' topological properties of a confining pore space, in addition to geometric ones.

*Poster

Diffusion of active swimmers in rough channels

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We investigate the diffusion properties of active particles in two-dimensional rough channels. The channel boundaries are modeled by hard walls represented by a bounded periodic function. The channel roughness is taken into account by superposing a hierarchy of periodic functions with different amplitudes and different periods, these make the pore length of the channel to increase. This increment of the channel length along with the roughness of the boundary, have profound effects on the diffusion properties of active particles.

*Poster

Wang-Landau type Monte Carlo study of crystallization in melts of short semi-flexible polymers

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Phase transitions in polymer melts have been under intensive experimental as well as theoretical investigation for many years. We present results of Wang-Landau Monte Carlo simulations of a melt of short semi-flexible polymer chains. The estimated density of states covers more than 5000 orders of magnitude and describes thermodynamical properties at the full energy range of the system. An analysis of the density of states shows that our model system undergoes a first-order phase-transition upon increasing the chain stiffness at constant density. The investigation of chain properties demonstrates crystallization of the model system into a rotator-like phase similar to rotator phases of n-alkane's melts. Because of the purely hardcore repulsive nature of bead-bead interactions, maximization of the entropy of the system is the main driving force of the phase transition. As a result, chains are stretching and nematicaly ordering at the transition temperature. Hexatic ordering perpendicular to the director is governed by the effective thickness of the chains similarly to the transition into a hexatic phase of 2d hard-disks systems. Due to weak but still significant size effects, the chains remain mobile along the nematic director. But in accordance to the real systems in the rotator-phase we found a tendency to organize in lammelae in the case of the least size effects. Consideration of the system in the phase coexistence region shows regimes of stability of different types of morphology which transitions are correlated with step-like changes of the inverse microcanonical temperature. We attribute these transitions to droplet evaporation-condensation transitions.

*Poster

Differential stability of DNA in the ionic solution

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Intracellular positive ions (cations) nullify the negative charges on the phosphates of DNA strand due to which the hydrogen bond gets more strength to hold together and that is the embodiment of enhanced stability of the system. The two strands are connected with each other through the hydrogen bonds between the bases on the opposite strands. However, the stability of DNA helix depends on the charge neutrality of the system. To counter the negative charges on the strands, the cellular environment require some positive charges in order to nullify the repulsion between negative charges. Nature develops positive ions from the salt that are dissolved in the body. The primary salts are $NaCl$ and $MgCl_2$ which on reaction with water release Na^+ and Mg^{2+}. The chlorine rearranges itself in form of hydrogen chloride (HCl). These cations act as the electrostatic screening agents by creating an attractive forces between the positive ions and the negative charges on the strands. The stability of DNA helix is governed by the balance between the attractive and repulsive forces exist in the system. These forces exist in the form of hydrogen bonding between the bases on the opposite strands, the stacking interaction along the strands, the repulsion between same kind of charges and attraction between opposite kind of charges. Various experiments followed by theoretical investigations on the role of salt in screening the repulsive forces in DNA revealed many interesting results. Not only the stability of DNA molecule but effect of salt on the $B-A$ transition, in the condensation of DNA molecule have been studied in detail by several researchers. In all these studies the stability of DNA has been studied under low or moderate (0.1-1.0 M) concentration of salt. Several experiments, conducted by groups of Owczarzy and SantaLucia revealed that short as well long DNA molecules becomes more stable as the content of cations in the solution increases. The stability of the structure were identified by calculating the melting temperature (T_m) of the molecule. In all these experiments, the melting temperature was found to have a logarithmic dependence on the amount of cations present in the solution. The theoretical work followed by these experiments attempt to explain the logarithmic dependence. These work were either based on semi-empirical formula or based on statistical models. The counterion theory proposed by Manning explains the stability of DNA molecule due to presence of salt in the solution. The stretching and unzipping behaviour of DNA molecule in the presence of cations are discussed by several groups. These results show that the mechanical stability of DNA molecule also increases with the content of cations. In another set of experiments that were executed at, relatively high salt concentration, people observed some strikingly different behaviour of DNA molecule. These experiments found that in this range of concentration the stability of DNA get shattered. Interestingly, in a similar kind of experiments, several research groups tested the condensation process and melting profile in DNA under different ethanol concentrations. One of the findings of the these experiments revealed that at relatively higher concentration of ethanol, the melting temperature of the system increases. As far as the role of cations *in vivo* is concerned, it is manifold. Keeping in the view the important aspect of the salt in the cell, we propose a theoretical description of the stability of DNA molecules at higher salt concentration. We consider one of the DNA sequences studied by Khimji *et al.*. They studied the DNA duplex stability in crowded polyanion solutions. For

*Poster

the current investigations we adopt the standard Peyrard Bishop Dauxois (PBD) model and modify the potentials appear in the model. In our earlier works, we showed that the PBD model has enough details which can be used to explain the thermal as well as mechanical stability of DNA molecule at lower strength of salt with varying salt concentration. 1. I. Khimji, J. Shin, and J. Liu, DNA duplex stabilization in crowded polyanion solutions, Chem. Commun., v49, p1306-1308 (2013) 2. K. Hatch, C. Danilowicz, V. Coljee, and M. Prentiss, Measurement of the salt-dependent stabilization of partially open DNA by Escherichia coli SSB protein, Nucleic Acids Research, v36, p294-299, (2008) 3. G.S. Manning, Counterion Condensation on a Helical Charge Lattice, Macromolecules, v34, p4650-4655, (2001) 4. Amar Singh and Navin Singh, Effect of salt concentration on the stability of heterogeneous DNA, Physica A, v419, p328 - 334, (2015) *and references therein*

Relaxation of a Single Star Polymer

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Relaxation of a single star polymer with the excluded volume interaction is studied by molecular dynamics simulations in the free draining limit. A star polymer consists of a center segment and f linear arms, each of which has M segments. Relaxation rates are estimated from the long-time behavior of the time-displaced autocorrelation functions of relaxation modes of an ideal star polymer with no excluded volume interaction. The behavior of the second slowest relaxation rate $lambda_2$ agrees well with the scaling prediction [3,4] for the relaxation of overall shape deformation $lambda_2 proptof^{u-(1/2)}M^{-2u-1}$. Here, $usimeq0.6$ is the Flory exponent. In contrast, the results for the slowest relaxation rate $lambda_1$ suggest the behavior $lambda_1 proptof^{u-1}M^{-2u-1}$, which corresponds to the exchange of the positions of two arms, rather than the scaling prediction [3] $lambda_1 proptof^{u-2}M^{-2u-1}$ for the rotational relaxation.
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*Poster

Numerical Study of Splash Detail Due to Grain Incident on Granular Bed

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Using the discrete element method (DEM), we study the splash processes induced by the impact of a grain on a randomly packed bed. Good correspondences are obtained between our numerical results and the findings of previous experiments for the movement of ejected grains. Furthermore, the distributions of the ejection angle and the vertical ejection speed for individual grains vary depending on the relative timing at which the grains are ejected after the initial impact. Obvious differences are observed between the distributions of grains ejected during the earlier and later splash periods: the form of the vertical ejection-speed distribution varies from a power-law form to a lognormal form with time, and this difference may determine the grain trajectory after ejection. In addition, we focus on the bulk dynamics inside the granular bed to relate the ejected grains behavior to the force propagations from the first impact to the ejection.

*Poster

Imbibition of Micro-Patterned Surfaces

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Wetting phenomena, such as water-repellency and imbibitions, have been familiar to us in daily life for a long time. Such phenomena and control of small amounts of liquid are important issues in various contexts including medical sciences to fuel delivery. By virtue of the progress of micro-fabrication technologies, imbibition of micro-patterned surfaces has actively been studied in these days; the imbibition length z scales with the square root of elapsed time t in the viscous regime [1], while another scaling law $z \sim t^{1/3}$ has been found for the imbibition of another type of textured surfaces [2] ($z \sim t^{1/3}$ was also reported for the dynamics of capillary rise into corners [3,4]). The difference between the exponents appearing in the scaling laws seems to be caused by geometries and sizes of micro structures on surfaces, however the crossover between the two dynamics has yet to be clarified. We experimentally and theoretically investigate imbibition of two different micro-patterned surfaces as follows: (1) Capillary rise on the surface of a leg of a small animal (wharf roach) and on the surfaces mimicking it [5]. In this work, we found a non-slowing down dynamics on a coarse-grained level for capillary rise on the surface of a sixth leg of the small animal, wharf roach. Motivated by this unusual feature, we also studied imbibition of artificial micro-patterned surfaces partially mimicking the surface of the sixth leg, then we confirmed that our composite model well describes experimental results although we could not reproduce non-slowing down dynamics. Furthermore, we found the capillary rise on the hybrid surfaces partially mimicking the surface of the leg is faster than the capillary rise on non-hybrid surfaces. (2) Capillary rise into "open-capillary" [6]. We carried out experiments with an open capillary tube whose cross-section is rectangular on a submillimeter scale, and then observed two regions in the tube: a liquid column in which the open capillary is almost completely filled with the liquid, and a precursor film that proceeds ahead of the liquid column. For the liquid column, we confirmed that scaling laws we developed for the statics and for the dynamics in the initial (viscous) and final (visco-gravitational) regimes well describe the experimental results. For the precursor film, we confirmed that its length h scales with $t^{1/3}$. Thus, the progress of the precursor film is regarded as capillary rise into the corners of the open capillary. Furthermore, we demonstrated two applications, multiple color changes of the BTB solution and the expression of Green Florescence Protein (GFP), in older to show capabilities of devices that utilize open channels and that are driven not by pumps but by capillary force. [1] C. Ishino, M. Reyssat, E. Reyssat, K. Okumura and D. Quéré, *Europhysics Lett.* **79**, 56005 (2007). [2] N. Obara and K. Okumura, *Phys. Rev. E Rapid Commun.* **86**, 020601 (2012). [3] A. Ponomarenko, D. Quéré and C. Clanet, *Journal of Fluid Mechanics* **666**, 146 (2011). [4] L. -H. Tang and Y. Tang, *J. Phys.II France* **4**, 881 (1994). [5] M. Tani, D. Ishii, S. Ito, T. Hariyama, M. Shimomura and K. Okumura, *PLOSOne* **9(5)**, e96813 (2014). [6] M. Tani, R. Kawano, K. Kamiya and K. Okumura, *Sci. Rep.* **5**, 10263 (2015).

*Poster

Reciprocating motion of active deformable particles in homogeneous media

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Active particles exhibit not only a simple translational motion but also other dynamical motions including active spinning (rotational) motion, spontaneous deformation, and self-replication. Recently the existence of reciprocating motion in a homogeneous medium has been found in several different experimental systems such as active droplets floating on aqueous phase and a vertically-vibrated water droplet. By reciprocating motion, we refer to a periodic back-and-forth motion in a straight line. Here we have carried out a systematic study on the reciprocating motion from a theoretical viewpoint. In order to keep our analysis general, we used a model derived from symmetry considerations for the centre-of-mass velocity and second- and third-mode deformations. We have found two routs to the reciprocating motion. One is due to Hopf instability of a motionless elliptically deformed state. The other is a transition from a rectilinear motion with an oscillatory speed. In both cases, the second-mode deformation breaks the symmetry of the homogeneous space to determine a axis of motion and, together with the third-mode deformation, induces front-rear asymmetry.

*Poster

The link between Capillary Wave and the Density Functional theories for liquid surfaces

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The extended version of the Capillary Wave Theory (CWT) describes the thermal fluctuations on the free surface of a liquid in terms of a wave-dependent surface tension $sigma(q)$ that represents the thermodynamic cost, per unit area increase, of a surface corrugation with a given wavelength $lambda = 2pi/q$. The spectrum of density-density fluctuations at the liquid surface should reflect the functional form of $sigma(q)$, but the use of apparently consistent density-functional (DF) routes to obtain that function have lead to qualitatively different results. The problem is examined here in terms of simple DF models and with a direct comparison with computer simulations, to provide a consistent view.

*Poster

Rheology of Critical Polymer-Colloid Mixtures.

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Polymer-Colloid mixtures are used as a model physical system for the study of phase transitions and their dynamics. Their usefulness comes from the easy control of interaction, and the wide range of observation tools. They exhibit many features of phase transitions, from metastable phases to critical points [1,2] . In this talk, I present a experimental study of a PMMA colloids with polystyrene polymer. In this system, although the colloids behave as hard spheres, there is an effective interaction through the depletion forces caused by the polymers. When the polymer to colloid size ratio is large enough, this system has a critical point at the transition from a single fluid to a liquid-gas mixture. This system gives rise to very large correlation lengths[3] of order 30 microns. This allows a direct visualization of critical processes that is not possible with molecular systems. After a short introduction on our experimental system and methods, and a study of the phase diagram of the system, we focus on the behavior of the system close to the critical point. We measure correlation lengths and dynamical properties. We focus especially on the rheology close to the critical point, and the link between structure and viscosity. We also present perspectives regarding the measurement of fluctuating forces in such systems. [1] Lekkerkerker, H. N. W., WC-K. Poon, P. N. Pusey, A. Stroobants, and P. B. Warren. “Phase Behaviour of Colloid+ Polymer Mixtures.” EPL (Europhysics Letters) 20, no. 6 (1992): 559. [2]Ilett, S. M., A. Orrock, W. C. K. Poon, and P. N. Pusey. “Phase Behavior of a Model Colloid-Polymer Mixture.” Physical Review E 51, no. 2 (February 1, 1995): 1344–52. [3]Patrick Royall, C., Dirk G. A. L. Aarts, and Hajime Tanaka. “Bridging Length Scales in Colloidal Liquids and Interfaces from near-Critical Divergence to Single Particles.” Nature Physics 3, no. 9 (September 2007): 636–40.

*Poster

Nonlinear adhesion dynamics of confined lipid membranes

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Lipid membranes, which are ubiquitous objects in biological environments are often confined. For example, they can be sandwiched between a substrate and the cytoskeleton between cell adhesion, or between other membranes in stacks, or in the Golgi apparatus. We present a study of the nonlinear dynamics of membranes in a model system, where the membrane is confined between two flat walls. The walls can be permeable or impermeable. We first derive a lubrication model for the membrane dynamics. The resulting dynamics is highly nonlinear and nonlocal. The solution of this model in one dimension exhibits frozen states due to oscillatory interactions between membranes caused by the bending rigidity. These dynamics can be understood whithin the frame of a revisited kink model based on the historical work of Kawasaki and Otha [†,‡,§]. In two dimensions, the dynamics is more complex, and depends strongly on the amount of excess area in the system. We discuss the relevance of our findings for experiments on model membranes, and for biological systems [¶].

*Poster

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Non-equilibrium triple line kinetics and instabilities in solid-state dewetting.

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Dewetting is the process by which thin films recede and break up into droplets. Liquid state dewetting, where mass transport is dominated by hydrodynamics, has been studied extensively for several decades. However in the past decade, surface diffusion induced dewetting has also been observed in various systems with nanometrically thin solid-state crystalline films under annealing, such as Si/SiO_2[†] and Metal/Oxide[‡]. In addition, it was also proposed recently that polymer films below the glass transition also exhibit surface-diffusion-limited solid-state dewetting[§]. Kinetic Monte-Carlo simulations[¶], and continuum approaches[‖] have been used to study this phenomena. Here, we propose a novel continuum model without discontinuity at the triple-line. Through the asymptotic study of this model, we have derived a set of non-equilibrium conditions at the triple-line, which generalize the equilibrium Young contact angle condition used in previous works[5]. We have systematically investigated the influence of these new boundary conditions on the dynamics of dewetting. We also study the effect of film-substrate wetting interactions on the breakup of the nano-scale films. Specifically the mass shedding effect[5] where the film breaks at a finite distance from triple line, is accelerated several order of magnitudes due to these interactions.

*Poster

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Statistical mechanics theory for modeling of water

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We developed a statistical model which describes the thermal and volumetric properties of water-like molecules. A molecule is presented as a three-dimensional sphere with four hydrogen-bonding arms. Each water molecule interacts with its neighboring waters through a van der Waals interaction and an orientation-dependent hydrogen-bonding interaction. This model, which is largely analytical, is a variant of a model developed before for a two-dimensional Mercedes-Benz model of water [1] and parameterized for 3D Mercedes-Benz model of water [2]. References [1] T. Urbic and K. A. Dill, J. Chem. Phys. 132, 224507(2010). [2] A. Bizjak, T. Urbic, V. Vlachy, and K. A. Dill, Acta Chim. Slov. 54, 532(2007).

*Poster

Linear and ring polymer chains in confined geometries

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Investigation of a dilute solution of ideal and real linear and ring polymer chains with excluded volume interactions in a good solvent immersed in a confined geometry of two parallel walls or confined in the solution of spherical colloidal particles of big size for different boundary conditions (b.c.) such as: Dirichlet-Dirichlet, Neumann-Neumann and Dirichlet-Neumann which correspond to the situation of two repulsive walls, two inert walls and for the mixed case of one repulsive and one inert wall were performed. Taking into account the well known correspondence between the field theoretical ϕ^4 O(n)-vector model in the limit n-¿ 0 and the behavior of long-flexible polymer chains in a good solvent and Derjaguin approximation for the case of big spherical colloidal particles the calculation of the correspondent depletion interaction potentials and the depletion forces were calculated for all above mentioned cases. It was found that the confining of ideal and real ring polymer chains with EVI to a slit geometry of two parallel walls with different boundary conditions leads to the loss of configurational entropy and to arising of the repulsive forces which exert ring polymer chains on the surfaces. The obtained results indicate, that the depletion interaction potential for the case of two big colloidal particles with repulsive surfaces is smaller than for the case of big colloidal particle near the surface. In general case introducing the curvature for two surfaces leads to the reducing of the correspondent depletion interaction potentials. The obtained results are in good qualitative agreement with previous theoretical investigations and with the results of Monte Carlo simulations.

*Poster

Dynamics of interacting colloids on a circumference: Temporal regimes and scaling laws.

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We report on the dynamics of N superparamagnetic colloidal particles moving on a circumference of radius R. We particularly focus on the temporal regimes obtained from the many-particle Langevin equation for curved manifolds. Our findings show that, regardless the linear density of colloids and the strength of the inter-particle interaction, the mean-square angular displacement, $< [\Delta\phi(t)]^2 >$, displays four temporal regimes of the form: free diffusion ($D_0 t$), (open) single-file diffusion ($\sqrt{D_0 t}$), cluster-like diffusion ($D_0 t/N$) and localization-like diffusion ($\pi^2/3$), where D_0 is the Stokes-Einstein diffusion coefficient. We furthermore demonstrate that the crossover times between these regimes follow scaling laws in terms of the system parameters.

*Poster

Self-assembly in binary mixtures of hard nematic rods and dipolar spheres

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Spatially periodic phase-separation patterns coupled to liquid-crystalline order arise already in mixtures of differently shaped particles with hard-body repulsion only [1]. Simulations have revealed a strikingly complex phase behavior with uni- or biaxial, smectic and lamellar structures in binary mixtures of rods and soft magnetic spheres of comparable diameter [2]. In this study, we aim at a theoretical description that allows us to trace phase boundaries and to explain some of these structures for a model mixture of hard, nematically ordered spherocylinders and hard dipolar spheres. Our semi-analytical description starts from a free-energy functional which governs the equilibrium component-density distributions of position and orientation. This functional is constructed using concepts of classical density functional theory and the modified mean-field approximation for the dipolar interaction [3]. A stability analysis provides first insights into the coupling of nematic order, component phase separation, and dipolar ordering (polarisation).
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*Poster

Enhancement of water evaporation on solid surfaces with nanoscale hydrophobic-hydrophilic patterns

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Using molecular dynamics simulations, we show that the evaporation of nanoscale water on hydrophobic-hydrophilic patterned surfaces is unexpectedly faster than that on any surfaces with uniform wettability. The key to this phenomenon is that, on the patterned surface, the evaporation rate from the hydrophilic region only slightly decreases due to the correspondingly increased water thickness; meanwhile, a considerable number of water molecules evaporate from the hydrophobic region despite the lack of water film. Most of the evaporated water from the hydrophobic region originates from the hydrophilic region by diffusing across the contact lines. Further analysis shows that the evaporation rate from the hydrophobic region is approximately proportional to the total length of the contact lines.

*Poster

Microrheology in Active Brownian

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A recent experiment on bacteria suspensions revealed a fascinating phenomenon: the viscosity of the suspensions under small shear decreases with the concentration (thinning), and may even reach a frictionless state [1]. This was interpreted as the result of force dipoles induced by hydrodynamics effects originating from self-propulsion [2]. However, a microscopic understanding of this novel phenomenon is still absent [3]. Alternatively, we studied the microrheology of active Brownian particles without hydrodynamics. Interestingly, our simulation results show a similar thinning effect due to activity: the effective friction (micro-viscosity) drops compared to passive Brownian particles[4][5]. An analytical calculation indicates that self-propulsion plays the role of an effective force dipole as well. We finally discuss the micro-mechanism leading to such thinning effects in active Brownian particles. [1] H. M. Lopez, J. Gachelin, C. Douarche, H. Auradou, and E. Clement, Phys. Rev. Lett. 115, (2015). [2] Y. Hatwalne, S. Ramaswamy, M. Rao, and R. A. Simha, Phys.Rev.Lett. 92, 118101 (2004). [3] M. C. Marchetti, Nat 525, 37 (2015). [4] T. Wang and M. Sperl, Phys. Rev. E 93, 022606 (2016). [5] T. Wang, M. Grob, A. Zippelius, and M. Sperl, Phys. Rev. E 89, 42209 (2014).

*Poster

Emergent Hyperuniformity in Periodically Driven Emulsions

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We present on the self-organization of microfluidic emulsions into anomalously homogeneous structures. Upon periodic driving confined emulsions undergo a first-order transition from a reversible to an irreversible dynamics. We evidence that this dynamical transition is accompanied by structural changes at all scales yielding macroscopic yet finite hyperuniform structures. Numerical simulations are performed to single out the very ingredients responsible for this suppression of density fluctuations. We show that, as opposed to equilibrium systems, the long-range nature of the hydrodynamic interactions are not required for the formation of hyperuniform patterns, thereby suggesting a robust relation between reversibility and hyperuniformity which should hold in a broad class of periodically driven materials.

*Poster

Droplet manipulation on fiber networks leading to the creation of multicompound droplets

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Recent works demonstrated that fiber networks may constitute new means of designing open digital microfluidic systems. In this work, we discuss the general behavior of water droplets interacting with a fiber array. Depending on their volume, droplets sliding along an inclined fiber can be stopped at a crossing of two fibers. We show that, by changing the angle between these fibers or their diameters, we can modify the critical volume above which the water droplets cross the nodes. The geometry of the fiber array is the key parameter to control the droplet motion. After the detachment, tiny residues remain trapped at the nodes and can be collected to create multicompound droplets. These microemulsions have numerous applications such as pharmaceutical drug delivery, biosensors, microreactors, ...

*Poster

Instabilities, motion and deformation of active fluid droplets

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We consider two minimal models of active fluid droplets that exhibit complex dynamics including steady motion, deformation, rotation and oscillating motion. First we consider a droplet with a concentration of active contractile matter adsorbed to its boundary. We analytically predict activity driven instabilities in the concentration profile, and then simulate the system to find the steady states. Secondly, we consider a droplet of active polar fluid of constant concentration. In this system we predict, motion and deformation of the droplets in certain activity ranges due to instabilities in the polarisation field. Both these systems show generic routes to motility and deformation in active fluid droplet systems which resemble dynamics of the cell cytoskeleton in animal cells.

*Poster

Intermolecular and Intramolecular vibrations of water molecules from the viewpoint of atoms

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By using the instantaneous normal mode (INM) analysis for two water models of flexible molecules, we investigate intermolecular and intramolecular vibrations of water molecules in a liquid phase from the viewpoint of atom [1]. Our investigations include three aspects of the INM spectrum of liquid water, which is separated into the unstable, intermolecular, bending and stretching bands. The first aspect is the O- and H-atom contributions in the four INM bands. Second, the inverse participation ratios (IPRs) of the O- and H-atoms and water molecules involved in INMs were formulated. With the IPRs, the localization characters of INMs in each band were studied. Thirdly, by classifying simulated molecules into subensembles according to their local environments or H-bond configurations, the local-structure effects on the bending and stretching INMs were examined.

*Poster

Numerical study on the role of hydrodynamics in microrheology of non-Brownian suspensions

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Colloidal suspensions exhibit rich rheological behaviours such as shear thinning and thickening. The problem has been studied intensively for a long time, but the presence of a fluid component and the resulting many-body hydrodynamic interactions (HIs) makes its phyiscal understanding very challenging. For example, the incompressibility of a fluid not only leads to long-range interactions between particles, but also gives rise to squeezing effects when particles approach each other. Furthermore, at high packing fractions, particles transmit forces via direct interparticle repulsive interactions. So there may be a non-trivial interplay between HIs and direct force transmission. Here we numerically study how hydrodynamic interactions affect the force transmission by using a microrheological approach. In our numerical simulations, a probe particle is dragged by a constant external force in bidisperse non-Brownian suspensions. Particles directly interact with each other via a soft-core repulsive potential. We neglect thermal fluctuations and interparticle frictions. In order to evaluate the effects of HIs, we compared numerical simulation results between with and without HIs, i.e. Fluid Particle Dynamics (FPD) [1] and Relaxation Dynamics (RD) method, respectively. The former fully takes into account the hydrodynamic degrees of freedom, whereas the latter does not. The drag coefficient of the probe particle increases with an increase in the particle packing fraction and eventually diverges towards critical packing fractions in both FPD and RD. We find that this divergence takes place at a lower packing fraction and the pressure coming from interparticle compression induced by the dragged probe particle propagates over a longer distance for FPD than for RD. These results indicate that the longer-range force transmission is responsible for the jamming at a lower packing fraction in the system with HIs. We will discuss the mechanism by which HIs enhance and stabilize force chains.

[1] H. Tanaka, and T. Araki, it Phys. Rev. Lett. bf 85, 1338 (2000).

*Poster

Spontaneous emergence of self-replicating cycles with colloidal spheres

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Biological systems are a source of inspiration for creating a new paradigm for material synthesis. This paradigm aims to design materials that can self-replicate, while providing functionality such as catalysis of multiple reactions. Ultimately, tuning the parameters of such systems would allow the possibility of evolving materials with either designed or unexpected properties by carrying out cycles of mutation and selection. Even though these ideas seem removed from realization in the laboratory, recent experimental advances in coating colloidal-scale objects with specific glues, like complementary DNA strands, have suggested theoretical models in which the possibilities of these ideas can be explored in a controlled way. I will describe our ongoing work on exploring these ideas through theory and computer simulations.

*Poster

The Proton Polarity of Interfacial Water Inhibits Heterogeneous Ice Nucleation

Xin Zhou * [1]

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It has been puzzled for a long time why many materials (e.g., silver iodide, and barium fluoride) have a similar lattice structure with ice, but very different abilities of facilitating ice nucleation. Based on atomistic molecular dynamics simulations, we show that the various rearrangements of hydrogen directions (the proton polarity) in the interfacial water (IW) dominates the formation of ice. While the oxygen atoms of IW form the same ice lattice, the partial ionic charges of these substrates can induce different proton polarity in the IW layers then increase the surface tension of ice nucleus on the layers, which increasing the contact angle of ice nucleus thus the free energy barrier of ice nucleation. Our results indicate that the reconstruction of IW on substrates, not only its oxygen lattice order but its hydrogen directionality, dominates water freezing, lattice-similar substrates can induce different hydrogen arrangements of the IW then have different effects on ice nucleation.

*Poster

Density determines the nature of the hexatic-liquid transition in two-dimensional melting of core-softened systems

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We find that both continuous and discontinuous hexatic-liquid transition can happen in the melting of two-dimensional solids of core-softened particles. For three typical model systems, Hertzian, Harmonic, and Gaussian-core models, we observe the same scenarios. These systems exhibit reentrant crystallization with a maximum melting temperature T_m happening at density ρ_m. The hexatic-liquid transition at a density smaller than ρ_m is discontinuous. Liquid and hexatic phases coexist in a density interval, which becomes narrower with increasing temperature and tends to vanish approximately at T_m. Above ρ_m, the transition is continuous, in agreement with the KTHNY theory. For these core-softened systems, density determines the nature of the hexatic-liquid transition, with the melting at ρ_m being a plausible transition point from discontinuous to continuous hexatic-liquid transition.

*Poster

Topic 7: Nonlinear physics -Posters

Singular diffusion in a confined sandpile

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We investigate the behavior of a two-state sandpile model subjected to a confining potential in one and two dimensions. From the microdynamical description of this simple model with its intrinsic exclusion mechanism, it is possible to derive a continuum nonlinear diffusion equation that displays singularities in both the diffusion and drift terms. The stationary-state solutions of this equation, which maximizes the Fermi-Dirac entropy, are in perfect agreement with the spatial profiles of time-averaged occupancy obtained from model numerical simulations in one as well as in two dimensions. Surprisingly, our results also show that, regardless of dimensionality, the presence of a confining potential can lead to the emergence of a power-law tail in the distribution of avalanche sizes.

*Poster

Equivalence between asynchronous and delayed dynamics in coupled maps

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Coupled map lattices are paradigmatic models of many collective phenomena. However, quite different patterns can emerge depending on the updating scheme. While in early versions, maps were updated synchronously, there is, in recent years, a concern to consider more realistic updating schemes, where elements do not change all at once. Asynchronous updating schemes and the inclusion of time delays are seen as more realistic than the traditional parallel dynamics, and, in diverse works, either one or the other, have been implemented separately. But are they actually distinct cases? For the synchronization of coupled map lattices with adjustable range of interactions, we prove, using both numerical and analytical tools, that an adequate delayed dynamics is exactly equivalent to an asynchronous one, providing a unified framework that embraces both dynamics.

*Poster

Sensitivity to initial conditions of d-dimensional long-range-interacting Fermi-Pasta-Ulam-like model: Universal scaling

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We introduce a generalized d-dimensional β-Fermi-Pasta-Ulam (FPU) model in presence of long-range interactions, and perform a first-principle study of its chaos for $d = 1, 2, 3$ through large-scale numerical simulations. The nonlinear interaction is assumed to decay algebraically as $d_{ij}^{-\alpha} (\alpha \geq 0)$, d_{ij} being the distances between N oscillator sites. Starting from random initial conditions we compute the maximal Lyapunov exponent λ_{max} as a function of N. Our $N >> 1$ results strongly indicate that λ_{max} remains constant and positive for $\alpha/d > 1$ (implying strong chaos, mixing and ergodicity), and that it vanishes like $N^{-\kappa}$ for $0 \leq \alpha/d < 1$ (hence approaching weak chaos, thus opening the possibility of breakdown of ergodicity). The suitably rescaled exponent κ exhibits universal scaling, namely that $(d+2)\kappa$ depends only on α/d and, when α/d increases from zero to unity, it monotonically decreases from unity to zero, so remaining for all $\alpha/d > 1$. The value $\alpha/d = 1$ can therefore be seen as a critical point separating the ergodic regime from the anomalous one, κ playing a role analogous to that of an order parameter. This scaling law is consistent with Boltzmann-Gibbs statistics for $\alpha/d > 1$, and q-statistics for $0 \leq \alpha/d < 1$.

*Poster

Adaptive Gyrotactic Swimmers in a Taylor-Green Vortex Flow: A Reinforcement Learning Approach

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For several species of phytoplankton and most zooplankton the ability to move vertically is important for survival. This capability is affected by hydrodynamic shear in the underlying flow, which can eventually cause accumulation of particles in specific regions and have a substantial effect on processes like competition for nutrients or reproduction. It is thus beneficial for these organisms to learn to actively control their spatial position in order to increase their adaptability. In this study we focused on gyrotactic swimmers, i.e. microorganisms for which the direction of motion depends on the balance between gravitational and viscous torques. We modeled the swimmers as point-like, neutrally buoyant, gyrotactic particles, immersed in a two dimensional steady Taylor-Green Vortex flow. The swimmers are able, using a reinforcement learning algorithm (Q-learning 1-step algorithm), to escape regions of high vorticity and swim upwards. We tested the algorithm at varying both the translational and rotational speed of the swimmer. We also assessed the robustness of the learning process results against different perturbations of the original flow. This work suggests that reinforcement learning algorithms represent a useful tool for modeling adaptability mechanisms observed in a number of real aquatic microorganisms.

*Poster

Waves spontaneously generated by heterogeneity in oscillatory media

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Wave propagation is an important characteristic for pattern formation and pattern dynamics. To date, various waves in homogeneous media have been investigated extensively and have been understood to a great extent. However, the wave behaviors in heterogeneous media have been studied and understood much less. In this work, we investigate waves that are spontaneously generated in one-dimensional heterogeneous oscillatory media governed by complex Ginzburg-Landau equations; the heterogeneity is modeled by multiple interacting homogeneous media with different system control parameters. Rich behaviors can be observed by varying the control parameters of the systems, whereas the behavior is incomparably simple in the homogeneous cases. These diverse behaviors can be fully understood and physically explained well based on three aspects: dispersion relation curves, driving-response relations, and wave competition rules in homogeneous systems. Possible applications of heterogeneity-generated waves are anticipated.

*Poster

Sivashinsky equation for flame dynamics, an experimental test

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The dynamics of unstable premixed flames is described by the Sivashinsky equation, a non linear integral equation which has simple solutions given by poles in the complex plane. The pole positions satisfy ordinary differential equations and are related to the crests observed on the flame front. We provide here precise experiments, using quasi two dimensional flames in a Hele-Shaw cell, to test quantitatively this model equation. The merging of neighboring small crests is found to be essentially a 2-body problem, and the front evolution for a large cell width can be predicted for a short time by the Sivashinsky equation. The role of gravity for flames propagating downwards, which can be added easily to the Sivashinsky equation but breaks the pole decomposition, will be discussed.

*Poster

Instantons, zero modes and fluctuations in the Kraichnan model of tubulent advection

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Self-similar instanton solutions of the stochastic dynamics of the full passive scalar field in the Kraichnan model of turbulent advection are arguably good candidates for describing the coherent motion of fluid particles leading to the production of strong gradients of the scalar and intermittency properties. There exists a whole continuum of them, with scaling index ranging between 1 (regular field) and 0 (discontinuous field). We show that they can be set in correspondence (by a Legendre transform) with the so-called zero modes which come out when one considers the evolution of clouds of a finite number of Lagrangian particles and are known, since the late 90s, to constitute the good mathematical framework for understanding and quantifying anomalous scaling in the Kraichnan model. Sticking to the classical level of approximation in the instanton approach, i.e., concentrating on trajectories realizing an extremum of the action, leads clearly to an overestimation of scaling exponents of the structure functions of the scalar. To get further and incorporate the effect of fluctuations, we rather use the instanton solutions as basic building blocks of trial many-body wave functions for zero modes. This approach gives surprisingly good estimates of scaling exponents even at low statistical orders (at least in 2d and for the values of parameters investigated so far), but still leaves some mystery about their ultimate behaviour at large orders where saturation is expected.

*Poster

Scattering theory of walking droplets

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Walking droplets that are sustained on the surface of a vibrating liquid, have attracted considerable attention during the past decade due to their remarkable analogy with quantum wave-particle duality. This was initiated by the pioneering experiment by Y. Couder and E. Fort, which reported the observation of a diffraction pattern in the angular resolved profile of droplets that propagated across a single slit obstacle geometry. While the occurrence of this wave-like phenomenon can be qualitatively traced back to the coupling of the droplet with its associated surface wave, a quantitative framework for the description of the surface-wave-propelled motion of the droplet in the presence of confining boundaries and obstacles still represents a major challenge. This problem is all the more stimulating as several experiments have already reported clear effects of the geometry on the dynamics of walking droplets. Here we present a simple model inspired from quantum mechanics to generalise the statistical description of the trajectory of a walking droplet in an arbitrary geometry. We propose to describe this trajectory using a Green function approach. The Green function is related to the Helmholtz equation with Neumann boundary conditions on the obstacle(s) and outgoing conditions at infinity. For a single slit geometry our model is exactly solvable and reproduces some of the features observed experimentally. It stands for a promising candidate to account for the presence of boundaries in the complex dynamics of a walker.

*Poster

Walking Droplets In Confined Geometries

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Lorsqu'on dépose délicatement une goutte sur un bain vibré verticalement, sous certaines conditions, nous parvenons à éviter le phénomène de coalescence. La goutte rebondit alors de façon permanente. En augmentant l'accélération de forçage, la goutte atteint un régime dynamique lui permettant de se déplacer horizontalement à la surface du liquide, à vitesse constante [1,2]. En se mouvant ainsi, la goutte marcheuse laisse dans son sillage des sources d'ondes stationnaires résultant de ses impacts sur la surface. Ce sont ces ondes qui sont à l'origine de la marche. Ces dernières années ont vu l'apparition de techniques de confinement de gouttes dans une géométrie bidimensionnelle : cavité cylindrique, potentiel harmonique ou encore force de Coriolis [3,4]. D'autre part, les interactions entre deux marcheurs identiques ont également été caractérisées [5]. Au cours de notre exposé, nous montrons qu'il est possible de confiner un marcheur dans une géométrie quasi 1d en utilisant des cavités submergées. En premier lieu, nous présentons des expériences menées dans des cavités rectangulaires, de largeurs proportionnelles à la longueur d'onde de Faraday. L'étude des vitesses transversales et longitudinales des marcheurs au sein de ces cavités, nous permet de trouver un critère pour obtenir un confinement à 1d optimal. En s'intéressant aux ondes de Faraday émises dans la cavité, nous proposons ensuite une analogie avec les guides d'ondes pour rendre compte de l'évolution de la vitesse des marcheurs dans les cavités. Dans une seconde partie, nous utilisons des cavités annulaires afin d'étudier les interactions inter-gouttes et montrons qu'une quantification des interdistances apparaît. Nous étudions la vitesse de binômes de gouttes, l'interdistance entre les gouttes influe sur leur vitesse de groupe : ces gouttes se déplacent plus vite lorsqu'elles sont proches. Nous portons enfin notre intérêt sur les chaînes de gouttes. Ces dernières partagent la même onde cohérente qui tend à autopropulser le système à une vitesse supérieure à celle d'une goutte seule. Nous discutons de l'influence du nombre de gouttes, mais également de la distance entre ces dernières sur la vitesse d'une chaîne. L'évolution de la vitesse d'une chaîne est le résultat d'interférences constructives entre chaque onde émise par chaque goutte. Nous proposons enfin un modèle rendant compte de la quantification des distances et de l'évolution des vitesses selon les différents paramètres [6].

1) Y. Couder, S. Protière, E. Fort, and A. Boudaoud, Nature 437, 208 (2005). 2) S. Protière, A. Boudaoud, and Y. Couder, J. Fluid Mech. 554, 85 (2006). 3) S. Perrard, M. Labousse, M. Miskin, E. Fort, and Y. Couder, Nat. Comm. 5, 3219 (2014). 4) M. Labousse and S. Perrard, Phys. Rev. E 90, 022913 (2014). 5) C. Borghesi, J. Moukhtar, M. Labousse, A. Eddi, E. Fort, and Y. Couder, Phys. Rev. E 90, 063017 (2014). 6) B. Filoux, M. Hubert, and N. Vandewalle, Phys. Rev. E 92, 041004(R) (2015).

*Poster

Crystal growth in nano-confinement

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Crystal growth with free interfaces has been studied for many decades. In constrat, the growth of crystals in nano-confined environments, which is relevant for many processes ranging from biology to geology, is still poorly understood. We present a generic continuum model describing growth or dissolution of a crystal in nano-confinement. Diffusion and hydrodynamics in the liquid film separating the crystal and a substrate are modeled within the lubrication approximation, leading to a highly non-linear evolution equation which governs the non-equilibrium dynamics of the growth front. Based on this model, we explore nonlinear dynamics and pattern formation associated with different questions such as the force of crystallization exerted by the growing crystal on the substrate, and the rate of dissolution of a crystal under a macroscopic load (also called pressure solution in the literature).

*Poster

Koopman Mode Analyses of Fluid Flows

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Analytical and computational studies of fluid and reacting flows are extremely challenging, due in part to nonlinearities of the underlying system of equations and long-range coupling. Recent developments in high-resolution high-frequency experimental data capture provide an alternative approach that relies on on modal decomposition of experimental data. We use Koopman mode analysis, a nonlinear generalization of normal mode analysis, to decompose a flow into its constituents. Koopman modes are global structures, each of which evolve with a single complex growth rate. Flow analysis also requires a method to differentiate constituents that are robust (i.e., common between nominally identical experiments) from noise and non-robust features. We introduce a technique for this task based on Koopman mode analysis. The methodology is used to identify critical flow constituents in (1) cellular patterns on flame fronts, (2) instabilities in reacting flows behind a barrier, (3) injector flows, and (4) swirling combustion.

*Poster

Study of translational flows in rough wall channel flows

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Despite many efforts, a fully satisfactory understanding of the interaction among the degrees of freedom excited at the onset of turbulence in wall-bounded shear flows is still lacking. Here, we report direct numerical simulations of a transitional square-duct flow using off-lattice Boltzmann schemes. We investigate the influence of the distribution and geometry of wall irregularities on both small and large scales fluctuations. We present detailed numerical results on the friction factor and the statistical properties of the energy flux.

*Poster

Energetics of hydrodynamic synchronization in coupled Stokes spheres

Yuki Izumida * [1], Hiroshi Kori, Udo Seifert

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Formulating energetics of hydrodynamic synchronization is of importance for understanding function of flagella and cilia of microorganisms in a viscous fluid. While mechanism of synchronization itself of such active objects is often analyzed by a language of nonlinear dynamics, a generic energetic aspect of synchronization could be revealed with the aid of nonequilibrium thermodynamics analysis. By simply modeling Stokes spheres as noisy coupled oscillators described by phase equations and using a framework of stochastic thermodynamics, here we present novel thermodynamics formula of the energy dissipation rate that can be applied to a simple setup of the rotating Stokes spheres on a circular trajectory in a viscous fluid [1]. Our concise formula is expressed by using measureable quantities of natural and mean frequencies of the spheres, and can universally be applied to any type of weak coupling between them. Our formula highlights the role of hydrodynamic synchronization in energetics, revealing that a characteristic change in the dissipation arises in association with frequency synchronization between the spheres as the coupling strength increases. [1] Y. Izumida, H. Kori, and U. Seifert, arXiv: 1602.07116.

*Poster

When Kraichnan model fails: effect of time correlations on turbulent mixing.

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Theoretical results regarding turbulent mixing are mostly based on the model of Kraichnan flows with zero correlation time. However, empirical evidence has been gathered showing that time correlations can give rise to qualitative changes in the dynamics of mixing, c.f. Boffetta et al, PRL v. 93, 134501 (2004), and Gotoh et al PRL v. 115, 114502 (2015). We pinpoint three physically different sources of mismatch between the tracer dynamics in Kraichnan flows, and in real time-correlated flows. Further, we show that in certain cases, it is possible to improve the matching between real flows and Kraichnan flows by adjusting the Kraichnan model parameters. In particular we introduce the concept of mixing dimension d_m which can take fractional values, c.f. Ainsaar et al, arXiv:1510.02854 (2015). For incompressible Kraichnan flows, the mixing dimension equals to the topological dimension d; for real flows, $d_m > d$. We show that this inequality gives rise to a local inhomogeneity of mixing — a phenomenon which cannot be observed for ideal flows, and has important implications, e.g. it impacts the rate of bimolecular reactions in turbulent flows, and the efficiency of small-scale kinematic dynamos. Finally, we provide qualitative and quantitative explanations of the empirical findings of Boffetta et al (2004) regarding anomalous behaviour of tracers in time-correlated compressible flows.

*Poster

Instabilities and relaxation to equilibrium in long-range oscillator chains

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We study instabilities and relaxation to equilibrium in a long-range extension of the Fermi-Pasta-Ulam-Tsingou (FPU) oscillator chain by exciting initially the lowest Fourier mode. Localization in mode space is stronger for the long-range FPU model. This allows us to uncover the sporadic nature of instabilities, i.e., by varying initially the excitation amplitude of the lowest mode, which is the control parameter, instabilities occur in narrow amplitude intervals. Only for sufficiently large values of the amplitude, the system enters a permanently unstable regime. These findings also clarify the long-standing problem of the relaxation to equilibrium in the short-range FPU model. Because of the weaker localization in mode space of this latter model, the transfer of energy is retarded and relaxation occurs on a much longer timescale.

*Poster

Self-Excited Oscillation and Shedding of Acoustically Levitated Water Drops

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Acoustic levitation is a technique for suspending matters in mid-air without material limitation by balancing gravity with the acoustic radiation force. Strong acoustic radiation force can be generated around the node of the acoustic standing wave field. In our experiment, by decreasing the static acoustic pressure below a threshold, we demonstrate the self-excited quasi-periodic oscillation, chaotic oscillation, and chaotic shedding of mm sized drops in a single-node cavity. The possible reason for sustaining and growing of the self-excited oscillation, dynamic process of shedding, and the mode interactions would be discussed.

*Poster

Assimilation by delay-coordinate nudging in spatially extended chaotic systems

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A new nudging method for data assimilation, delay-coordinate nudging, is presented. Delay-coordinate nudging makes explicit use of present and past observations in the formulation of the forcing driving the model evolution at each time-step. Numerical experiments with a low order chaotic system show that the new method systematically outperforms standard nudging in different model and observational scenarios, also when using an un-optimized formulation of the delay-nudging coefficients. A connection between the optimal delay and the dominant Lyapunov exponent of the dynamics is found based on heuristic arguments and is confirmed by the numerical results, providing a guideline for the practical implementation of the algorithm. Delay-coordinate nudging preserves the easiness of implementation, the intuitive functioning and the reduced computational cost of the standard nudging, making it a potential alternative especially in the field of seasonal-to-decadal predictions with large Earth system models that limit the use of more sophisticated data assimilation procedures.

*Poster

Nonautonomicity and living systems

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Most systems in nature exchange energy and matter with their environment, and as such are open systems. This environment in general varies over time, which makes the system nonautonomous: its dynamics are time-varying. This often yields seemingly complicated oscillatory time evolutions of those systems, e.g. the heart rate [1]. Traditionally, oscillations in living systems are modelled either by autonomous limit-cycles [2] or stochastic models [3]. Whilst the latter do not allow the phase of the limit cycle to be stable, the former does not provide much insight about the internal structure of the system and its interaction with its environment. A theory of nonautonomous dynamical systems has seen continuous development amongst the mathematical community over the past decades [4]. However, very few truly nonautonomous modelling approaches and techniques are adopted in the life sciences. Chronotaxic systems [5] – nonautonomous oscillators with stable amplitude and stable phase – is one example of such approaches. Mathematically, any nonautonomous system of dimension n evolving in state space $mathcalMsubseteqmathbbR^n$ can be rewritten as an autonomous system with one extra dimension accounting for time ($x_{n+1} = t$), and hence one extra equation for that variable: $dotx_{n+1}(t) = 1$. One might then argue that all nonautonomous models can be rewritten as autonomous and analysed, using well established concepts and techniques traditionally used for autonomous systems, as suggested in [6], for example. However, does this approach yield correct results about the system? The above approach is in general misleading, and the use of genuinely nonautonomous concepts and techniques have in general to be adopted to deal with such systems. We will discuss these issues by analysing a simple nonautonomous low-dimensional theoretical example with the approach described above. Particular cases and difference between periodic and non-periodic external forcing will also be discussed. In particular, when the nonautonomous component of the systems is periodic or composed or periodic terms, other ways of turning the system autonomous can be used. However, we will show that, in general, turning nonautonomous systems into autonomous version and analysing them with methods designed for autonomous systems is misleading. [1] P. T. Clemson, et al. Phys. Rev. E, 89(3):032904, 2014. [2] A. Goldbeter. Biochemical Oscillations and Cellular Rhythms. Cambridge University Press, Cambridge, 1997. [3] D. Gonze, et al. Int. J. Quant. Chem., 98(2):228–238, 2004. [4] P. E. Kloeden and M. Rasmussen. Nonautonomous Dynamical Systems. Amer. Math. Soc., Providence, 2011. [5] Y. F. Suprunenko, et al. Phys. Rev. Lett., 111(2):024101, 2013. [6] S. H. Strogatz. Nonlinear Dynamics and Chaos: with Applications to Physics, Biology, Chemistry, and Engineering. Westview Press, Boulder, 2nd ed., 2014.

*Poster

Dual energy cascades in rotating stratified geophysical flows

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We present a work focusing on the study of stably stratified Boussinesq flows with rotation by means of direct numerical simulations (DNS). In this framework results from high-resolution DNS are provided to describe characteristics of the energy cascade in rotating stratified fluids and to investigate energy transfer processes in geophysical flows. First unambiguous evidences on the existence of dual constant-flux energy cascades in rotating stratified flows are presented and a simple scaling model for the ratio of the fluxes to large and to small scales is here introduced. It is also argued how the outcome of this work sheds new light on the apparent paradox of the coexistence of large-scale balanced dynamics and small scale dissipation in the global ocean.

*Poster

Nonequilibrium fluctuations in the ring of material points with gravity

E. A. Melkikh * [1], A. V. Melkikh

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A model of the ring of the identical material points interacting with each other on the basis of gravitational forces is considered. As the initial condition a random distribution of points on the angles is selected, with the points located on the orbits spaced apart by the same initial distance. The nearest point of the ring is located at a distance of 1 AU, the latter at a distance of 30 AU. The initial velocities were chosen with direction tangentially to a circular orbit. Masses ranged from 40 to 200 Earth masses. We studied the initial stages of evolution for the case of different virial ratios. The calculations were performed by the method of molecular dynamics. As a result, we calculated the distribution function of the points in space for different virial ratios. The dependence of the relative mean square fluctuations of "evaporating" particles on the number of particles in the system is investigated. The number of particles N ranged from 20 to 100. As a result, it was found that this quantity is proportional to N^{α} ($\alpha = -0.7$ for the ratio $8K = -U$ and $\alpha = -0.75$ for $2K = -U$).

*Poster

Trapping scaling for bifurcations in Vlasov systems

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We study non oscillating bifurcations of non homogeneous steady states of the Vlasov equation, a situation occurring in galactic models, or for Bernstein-Greene-Kruskal modes in plasma physics. We show that resonances are strongly suppressed, leading to very different phenomena with respect to the homogeneous case. Through an unstable manifold expansion, we show that the dynamics is very sensitive to the initial perturbation: the instability may saturate at small amplitude -generalizing the "trapping scaling" of plasma physics- or may grow to produce a large scale modification of the system. These analytical findings are illustrated and extended by direct numerical simulations with a cosine interaction potential.

*Poster

Attractor non-equilibrium stationary states in perturbed long-range interacting systems

Jules Morand * [1], Pascal Viot, Michael Joyce

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Long range interactions concern numerous natural systems. A notable example is the one of gravitation which is especially relevant in the study of a stars system or a galaxy cluster. In particular, these systems do not respect the additivity of thermodynamical potential and presents a dynamics dominated by collective (mean-field) effects. One of the most remarkable feature is that, after a very rapid evolution, these systems remain trapped into quasi-stationary states up to a very long time (diverging with the system size). Simulations have shown that if such systems relax to thermal equilibrium, it happens only on time scales diverging with the system size. Quasi-stationary states are theoretically interpreted as stationary solutions of the Vlasov equation. Derived in the limit of a large number of particles, for which the two point and higher correlation function may be neglected, this kinetic equation, represents a very good approximation of the dynamics of long range systems. This equation is valid for strictly Hamiltonian system, and the quasi-stationary state are supposed to appear in this strictly conservative context. A natural question that arises is: are these states resistive to non-Hamiltonian perturbations? In adding extra term to the Vlasov equation, we have studied, how different kind of non-Hamiltonian perturbation modify the dynamics of such system. The results obtained have been derived in a perturbative limit i.e. in a limit such that the time scale of the mean-field dynamics and the one of the perturbation are separated. Simulations of the one dimensional self-gravitating sheet model subjected to such perturbations have been performed to investigate the dynamics and to corroborated theoretical predictions made with the kinetic theory. The main result is that quasi-stationary states are found to be robust to such perturbations and that irrespectively of the initial condition, the system is driven to a non-gaussian steady state depending on the kind of perturbation added.

*Poster

Lagrangian irreversibility in two-dimensional turbulence.

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In this talk we address the question whether or not it is possible to detect and quantify the degree of irreversibility of a two-dimensional turbulent flow following the trajectory of a fluid tracer. In particular we consider the regime of the direct enstrophy cascade, which develops at scales larger than the viscous scale and smaller than the correlation scale of the external forcing which sustains the flow. We show that the statistics of enstrophy time increments computed along Lagrangian trajectories is characterized by a negative skewness, which allows to discriminate the backward and forward dynamics. We find that the time asymmetry persists also for the time derivative of the enstrophy, and violates the fluctuation theorem of statistical mechanics. We analyze the different contributions due to the external force and the viscous forces, showing that the time asymmetry is originated by strong dissipative events, spatially localized in thin vortex filaments. We also discuss the universality of this phenomenon with respect to the forcing mechanism.

*Poster

Defect mediated turbulence in ribbons of viscoelastic Taylor-Couette ow

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The addition of a small amount of polymers with high molecular mass to a Newtonian solvent brings viscoelastic properties to the resulting solutions. Under shear with a rate, polymer solutions exhibit vis- coelastic properties via the shear-thinning, the relaxation time and the normal stress differences that do not ex- ist in Newtonian liquids. The Taylor-Couette system that consists of a ow confined in the gap between two coaxial differentially rotating cylinders is one of the ow systems that is suitable for investigation of the viscoelas- tic properties of polymer solutions. Transition to defect-mediated turbulence in the ribbon patterns observed in a viscoelastic Taylor- Couette ow is investigated when the rotation rate of the inner cylinder is increased while the outer cylinder is fixed. In four polymer solutions with different values of the elasticity number, the defects appear just above the onset of the ribbon pattern and trigger the appearance of disordered oscillations when the rotation rate is increased. The flow structure around the defects is determined by PIV measurments and the statistical properties of these defects are analyzed in the framework of the complex Ginzburg-Landau equation. For each working viscoelastic solution, the curves of variation of the mean number of defects, of the correlation time and correlation length exhibit a divergence-like behavior near a given value of the control parameter (Taylor number Ta) corresponding to the transition to the defect mediated turbulence.

*Poster

Geometric classes controlling spatiotemporal expression in repressor chains

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We propose a family of repressor networks, which we call repressor chains, as a simple model of chemical networks in cells. The model is described by coupled ordinary equations where the time evolution of concentration of each chemical species is governed by production terms repressed by the other chemical species and a degradation term. The geometric structure of repressive interactions is described by a one-dimensional lattice with long-range interactions, including repressilator as a certain case, which has played an important role in synthetic biology. In this model, it is easily understood that non-interacting chemical species only show homogeneous stationary states. We derive general conditions for the instabilities of homogeneous stationary states, and characterize geometric classes of the repressor chains, each of which shows different instabilities. Thus, the instabilities are purely a consequence of the repressive interactions. By focusing on some examples of the repressor chains with different geometric properties, we numerically investigate the arising spatiotemporal expressions such as traveling waves, spatiotemporal crystal, or quasicrystal in more detail.

*Poster

Cahn-Hilliard-Navier-Stokes Turbulence

Rahul Pandit * [1], Nairita Pal, Prasad Perlekar, Anupam Gupta

[1] Indian Institute of Science – India

We demonstrate how the coupled Cahn-Hilliard and Navier-Stokes (CHNS) equations provide a natural theoretical framework for studying turbulence in binary-fluid mixtures by using some of our recent studies: (a) the turbulence-induced suppression of phase separation in a symmetric binary-fluid mixture; (b) turbulence-induced multifractal dynamics in a droplet of the minority phase in a background of the majority phase; and (c) the reaction of the fluctuations of such a droplet on the turbulent fluid, which lead, eventually, to dissipation reduction. We first study two-dimensional (2D) binary-fluid turbulence by carrying out an extensive direct numerical simulation (DNS) of the forced, statistically steady turbulence in the coupled CHNS equations. In the absence of any coupling, we choose parameters that lead (a) to spinodal decomposition and domain growth, which is characterized by the spatiotemporal evolution of the Cahn-Hilliard order parameter ϕ, and (b) the formation of an inverse-energy-cascade regime in the energy spectrum $E(k)$, in which energy cascades towards wave numbers k that are smaller than the energy-injection scale k_{inj} in the turbulent fluid. We show that the Cahn-Hilliard-Navier-Stokes coupling leads to an arrest of phase separation at a length scale L_c, which we evaluate from $S(k)$, the spectrum of the fluctuations of ϕ. We demonstrate that (a) $L_c \sim L_H$, the Hinze scale that follows from balancing inertial and interfacial-tension forces, and (b) L_c is independent, within error bars, of the diffusivity D. We elucidate how this coupling modifies $E(k)$ by blocking the inverse energy cascade at a wavenumber k_c, which we show is $\simeq 2\pi/L_c$. We then study the advection of an active, deformable, finite-size droplet by a turbulent flow via a DNS of the CHNS equations. In these equations, the droplet has a natural two-way coupling to the background fluid. We show that the probability distribution functions of the droplet center of mass acceleration components exhibit wide, non-Gaussian tails, which are consistent with predictions based on pressure spectra. We also show that the droplet deformation displays multifractal dynamics. Our study reveals that the presence of the droplet enhances the energy spectrum $E(k)$, when the wavenumber k is large; this enhancement leads to dissipation reduction.

*Poster

Transition of a nanomechanical impact oscillator towards the chaotic regime

Hee Chul Park * [1], Joon Hyong Cho, Minah Seo, Taikjin Lee, Jae Hun Kim, Young Min Jhon, Chulki Kim, Seong Chan Jun, Robert H. Blick, Kang-Hun Ahn

[1] Center for Theoretical Physics of Complex Systems – South Korea

We realize a nanomechanical impact oscillator driven by a radiofrequency signal. The mechanical impact of the oscillator is demonstrated by increasing the amplitude of the external radiofrequency signals. Electron transport in the system is dramatically modified when the oscillator is strongly driven to undergo forced impacts with electrodes. We exploit this nonlinear kind of electron transport to observe the current response in the chaotic regime. Our model adopting the Sharvin conductance when in impacts reproduces the characteristic feature of the rectified current via the impact oscillator in the linear regime, revealing a path towards chaos. These findings open new perspectives to investigate unexplored regimes of nanomechanical electron transport.

*Poster

Enhancing energy-harvesting via coupling monostable oscillators

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The performance of a ring of linearly coupled, monostable nonlinear oscillators is optimized towards its goal of acting as energy harvesters (through piezoelectric transduction) of mesoscopic fluctuations which are modeled as Ornstein-Uhlenbeck noises. For a single oscillator, we study the overall efficiency as a function of the potential's stiffness. We find that a soft linear spring performs most optimally. Considering several units, we seek for the optimal number of units and analyze the effects of a bi-linear coupling among units. Whereas in-phase coupling worsens the performance, we find that counter-phase coupling can largely improve the performance.

*Poster

Multifractal closure for the velocity gradient evolution in Lagrangian turbulence

Rodrigo M. Pereira * [1], Luca Moriconi, Laurent Chevillard

[1] Universidade Federal do Rio de Janeiro – Brazil

We present a new closure for the evolution equation of the velocity gradient tensor $A_{ij} \equiv \partial_j u_i$ based on the multifractal nature of turbulent fluctuations. In particular, we adapt the strategy of Girimaji & Pope (1989), that assumed an Ornstein-Uhlenbeck process for the pseudo-dissipation and then looked for a compatible equation for A_{ij} starting from the restricted Euler model. We now impose a multifractal process starting from existing closures known to contain important physical aspects of the velocity gradient tensor, such as the Recent Fluid Deformation approximation developed by Chevillard & Meneveau (2006). This allows us to reach much higher Reynolds numbers than the original closure and reproduce the correct multifractal scaling of important physical quantities.

*Poster

Two effects of fluctuations on the dynamo instability

F. Pétrélis * [1], A. Alexakis, C. Gissinger, K. Seshasayanan

[1] LPS-Ecole Normale Supérieure – France

The dynamo instability is the generation of magnetic field by the flow of an electrically conducting fluid. Very generically, the dynamo flows are highly turbulent. We are then in the context of an instability occuring over a fluctuating background. I will present two situations where fluctuations affect the dynamo process. First, I will consider the case of a nonuniform fluid, in which the electrical conductivity varies spatially and temporally. A new dynamo mechanism exists, that provides a way to bypass anti-dynamo theorems. I will discuss the implication of this result for astrophysical objects and experiments. Second, it times permits, I will discuss how fluctuations of the amplitude of a velocity field affect the growth rate of an alpha-dynamo. In the limit of scale separation the problem is mapped onto the classical problem of injection of energy in an out-of-equilibrium system. Analytical results can thus be derived and I will compare them with the case of Kazantsev-dynamo.

*Poster

Formation and dynamics of striations in an annular inductive plasma

Nicolas Plihon * [1], V. Désangles, A. Poyé, P. Chabert, J.-L. Raimbault

[1] Laboratoire de Physique, Ecole Normale Supérieure de Lyon and CNRS – France

We present an experimental characterization of the dynamics of a low pressure, radiofrequency inductively coupled plasma with an internal coil (resulting in an annular geometry) as described in [1]. At low pressure, the resulting plasma equilibrium is axisymmetric. We show that the cylindrical symmetry of the system is broken at sufficiently high pressure (above 20 mTorr) and low coupled power. In these non-axisymmetric configurations, striations occur along the azimuthal direction (i.e. plasma parameters are azimuthaly modulated). The azimuthal mode of the striations (the number of plasma lobes) increases as pressure increases (from 2 to 7 lobes as pressure increases from 50 to 2500 mTorr). Both stationary and rotating structures have been observed. The transition between the axisymmetric configuration and non-axisymmetric configurations is shown to be subcritical, resulting in bistability. The transitions between non-axisymmetric configurations with various numbers of lobes are supercritical. High-speed imaging of the emitted light allow to precisely characterize the dynamics of the lobes, as well as the transitions between configurations. Similar behaviors have already been re- ported [2], but with no detailed characteriza- tion and no modeling. Here, we support our experimental observations by computations based on a fluid model including transport coefficients computed from kinetic distribution functions – in particular incorporating a thermoelectric coefficient. The properties of such a model is investigated to explain the basic features leading to the development of striations. [1] J. Arancibia Monreal, P. Chabert and V. Godyak, Phys Plasmas, 20, 103504 (2013) [2] A. S. Penfold, J. A. Thornton, R. C. Walder, Czech. J. Phys. B 23 431-435 (1973)

*Poster

The fate of dynamical localization for two interacting quantum kicked rotors

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The kicked rotor model is described as a single particle move on a ring with kicked driven potential. There is a well known dynamical property called dynamic localization. This property tell us if the period of the kicked drive take irrational multiple of 2π, the particle will localize in the momentum space. However, if considering two quantum kicked rotors with very short range interaction—δ function interaction, what is the fate of this dynamic localization? In my talk, different decay behaviors of the matrix element of the time evolution operator in the momentum space will be exhibited first. Compared to the exponential law decay of the matrix element in the kicked rotor model, we show that, the matrix element of the two interacting quantum kicked rotors have similar exponential law decay in the center of mass coordinate direction, but the power law decay in the relative coordinate direction. By using the second moments, the property of the dynamic evolution will be indicated in the talk.

*Poster

Measure Synchronization Goes Quantum

Haibo Qiu * [1], Bruno Julia-Diaz, Miguel Angel Garcia-March, Artur Polls

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Measure synchronization (MS), as a special concept which stands for collective dynamics shown in coupled Hamiltonian systems, has received little attention since it was proposed in 1999. In this talk, I will explain our work on MS, in which we extend the original classical concept of MS into the quantum many-body regime. The quantum-classical correspondence, quantum correlations, and dynamical mechanism of MS will be discussed.

*Poster

Particle transport in fluids with periodic forcing

Gerardo Ruiz Chavarria * [1], Erick Javier López Sánchez

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Particle transport in fluids is a subject which has deserved considerable attention in the last decades due to fundamental aspects involved in his study and also to applications in industry and in natural systems. In this work we present experimental and numerical results of particle transport in a periodic forced flow in a channel flushing into an open domain. This kind of flow can be observed in coastal systems under the actions of tides. For this purpose the Navier-Stokes and continuity equations are solved with the finite volume method, for a range of Reynolds numbers between 1000 and 20000. The velocity field obtained in this stage is used to solve the equation of motion for spherical particles inside the flow. The forces considered in this work are the drag, the gravity, the buoyancy, the added mass and the history force. With regard the experiments, we produce a periodic forced flow in a system of two basins connected by a channel. We put small particles (sand) inside the flow and we follow their evolution through a long time interval as compared with the forcing period. In the flow under study a vorticity dipole and a spanwise vortex are present. The dipole enhances displacement of particles because flow between vortices behaves like a jet and the spanwise vortex produces the lifting and deposition of particles from/to the bottom. We observe clustering of particles both into the channel and in the open domain as observed in coastal systems. Other aspect envisaged is the evaluation of different forces, in particular those related to the no stationarity of the flow. Finally, the influence of the finite size of particles is considered.
Acknowledgment: the authors acknowledge DGAPA-UNAM by support under project PAPIIT IN115315 "Ondas y estructuras coherentes en dinámica de fluidos"

*Poster

Dynamics in quasiperiodic environments

David P. Sanders * [1], Atahualpa S. Kraemer

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We present analytical and numerical results on billiard dynamics in a quasiperiodic Lorentz gas environment, consisting of point particles bouncing elastically off of fixed, hard discs arranged in a quasiperiodic lattice. We show how an efficient numerical method for simulating the system can be developed. This also gives rise to a new way to look at the system, showing that any such quasiperiodic structure contains channels which are devoid of obstacles [1], [2]. We will discuss the interplay of such channels with the diffusive properties of the system, in particular superdiffusion. [1] Horizons and free path distributions in quasiperiodic Lorentz gases Atahualpa S. Kraemer, Michael Schmiedeberg & David P. Sanders Phys. Rev. E 92, 052131 (205) [2] Embedding quasicrystals in a periodic cell: Dynamics in quasiperiodic structures Atahualpa S. Kraemer & David P. Sanders Phys. Rev. Lett. 111, 125501 (2013)

*Poster

Levy-Clifford algebra and multifractal calculus for analysis and simulation of spatial chaos

Daniel Schertzer * [1], Loulia Tchiguirinskaia

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There have been many attempts to analyse and simulate the fluctuations of chaotic systems whose spatial extension is of prime importance, such as turbulence, weather and climate. This was done at first with mono/uni-scaling approaches (e.g. structure functions, rescaled range or spectral analyses), however multifractal techniques are required to grasp the fundamental feature of intermittency, to track and simulate the scaling singularities of the underlying equations instead of relying on numerical, scale truncated simulations of these equations (e.g. Royer et al., 2008, Lovejoy and Schertzer, 2013 for climate).
Multifractals are indeed rather independent of the domain dimension, which can arbitrarily large, but on the contrary have been rather limited to scalar valued fields, i.e with 1D codomains. This prevents to deal with the key question of complex component interactions and their non trivial symmetries. The latter are unfortunately indispensable to answer to challenging questions such as the climatology of (exo-) planets based on first principles (Pierrehumbert, 2013) or to fully address the question of the relevance of quasi-geostrophic turbulence and to define an effective, fractal dimension of the atmospheric motions (Schertzer et al., 2012).
Fortunately, considering the Lie algebra of stochastic generators of cascade processes enabled to generalize multifractals to arbitrarily large codomains, e.g. large dimensional manifolds. In particular, we have recently investigated the neat example of stable Levy generators on Clifford algebra that have a number of seductive properties, e.g. universal statistical and robust algebra properties, both defining the basic symmetries of the corresponding fields (Schertzer and Tchiguirinskaia, 2015).
These properties provide the basis for a convenient multifractal calculus that should help to overcome current obstacles to the use of multifractal analysis and simulation at their full extent.
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*Poster

Critical bubble length controls gas-liquid flow in a solid foam

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This work combines global chemical engineering objectives with local physical methods to study hydrodynamics of a multiphase gas-liquid flow inside an innovating catalytic support: metallic open cell solid foams. The gas phase is nitrogen and the liquid phase is ethanol. The multiphase flow is constrained in a milli-channel in order to maintain a Taylor flow at the inlet of the porous medium. The proportion of liquid inside the porous medium varies in time with a typical main frequency. The analysis of this latter, depending on the initial flow rate conditions, leads to the identification of two hydrodynamic regimes. A scaling study is proposed to quantify the dimensionless parameter driving the transition between them. The bubble length fixed by the Taylor flow upstream the porous medium is identified to be the control parameter of this transition. A scaling model is proposed in order to predict the bubble length from which the regime transition occurs, called the critical bubble length.

*Poster

Origin of Instability derived from breakup and deformation of a droplet falling in miscible solution

Michiko Shimokawa * [1], Toshiya Takami, Hidetsugu Sakaguchi

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When a droplet with a higher density falls in a miscible solution with a lower density, the droplet deforms into a vortex ring and breaks up. The instability of the vortex ring is important for the breakup. An origin of the instability, however, has not been understood yet. To determine the origin, the wavelengths and thicknesses of the vortex rings were investigated at the time when the instability occurs in our experiments. The experimental results almost agree with the calculated results for Rayleigh–Taylor instability using the thickness of a higher-density solution. These results imply that the Rayleigh–Taylor instability plays a dominant role in the instability of vortex rings, which leads the breakup of a droplet.

*Poster

Statistical Theory of Reversals in Two-dimensional Confined Turbulent Flows

Vishwanath Shukla * [1], Marc Brachet, Stephan Fauve

[1] Indian Institute of Science – India

Motivated by the experimental observation of reversals in two-dimensional (2D), confined turbulent flows; we conduct a comprehensive theoretical and numerical study of the Kolmogorov flows, characterized by spatially periodic forcing. Our numerical simulations of the 2D Navier-Stokes equation with free-slip boundary conditions show that as the large-scale-friction is reduced, the following sequence of flow-regimes are observed: laminar flow, transition to chaos, turbulence with Gaussian velocity probability distribution functions (pdf), states with bi-modal velocity pdfs exhibiting random reverals of large-scale-circulation (LSC), and finally, a condensate state with dominant non-reversing LSC. The inverse cascade of energy can give rise to LSC; therefore, we ask, can we understand this observed behavior in terms of the inviscid dynamics of the large scale modes? To answer this, we make use of the two possible candidates for the statistical theory of 2D, Euler equation: (i) point vortices and (ii) Fourier truncated Euler equation. Our studies of the truncated, 2D, Euler equation and a simplified, minimal set of ordinary-differential equations for the large-scale modes, derived from it, with an absolute equilibrium initial conditions demonstrate that the statistical properties of the experimentally and numerically observed flow-regimes are qualitatively reproduced by an equilibrium system. Furthermore, we investigate the relationship between the reversals of the LSC and the presence of 1/f-noise in this system.

*Poster

Prediction and control of slip-free rotation states in sphere assemblies

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In a fixed assembly of rotating spheres in contact, spheres can influence each others rotation through sliding friction. From any initial state, sliding friction drives an assembly toward a slip-free rotation state. For bipartite assemblies, which have only even loops, this state is degenerated with at least four degrees of freedom. For exactly four degrees of freedom, we analytically predict the final state, which we proof independent of the strength of sliding friction, from an arbitrary initial one. With a tabletop experiment we show how to impose any slip-free rotation state by only controlling two spheres, regardless of the total number.

*Poster

Removal of phase transition of the Chebyshev quadratic and thermodynamics of Hénon-like maps near the first bifurcation

Hiroki Takahasi * [1]

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We treat a problem at the interface of dynamical systems and equilibrium statistical physics. It is well-known that the geometric pressure function

$$t \in \mathbb{R} \mapsto \sup_{\mu} \left\{ h_\mu(T_2) - t \int \log |dT_2(x)| d\mu(x) \right\}$$

of the Chebyshev quadratic map $T_2(x) = 1 - 2x^2$ ($x \in \mathbb{R}$) is not differentiable at $t = -1$. We show that this phase transition can be "removed", by an arbitrarily small singular perturbation of the map T_2 into Hénon-like diffeomorphisms. A proof of this result relies on an elaboration of the well-known inducing techniques adapted to Hénon-like dynamics near the first bifurcation.

*Poster

1D Cahn-Hilliard dynamics for pattern formation : Transition modes and stability criteria

Simon Villain-Guillot * [1], Mahdi Mcheik

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The Cahn-Hilliard equation describes the dynamics of phase separation in the conservative case (first order phase transition). This process is driven by the minimization of the free energy, especially of its interfacial part during the Ostwald ripening, or coarsening [1]. In 1D however, the lower energy state that should end the dynamics is very slow to reach. This is even more the case when the Cahn-Hilliard dynamics is modified to take into account long range interaction terms [2]: the lower energy state is then only reached for particular initial states. A criterion proposed by Misbah and Politi [3] to predict the end of the coarsening process (and the final wave length of the pattern) shows results that differ from the simple minimization of the free energy. In order to understand this difference, we have investigated possible transition modes that may describe the dynamic of coarsening in those systems. We have also explored a model where the Cahn Hilliard dynamics is coupled with a diffusion equation for the surfactant that favors interfaces. This scenario enables to speed up the dynamics and favors pattern formation or micro-structuration. Références [1] 1D Cahn-Hilliard dynamics : coarsening and interrupted coarsening pages 153-168 in "Discontinuity and Complexity in Nonlinear Physical Systems", Editors: J. Tenreiro Machado, Dumitru Baleanu, Albert Luo. Springer (2014) [2]] Dynamics versus energetics in phase separation P. Politi and A. Torcini J. Stat. Mech. P03016 (2015) [3] When does coarsening occur in the dynamics of one-dimensional fronts? P.Politi and C. Misbah, Phys. Rev. Lett. 92, 090601 (2004).

*Poster

Explicit computation of Reynolds stresses and velocity profile for Jupiter turbulent jets

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It is extremely uncommon to be able to predict analytically, from first principle, the velocity profile of turbulent flows and being able to compare it to observations. The self organization of barotropic turbulence into large scale stable structures evolving much slower than the typical time of eddies offers a unique opportunity for such an achievement through non-equilibrium statistical mechanics approaches. Jupiter's jets are a unique example, offering both this simple dynamical setup and a large amount of observations. We model the dynamics of Jupiter's jets by averaging the dynamics of eddies, in a barotropic beta-plane model, and explicitly predicting the balance between Reynolds' stresses and dissipation, thus predicting the average velocity profile explicitly [2]. In order to obtain this result, we adopt a non-equilibrium statistical mechanics approach. We consider a relevant limit for Jupiter troposphere, of a time scale separation between inertial dynamics on one hand, and stochastic forcing and dissipation on the other hand. A kinetic theory based on a quasilinear approach has been proven to be self consistent and exact in this inertial limit [1], however not giving fully explicit results. Starting from this kinetic theory and assuming further that the forcing acts on scale much smaller than the jet scale, we obtain a very simple explicit relation between the Reynolds stress, the energy injection rate, and the average velocity shear, valid far from jet edges (average velocity extrema) [2]. A specific asymptotic expansion close to jet edges unravel an asymmetry between eastward and westward, velocity extrema. We recover Jupiter's jet specificities: a cusp on eastward jets and a smooth parabola on westward jets. While obtaining such analytic theory of barotropic jet, in accordance with Jupiter's observation is extremely encouraging, it may not be sufficient to describe all the processes at hand on Jupiter's troposphere. We discuss possible future generalization to more comprehensive model, including for instance baroclinic instabilities.

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[2] E. WOILLEZ, and F. BOUCHET, 2016, Explicit computation of Reynolds stresses and velocity profile for Jupiter turbulent jets, to be available soon on ArXiv and Hal.

*Poster

Topic 8: Interdisciplinary and complex systems -Posters

Maximal synchronizability of networks and the role of edges

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We study synchronizability of networks of coupled oscillators as a function of number of edges while the node number is fixed. In many coupled oscillators systems, the synchronization state is stable in a finite interval of coupling parameter (ε). We define this finite interval of coupling parameter as *synchronization length* (l_ε). The number of edges in a network plays a crucial role in determining its synchronization length. We observed that, in most of the networks, there exists a perfect number of edges for which the synchronization length is maximum and we call these networks as the *maximally synchronizable* networks. Too less or too many edges reduce the synchronization length leading to worse synchronization performance of the network.

*Poster

Payoff heterogeneity in evolutionary game theory

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Evolutionary game theory is a common framework to study the evolution of cooperation, where it is usually assumed that the same game is played in all interactions. Here we depart from this assumption by considering mixed games, where the game played at each interaction is drawn uniformly at random from a set of two different games. Using the master equation approach we show that the random mixture of two games is equivalent to play the average game in well-mixed populations. Nevertheless in structured populations this is not always the case. We studied diverse topologies and update methods using Monte-Carlo Simulations and show that the outcome is in fact strongly dependent on the distance of separation of the two games in the parameter space. Effectively, this distance introduces payoff heterogeneity, and the average game is returned only if the heterogeneity is small. For higher levels of heterogeneity the distance to the average game grows, which often involves the promotion of cooperation. The presented results support preceding research that highlights the favorable role of heterogeneity regardless of its origin, and they also emphasize the importance of the population structure in amplifying facilitators of cooperation.

*Poster

Monte Carlo simulations of lasers: from mode locking to replica symmetry breaking

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When the number of electromagnetic modes in an optical system is large enough, statistical mechanics can be employed to study the system via a model at effective equilibrium. This approach is in particular powerful to study the properties of nonlinear lasing system. Within this context, we have employed an extensive numerical analysis of vector models with four-body interactions through Monte Carlo simulations with varying degree of disorder. These models have a direct interpretation in the optical counterpart, ranging from standard mode locking lasers to random lasers. Our numerical analysis extends known results of analytical mean field studies and allow to investigate situations closer to real systems, like the presence of well definite frequencies for the electromagnetic modes. We discuss the thermodynamic properties of these systems and the experimental implications for the optical counterpart, in particular with respect to the evidence of replica symmetry breaking in random lasers.

*Poster

Study of the Fixation time in Evolutionary Graphs

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How does a new species take over the whole a population of a fixed number of individuals? This is one the crucial problems in Evolutionary Dynamics. Fixation probability and fixation time, are two quantities that used to quantify this issue. These quantities are related to the structure of a network. However there is not any clear relation between them. In this study, we focus on the fixation time by analytical and simulation approaches. First, we introduce an approach for exact calculation of fixation time. We consider two different kinds of graph topologies. Then we study the effect of heterogeneity of graphs on the fixation time for a number of known structures by simulation. This study shows that the effects of heterogeneity on the fixation probability and the fixation time are quite different.

*Poster

Complex dynamics outcomes from a simple stochastic cellular automaton on infectious diseases

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A cellular automaton (CA) is an extension of difference equations in which we are able to follow the dynamics of one or more variables or elements which reside in a lattice or grid [1]. Usually, each cell of the grid can be occupied by no more than one element y, which status at a given time t depends on both its status at the previous time $t-1$, as well as the status of its neighbours at the same previous time. On a 1D-CA, each cell has two neighbours (as the borders touch, forming a torus), x and z. Formally,

$$y_t = f(x_{t-1}, y_{t-1}, z_{t-1}) \tag{6}$$

Early epidemic 1D-CA models considered a contact process in which susceptible elements S and infectious elements I were randomly allocated on a lattice [2]. An S element becomes an I element at rate γ at time $t+1$ if at the previous time t it has an I neighbour. At rate γ, I elements become S elements again, resembling a classic SIS model. By using probabilities instead of rates, I developed a relative simple 1D-CA that is able to simulate, SIS models, SIR models, long-range local infections and long-range foreign infections by changing parameter values. All cells are populated with either S, I or R elements. At baseline ($t=0$) R elements are not present. The "updating rules" are relative simple, but stochastic. If an S element has an I neighbour at time t, then it becomes an I element with probability p_{infect} at time $t+1$. An I element keeps its current status for t_{infect} discrete times. After $t = t_{infect}$ time steps, an I element becomes an R element with probability p_{memory} or an S element with probability $1 - p_{memory}$. Long-range local infections occur with probability p_{local} if an S element was not infected by its neighbours but there were infectious elements on the previous time. Long-range foreign infections occur with probability $p_{foreign}$ if an S element was not infected, regardless of whether or not there were infectious elements on the previous time. Simulations give rise to simple dynamics (e.g., fixed points on classic SIS), oscillations (e.g. classic SIR), as well as complex dynamics (when long-range infections are allowed).

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[2] Harris, TE (1974). Contact interactions on a lattice. *Ann Probab*, 2: 969-988.

*Poster

The Instantaneous Time Mirror : Performing a Loschmidt Daemon in Wave Physics

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Can we time reverse at once the evolution of a system, so that everything in its future evolution happens as though time would be going backwards ? In general this is the case if the dynamics is time symmetric. This reversibility has been at the heart of a well known dispute between Boltzmann and Loschmidt. Boltzmann's famous statistical theory of gases describes how irreversibility at the macroscopic level and entropy growth can arise from the statistical properties of the motion of the particles. Although Boltzmann's work can be considered as the fundament of modern statistical physics, the fundamental question of how these statistical properties emerge from microscopic molecular interactions remains open. Furthermore, there is in principle a contradiction between Boltzmann's "molecular chaos" assumption and the time reversibility of the dynamical equations of motions known to hold at the molecular level. This paradox was pointed out by Loschmidt who suggested considering a Gedankenexperiment in which a "daemon" would be able to stop the motion of all the particles of a gas at a given instant and send each of them back with a velocity exactely opposite of the velocity they had before. This corresponds to an instantaneous transformation of the position $\overrightarrow{r}$ and the velocity $\overrightarrow{v}$ for each particle :

$$(\overrightarrow{r}(t^-), \overrightarrow{v}(t^-)) \rightarrow (\overrightarrow{r}(t^+), \overrightarrow{v}(t^+)) = (\overrightarrow{r}(t^-), -\overrightarrow{v}(t^-)). \tag{7}$$

In such a scenario, owing to the time reversibility of the microscopic dynamics, all particles would move back as though the time was running backwards, converting say an explosion into a collapse. Modern day chaos theory has shown that the realization of such a daemon is impossible in practice since small perturbations or errors will grow exponentially. Here we experimentally demonstrate for the first time that a Loschmidt daemon can however be achieved in wave physics. For a wave field ϕ, the corresponding transformation is :

$$(\phi(t^-), \frac{\partial \phi}{\partial t}(t^-)) \rightarrow (\phi(t^+), \frac{\partial \phi}{\partial t}(t^+)) = (\phi(t^-), -\frac{\partial \phi}{\partial t}(t^-)) \tag{8}$$

A sudden and brief change of the effective phase velocity performed in the whole medium at once suffices in order to produce an exact time reversed backward propagating wave. We show this backward wave is the equivalent of the result of Loschmidt's daemon transformation. We baptize this concept the instantaneous time mirror. It can be implemented for any type of wave. In our experimental implementation with water waves on the surface of a liquid, we act on the bath by submitting it to a strong vertical jolt (acceleration of the order of ten times the gravity during a few milliseconds). At the instant of the jolt, a backward propagating wave instantaneously appears which refocuses at the original emission spot. This backward wave packet is the time reverse of the original one.

*Poster

Combination of Tit-for-Tat and Anti-Tit-for-Tat Remedies Problems of Tit-for-Tat

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One of the most important questions in game theory concerns how mutual cooperation can be achieved and maintained in a social dilemma. In Axelrod's tournaments of the iterated prisoner's dilemma, Tit-for-Tat (TFT) demonstrated the role of reciprocity in the emergence of cooperation. However, the stability of TFT does not hold in the presence of implementation error, and a TFT population is prone to neutral drift to unconditional cooperation, which eventually invites defectors. We argue that a combination of TFT and anti-TFT (ATFT) overcomes these difficulties in a noisy environment, provided that ATFT is defined as choosing the opposite to the opponent's last move. According to this TFT-ATFT strategy, a player normally uses TFT; turns to ATFT upon recognizing his or her own error; returns to TFT either when mutual cooperation is recovered or when the opponent deviates from expected moves by defection. The proposed strategy provides simple and deterministic behavioral rules for correcting implementation error in a way that cannot be exploited by the opponent, and suppresses the neutral drift to unconditional cooperation.

*Poster

Biologically-inspired functional clustering in logical networks and games

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How much of the functional organization of an artificial system can one recover by mimicking empirical approaches from biology, devised to reverse-engineer molecular, neural and ecological networks? I take interest in basic methods, such as knockouts and substitutions, that do not target specific structural or dynamical features but functionality, i.e. the role played by one element in the system's response to external selection. By testing them on simple abstract systems - logical networks and combinatorial games - I attempt to shed light on their explanatory power, and on their limitations: What sort of structures confound them? Can they deal with multiple levels of abstraction? Are they robust under refactoring? The main result is that the existence of distinct failure modes for the system greatly helps with functional identification.

*Poster

Measuring cultural evolution with statistical physics: the analysis of American baby names

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The quantitative description of cultural evolution is a challenging task. The most difficult part of the problem is probably to find the appropriate measurable quantities that can make more quantitative such evasive concepts as, for example, dynamics of cultural movements, behavioral patterns, and traditions of the people. A strategy to tackle this issue is to observe particular features of human activities, i.e., cultural traits, such as names given to newborns. We study the names of babies born in the United States from 1910 to 2012. Our analysis shows that groups of different correlated states naturally emerge in different epochs, and we are able to follow and decrypt their evolution. Although these groups of states are stable across many decades, a sudden reorganization occurs in the last part of the 20th century. We unambiguously demonstrate that cultural evolution of society can be observed and quantified by looking at cultural traits. We think that this kind of quantitative analysis can be possibly extended to other cultural traits: Although databases covering more than one century (such as the one we used) are rare, the cultural evolution on shorter timescales can be studied due to the fact that many human activities are usually recorded in the present digital era. [1] Barucca P., Rocchi J., Marinari E., Parisi G. and Ricci-Tersenghi F., Proceedings of the National Academy of Sciences 112 (2015) 7943.

*Poster

Information Based Price Formation in Race Track Odds

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We explore price-odds formation in the domain of horse track racing using information perception models. The horse racing odds considered in this study are in-play, referring to data collected once the race has started, up to the point when the race has finished. From the in-play data set, we use the Last Price Matched signals which are converted to probabilities, and only winning horses are considered. We extend a pioneering approach to financial asset pricing known as the Brody-Hughston- Macrina framework [1] or information based asset pricing. This is used as a means to calibrate a model where a group of agents acquire their own individual perspectives of what they believe the price of an asset to be, given a stochastic process of the arrival of information. This information model gives the flexibility that agents can adjust their pricing kernel according to price changes caused by information. The informational impact on price may occur even if the agents' preferences are unchanged, and hence we can view the dynamics of the price movement as emergent. When fitting the model to data we find that the odds of the ultimately winning horse, as perceived by a representative agent, evolve in a fashion that can be interpreted in terms of the arrival and perception of information. We find that the fitted information rate parameter varies with race distance according to a power law. References [1] D.C. Brody, L.P. Hughston, and A. Macrina. Information-based asset pricing. International Journal of Theoretical and Applied Finance, 11(1):107?142, 2008.

*Poster

Spatial distribution of zebrafish groups in heterogeneous environment

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Aggregative behavior is observed in many different fish species. It can in particular be observed around natural floating objects that compose their environment. Our study on zebrafish (Danio rerio) demonstrates its aggregative behavior around floating objects and shows it is influenced by both social and environmental factors. We tested groups composed of different numbers of fish (1, 5, 25) and confronted them with two separate environmental conditions, one a circular tank with two heterogeneities (floating objects) and the other a circular tank without heterogeneities. Fish displayed an inhomogeneous spatial distribution in the tank for both environmental conditions. They showed a clear attraction to the edge of the tank and aggregated mainly under the floating objects when confronted with them. They globally did not show a preference between either of the floating objects and alternated between them. This is in stark contrast to the dynamics observed in other species which show an irreversible group choice between resources (e.g. social insects, mammals).

*Poster

The Braess' paradox in a network of totally asymmetric exclusion processes

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We present a Monte Carlo study of the Braess' paradox in a network with totally asymmetric exclusion processes (TASEPs) on the edges. The Braess paradox describes the situation, where adding more capacity, i.e. a new link, to a network leads to a worsening of the network performance. Traveltimes on the TASEPs are nonlinear in the density and jammed states can occur due to the microscopic exclusion principle. Furthermore the individual edges influence each other. This leads to a much more realistic description of traffic-like transport on the network than in previously studied linear macroscopic models. Furthermore the stochastic dynamics allows to explore the effects of fluctuations on the network performance. We observe that for low densities the added edge is useful, then for slightly higher densities the Braess paradox in its classical sense occurs in a small density regime. In a large regime of intermediate densities strong fluctuations in the traveltimes dominate the system's behaviour. These fluctuations are due to links being in the domain wall or coexistence phase. While we cannot predict the actual state of the system, we can still conclude that the added link does not improve the whole system since the system optimum is equal to that of the system without the new link. At high densities the added link is observed to be useful again. We present a phase diagram predicting, in which state the system will be, depending on the global density and crucial length ratios.

*Poster

Disease-induced resource constraints can trigger explosive epidemics

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Advances in mathematical epidemiology and network science have led to a better understanding of the risks posed by epidemic spreading and informed strategies to contain disease spread through prevention and treatment. However, a challenge that has been overlooked is that, as a disease becomes more prevalent, it can limit the availability of the capital needed to effectively treat those who have fallen ill. Here we use a simple mathematical model to gain insight into the dynamics of an epidemic when the recovery of sick individuals depends on the availability of healing resources that are generated by the healthy population. We find that epidemics spiral out of control into explosive spread if the cost of recovery is above a critical cost. This can occur even when an epidemic would not be predicted by a standard model that does not consider the reduction in resource generation as individuals fall ill. Through simulations and analytical solutions we show that the onset of explosive epidemics is very sudden, exhibiting a discontinuous transition under very general assumptions. We also determine analytically the critical cost and the size of the explosive jump in infection levels in terms of the parameters that characterize the spreading process. Our model and results apply beyond epidemics to other contagion dynamics that self-induce constraints on recovery, thereby amplifying the spreading process.

*Poster

Analytic solutions for links and triangles distributions in finite Barabási-Albert networks.

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Barabási-Albert model describes many different natural networks, often yielding sensible explanations to the subjacent dynamics. However, finite size effects may prevent from discerning among different underlying physical mechanisms and from determining whether a particular finite system is driven by Barabási-Albert dynamics. Here we propose master equations for the evolution of the degrees, links and triangles distributions, solve them both analytically and by numerical iteration, and compare with numerical simulations. The analytic solutions for all these distributions predict the network evolution for systems as small as 100 nodes. The analytic method we developed is applicable for other classes of networks, representing a powerful tool to investigate the evolution of natural networks.

*Poster

Assessing the degree of chaos of the Kuramoto model

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The Kuramoto model of coupled phase-oscillators is widely used in non-linear sciences. In spite of its simple structure, it gives rise to a wealth of dynamical phenomena that can be observed in various setups that range from chemical oscillators to firing neurons. It is well known that a finite ensemble of such oscillators is characterized by a chaotic dynamics, but very little efforts have been made to investigate the scaling properties of the chaotic dynamics on both the system size and the coupling strength. Here, we mostly focus on the maximum Lyapunov exponent, going beyond a mere scaling analysis. More precisely, we study its dependence on the realization of the natural frequencies, the importance of the intrinsic fluctuations of the phase evolution, and perform some analytical calculations in the limit of a few oscillators.

*Poster

Statistical physics models of Language Dynamics: Role of Diversity

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The dynamical nature of a societal phenomenon is based on the collective behavior of a myriad number of interacting agents, and hence has many features in common with interacting systems in statistical physics. Interdisciplinary studies based on such phenomena have given rise to a new area, popularly known as "Sociophysics". Among such sociophysics problems, language dynamics has become an important issue. Several models have been proposed to mimic the language dynamics. Despite languages being treated as non-evolving entities, a quantitative description of their interactions, diffusion, and extinction processes, is certainly relevant also for a better understanding of their history and distribution [1, 2, 3], which still represent open problems. In a typical situation, only one of the two languages survives [4]. However, there are cases of languages which do not seem to risk extinction and survive despite their limited diffusion and the interaction with other more diffused languages. Here, we study a set of novel two- and three-state models of language dynamics inspired by older analogous models [5], beginning with the well-known Abrams-Strogatz model [6] and the Baggs-Freedman model [7]. In our models, we add further elements which make these simple models more realistic and relevant, such as (i) the addition of population dynamics terms (in the form of a logistic term), and (ii) the heterogeneity of the individuals in some of their parameters, emphasizing the importance of diversity in "Complex Systems" [8]. The study, carried out both within a mean field approach and through numerical simulation of individual-based models, reveals how simple models of cultural dynamics can present surprisingly complex dynamics. We also discuss the link between some real examples of language competition and the corresponding range in the parameter space. References [1] R.D. Gray. Q.D. Atkinson, Language-tree divergence times support the Anatolian theory of Indo-European origin, Nature 426 (2003) 435. [2] J.R. Diamond, Linguistics: The language steamrollers, Nature 389 (1997) 544. [3] J.E. Terrell, J. Hines, T.L. Hunt, Language steamrollers? Nature 391 (1998) 547. [4] M. Patriarca and T. Leppanen, Modelling language competition, Physica A 338 (2004) 296. [5] M. Patriarca, E. Heinsalu, and A. Chakraborti: Basic kinetic wealth-exchange models: common features and open problems, Eur. Phys. J. B 73 (2010) 145. [6] D.M. Abrams, S.H. Strogatz: Modeling the dynamics of language death, Nature 424 (2003) 900. [7] I. Baggs, H.I. Freedman: A mathematical model for the dynamical interactions between a unilingual and bilingual population: Persistence versus extinction, J. Math. Sociology 16 (1990) 51. [8] The role of diversity in Complex Systems, Institutional Research Funding IUT (IUT39-1) of the Estonian Ministry of Education and Research.

*Poster

Rubik's cube: an energy perspective

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What if we played the Rubik's cube game by simple intuition? We would rotate the cube, probably in the hope of getting a more organized pattern in each next step. Yet frustration occurs easily, and we soon find ourselves trapped as the game progresses no further. Played in this completely strategy-less style, the entire problem of the Rubik's cube game can be compared to that of complex chemical reactions such as protein folding, only with less guidance in the searching process. In this work we look into this random-searching process by means of thermodynamics and compare the game's dynamics with that of a faithful stochastic model constructed from the statistical energy landscape theory (SELT). This comparison reveals the peculiar nature of SELT, which relies on the random energy approximation and often chops up energy correlations among nearby configurations. Our observation provides a general insight for the use of SELT in the studies of these frustrated systems.

*Poster

q-neighbor Ising model on complex networks

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We modify the kinetic Ising model with Metropolis dynamics, allowing each spin to interact only with q spins randomly chosen from the whole system, which corresponds to the topology of a complete graph. We show that the model with $q \geq 3$ exhibits a phase transition between ferromagnetic and paramagnetic phases at temperature T^*, which linearly increases with q. Moreover, we show that for $q = 3$ the phase transition is continuous and discontinuous for larger values of q. For $q > 3$ the hysteresis exhibits oscillatory behavior – expanding for even values of q and shrinking for odd values of q. If only simulation results were taken into account, this phenomenon could be mistakenly interpreted as switching from discontinuous to continuous phase transitions or even as evidence of the so-called mixed phase transitions. Due to the mean-field like nature of the model we are able to derive the analytical form of transition probabilities and, therefore, calculate not only the probability density function of the order parameter but also precisely determine the hysteresis and the effective potential showing stable, unstable and metastable steady states. Our results show that a seemingly small modification of the kinetic Ising model leads not only to the switch from a continuous to a discontinuous phase transition but also to an unexpected oscillating behavior of the hysteresis.
The analysis of the q-neighbor Ising model on complete graph is presented in [1]. In the case of a random regular graph, where the degree of node k is sufficiently larger than q, we observe the same behavior as for the complete graph (oscillating behavior of the hysteresis). In a spirit of [2], we generalize the q-neighbor Ising model for multiplex networks. A node will change the state only if both levels suggest the change (AND -rule). In case of duplex networks we observe only continuous phase transition, for all values of q.

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[2] A. Chmiel, K. Sznajd-Weron *Phase transitions in the q-voter model with independence on a duplex clique*, Phys. Rev. E **92**, 052812 (2015).

*Poster

Comprehensive studies of phase transitions in a two-step contagion model

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Recently hybrid phase transition (HPT) that exhibits natures of both first-order and second-order transitions at the same transition point has been observed in diverse systems. One of the fundamental questions is how the critical behavior of HPT is exerted by the discontinuity of the order parameter. Recent studies for the HPT focused on the behavior of the order parameter. However, such studies are not sufficient to understand the critical behavior of the HPT. Here we investigate the critical behavior of the HPT more deeply including the behaviors of the fluctuations of the order parameter and the correlation funciton using finite-size scaling analysis for a two-step contagion model. The hyperscaling relation is also examined.

*Poster

A bistable belief dynamics model for radicalization within sectarian conflict

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We introduce a two-variable model to describe spatial polarization, radicalization, and conflict. Individuals in the model harbor a continuous belief variable and a discrete radicalization level expressing their tolerance to neighbors with different beliefs. A novel feature of our model is that it incorporates a bistable radicalization process to address memory-dependent human social behaviors. We demonstrate how bistable radicalization may explain contradicting observations regarding whether social segregation exacerbates or alleviates conflicts. We also extend our model by introducing a mechanism for institutional influence and examine its effectiveness. In some parameter regimes, institutional influence may suppress the progression of radicalization and allow a population to achieve social conformity over time. In other cases, institutional intervention may exacerbate the spread of radicalization through a population of mixed beliefs. In such instances, our analysis implies that social segregation may be a viable option against sectarian conflicts.

*Poster

Phase transitions of cooperative contagions on complex networks

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The generalized epidemic process (GEP) [1, 2] is a simple model of cooperative contagions, in which the probability of infection changes according to the number of infected neighbors. For regular lattices, it is known that the model exhibits both continuous and discontinuous phase transitions, with (tri)critical exponents near the upper critical dimension derived by a field theory [2]. Similar phenomena were also observed in networks, but the studies have been limited to the phase diagram of Poisson random networks [3]. Extending an analytical technique based on the representation of a network as a tree of node clusters, we propose a self-contained theoretical framework [4] that describes the phase diagram and (tri)critical behaviors of the GEP on a broader range of complex networks, which includes modular networks and scale-free networks. While the modularity simply affects the epidemic threshold [5], the structural heterogeneity of scale-free networks has nontrivial consequences on the transition properties of the GEP. Most notably, when the power-law exponent characterizing the degree distribution lies between 2 and 3, our theory predicts a discontinuous transition at zero epidemic threshold for a properly chosen order parameter. The theoretical predictions are also compared with numerical results, which also provide information about finite-size scaling that has been missing in previous studies. [1] P. S. Dodds and D. J. Watts, Phys. Rev. Lett. 92, 218701 (2004). [2] H.-K. Janssen, M. Mueller, and O. Stenull, Phys. Rev. E 70, 026114 (2004). [3] G. Bizhani, M. Paczuski, and P. Grassberger, Phys. Rev. E 70, 011128 (2012). [4] K. Chung, Y. Baek, M. Ha, and H. Jeong, arXiv:1512.04457; accepted in PRE. [5] K. Chung, Y. Baek, D. Kim, M. Ha, and H. Jeong, Phys. Rev. E 89, 052811 (2014).

*Poster

Monte Carlo and molecular dynamics simulations of capillary bridges.

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The theory of capillarity was created in the early 1800's, and it is applicable to macroscopic, mesoscopic and some nanoscopic systems, ranging from diagnosis of airways condition in the lung to wetting. Here, we conducted two studies in which the capillary theory (CT) and, Monte Carlo (MC) and molecular dynamic (MD) simulations were used to comprehend the processes of occlusion of small airways in the lung, and to test the applicability of capillarity concepts to nanoscopic systems. In the first study, we focus on the blocking of airflow of small airways by capillary bridges due to abnormal mechanical instabilities. The formation of capillary bridge during exhalation can cause the crackling adventitious lung sound, which can be heard using a simple stethoscope. To understand this phenomenon, we study the capillary bridge between two parallel planes, using both Monte Carlo simulation of a lattice gas model and variational calculus based on minimization of the surface area with the volume and the contact angle constrained. The simulation results are in agreement with the capillarity analytical solution, and we observed a difference in free energy prior and after the bridge formation, indicating the cause of the crackling adventitious lung sound. In the second study, we focus on the test of capillarity theories at the nanoscale. It is expected that macroscopic theories fail at the < 10 nm scales, once molecular details may become relevant. Specifically, we perform atomistic MD simulations of water capillary bridges in contact with various hydroxilated (crystalline) silica surfaces, which are modified to cover a wide range of hydrophobicity/hydrophilicity. In agreement with CT, it is found that water contact angle depends only on the hydrophobicity/hydrophilicity of the surface employed. In addition, CT provides the correct capillary bridge profile for all surfaces considered. We also calculate the capillary forces between the different surfaces induced by water capillary bridges. These forces allowed us to calculate the water surface tension. This study confirm the self-consistency of CT at $2 - 10$ nm scales.

*Poster

Exploiting resources: evolutionarily stable strategy with no conflicts and emergence of property rights

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In a game theoretic approach to the study of the evolution of animal conflicts, it has been shown that choosing an initial asymmetric feature (such as first arrived to the good) to settle a contest is evolutionarily stable, and that in such circumstances animal fights are generally avoided. In this context, we investigate the optimal strategy that could be adopted by N animals competing for N resources providing different payoffs, in a situation in which animals avoid conflicts. For this purpose we consider that each resource can be exploited only by one animal at a time, and if an animal finds a resource already occupied, it looks for another resource, which implies a certain cost.
We first obtain the mean-field solution for the Nash equilibrium in which animals use a mixed strategy. Surprisingly, this solution coincides with the mean optimal strategy resulting from a Monte Carlo simulation of a system in which each animal improves its own strategy by learning. Moreover, further analysis of the behavior of the animals in the simulation reveals that each of them adopts actually a different strategy, avoiding each other while obtaining the same mean payoff, resulting in a situation in which individuals meet rarely and spread optimally over the system. Finally, we highlight places favorable for the emergence of settlers among the animals, whose pure strategy leads to a better payoff. This approach can help for instance to understand the repartition of animal strategies for exploiting resources in an ecosystem.

*Poster

Self-organized groups in a tortuous domain:hydrodynamic aspects

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Examples of self-organization and cooperation in living species surround us daily. The most common ones are represented by the motion of flocks of birds, schools of fishes and swarms of insects, which tend to arrange in orchestrated organized spatial structures. Usually, numerical models for predicting their collective behavior idealize the individuals as point wise self-propelled particles without mass. Moreover, the role of the surrounding medium is disregarded. Here, we investigate the problem of a leader that wants to guide a group in a tortuous domain as they are immersed in a fluid. We propose to combine the collective laws with a hydrodynamic solver based on a combined lattice Boltzmann-immersed boundary approach. We find that the presence of the fluid plays a crucial non-linear role in spreading the consensus within the group, thus affecting the performance of the leader.

*Poster

Pattern forming instabilities leading to the formation of hexagonal clusters

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It is well known amongst physicists that seemingly distinct systems can sometimes exhibit strikingly similar behaviors under some circumstances. Here, we draw a parallel between two comparable cases of clustering observed in very different models : on the one hand, Brownian particles interacting via a "soft potential", purely repulsive but allowing overlaps between particles (two characteristics typical of various types of polymeric macromolecules like polymer chains or dendrimers for example). On the other hand, a model of population dynamics with neighborhood dependent birth and death rates, accounting for the spatial heterogeneity of the competition between individuals. Both of these systems exhibit a similar phase transition leading to a segregation of their particles into clusters arranged in hexagonal patterns. Macroscopic equations can be derived for the two models and their structures are quite comparable, despite the fact that the number of particles is not conserved in the second case. Their linear stability analysis shows that this clustering is induced by an instability of the homogeneous state, triggered by the non-local mutual interactions.

*Poster

Smoldering combustion ? a new laboratory for research on complexity

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While ordinary flaming combustion involves reactions in gas phase, smoldering combustion is a set of reactions with oxygen that occur directly at the surface of a solid fuel. Thus, during smoldering combustion there are no flames, but smoke is produced. From a safety perspective, smoldering is a challenge: it can survive at low oxygen concentrations and is difficult to extinguish. Examples are fires in coal mines, which may last for years. Furthermore, the fundamentals of smoldering as such are poorly understood. Both from applied and basic research, smoldering combustion has received far less attention than various forms of flaming combustion. The ignition of smoldering, its propagation and its possible spontaneous transition to flaming fire depend on an intricate interplay between material (fuel) properties, heat generation, heat loss and exchange of gases. Ignition occurs at relatively low temperatures, through a series of endothermal and exothermal irreversible reactions. Thus, ignition of smoldering, as a function of temperature, is far more complex than a simple phase transition. Similarly, the propagation of a (self-sustained) smoldering fire may take surprising routes, and secondary combustion processes occur in an stochastic way in partly combusted material. In this contribution, an overview will be given of results on smoldering fires in several experimental configurations and using several materials, as obtained by five groups in an international collaboration (see http://www.hsh.no/fou/fouprogram/ts/emris). Keywords: 'transition' between non-ignition and ignition, hysteresis, front propagation, 'transition' to flaming fire. With a series of scenarios with smoldering fires largely unexplored, there is a potential for refinement of concepts from the statistical-physics toolbox.

*Poster

Nature of phase transitions in Axelrod-like coupled Potts models in 2D

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In this communication I will present a recently published paper about the nature of phase transitions in Axelrod-like coupled Potts models over lattices. I will explain the motivation related to some social models, for our system, consisting of F coupled q-state Potts models embedded in a two- dimensional square lattice. I will present the properties of the geometrical clusters, which allows to determine the fractal dimension D of the incipient infinite cluster and to examine the finite-size scaling of the cluster number density via data collapse. I will show that data collapse can be obtained, no only in the continuous (F=2,q=2), but also in the weakly first order (F=3,q=2) phase transition. Contrary to the one-dimensional case, in two spatial dimensions we have found that the thermodynamical version of the Axelrod model and the out-of-equilibrium original model with noise show a different qualitative behaviour in the limit of infinite size. This comparison is an example of the possible interesting connections that can be drawn between statistical mechanics and complex systems.

*Poster

Steady-State Immiscible Two-Phase Flow in Porous Media: Some New Aspects

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Immiscible two-phase flow in porous media under steady-state conditions is a simpler problem than when one fluid is invading the space of another. However, the latter has been studied extensively compared to the first. In the steady-state problem, both fluids complete for the same pore space leading to self organization. We present a number of results concerning such flow including equations that relate the flow rates of each fluid and equations that relate total flow rate to pressure difference.

*Poster

Time and space patterns in a pedestrian dynamic simulation

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In this work we show a variation in the model for pedestrian dynamics proposed by Helbing and Molnár in 1995 (1). Three kinds of interactions are considered. Firstly, there is a "trend force" responsible for each pedestrian tending to have a desired speed in a desired direction. Secondly, there is a repulsive force between every pair of pedestrian so that they avoid disturbing each other during their movement. Finally, it is also taken into account a force between the pedestrians and some boundaries. Computer simulations were carried out including 250 pedestrians in a 900 m2 square. Pseudo-periodic boundary conditions were applied in the directions available to the pedestrian movements. We show results on the dynamics of two different groups of pedestrians with different desired velocities. When the desired velocities are parallel in opposite directions the pedestrians self-organize on lanes with alternating directions. We also study situations where the pedestrians move in non-parallel directions and a pattern of alternating lanes is observed in the direction of the vector difference between the desired velocities. An analogy is developed between these situations and a hydrodynamic instability produced when two fluids of different densities are in contact under the influence of gravity. A special situation is considered when two groups of pedestrians try to go trough a door in opposite directions leading to two pedestrian flows that in this case alternate in time. An analogy is thus developed between this latter situation and the so-called density oscillator (2). 1.-Helbing, D., and Molnar, P. Physical Review E 51 (5): 4282-4286 (1995) 2.-Steinbock, O., Lange, A., and Rehberg, I. Physical Review Letters 81 (4): 798-801 (1998)

*Poster

From binding stoichiometry to the parking lot problem

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Consider a macromolecule, containing several equivalent and non-interacting binding sites, reacting with ligands. One is interesting in determining the binding stoichiometry of the reactants that is the key element of the macromolecule-ligand interaction. Once this quantity is known, the fraction of bound ligands can be calculated for given conditions of the reaction. This problem can be mapped onto the parking lot problem in which the jamming coverage can be related to the binding stoichiometry. We have studied the discrete version of the reversible car parking lot problem in which M identical particles (of a given size) reversibly bind and detach on a line with N binding sites. In this work, we are interested in the density of occupied sites at the equilibrium state as a function of various parameters: binding particle size, adsorption rate / desorption rate, number particles / number of binding sites. We have derived an analytical expression for the density of occupied sites that is in very good agreement with simulations. Finally, the relation with the binding stoichiometry problem is discussed.

*Poster

Long-range correlations in time series data and the method of detrended fluctuation analysis revisited

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Long-range correlation is an important phenomenon found in many time series, such as in hydrology, climate, and finance. Since its first discovery by Hurst analyzing Nile river flows in 1951, there has been a fruitful debate on the reliable distinction of long-range correlated noise and external non-stationarities such as trends. In this talk, we investigate analytically the influence of long-range correlations on the estimation of linear trends and their detection with the method of detrended fluctuation analysis, thereby we found new insights on this field of study. First, we provide an analytical study on the estimation of linear trends for time series with long-range correlations and show, that the longer the correlations the higher is the uncertainty of estimated trends. We apply our framework on the long-term daily air temperature record in Potsdam. Then, we focus on the detection of long-range correlations in time series and propose the fluctuation function as an integral transform of the autocorrelation function with kernel working as filter. This function enables us to estimate the autocorrelation function indirectly via segmentation of the time axis. We show, that this form of the fluctuation function represents the fluctuation function of the well-known method of detrended fluctuation analysis (DFA). Finally, we investigate the DFA analytically. We show, that short-range correlated series causes a crossover behaviour on the scaling of the fluctuation function and we also investigate how DFA works on the intrinsic non-stationary fractional brownian motion.

*Poster

Self-Elongation with Sequential Folding of a Filament of Bacterial Cells

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Under hard-agar and nutrient-rich conditions, a cell of *Bacillus subtilis* grows as a single filament owing to the failure of cell separation after each growth and division cycle. The self-elongating filament of cells shows sequential folding processes, and multifold structures extend over an agar plate. We report that the growth process from the exponential phase to the stationary phase is well described by the time evolution of fractal dimensions of the filament configuration. We propose a method of characterizing filament configurations using a set of lengths of multifold parts of a filament. Systems of differential equations are introduced to describe the folding processes that create multifold structures in the early stage of the growth process. We show that the fitting of experimental data to the solutions of equations is excellent, and the parameters involved in our model systems are determined.

*Poster

Congestion in a traffic model with decision-making

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We study the statistical physics in the strategy evolution of a traffic model, which involves a decision-making process to avoid the congestion charge. We investigate theoretically and systematically the effects of drivers' decision-making on traffic congestion. We explore the basic mechanisms and various scaling properties. We examine the characteristics of branching behavior triggered by the decision-making processes on complex networks. We analyze the branching effects in the basic model and study the correlations between branching and congestion. We also evaluate the effectiveness of various control schemes to suppress the traffic congestion.

*Poster

Putting the electric double layer to work - harvesting sustainable energy using variable capacity engines

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In recent years there has been a growing interest in so-called ?blue energy?, energy harvested from the salt concentration differences between sea and river water. Next to membrane-based engines, of which a pilot-plant is currently being tested, a new capacitive blue engine was proposed recently [1]. This engine operates by cyclically charging and discharging nanoporous supercapacitors immersed in salty and fresh water, respectively. We show that a temperature difference between sea and river water has a dramatic effect on the work performed during operation cycles: it can lead to a threefold increase in the energy harvested if warm fresh water is mixed with cold sea water [2,3]. Heating the water with low-grade waste heat, abundantly available as a by-product from industrial processes, synergistically combines two vast energy reservoirs which are currently poorly exploited. Moreover, similar reasoning can be employed to construct a novel type of heat-to-current converter [4], as well as a microfluidic device which harvests electric energy from small ambient vibrations [5,6]. [1] D. Brogioli, *Phys. Rev. Lett.* **103**, 058501 (2009). [2] M. Janssen, A. Härtel and R. van Roij, *Phys. Rev. Lett.* **113**, 268501 (2014). [3] A. Härtel, M. Janssen, S. Samin and R. van Roij, *J. Phys.:Condens. Matter* **27**, 194129 (2015). [4] A. Härtel, M. Janssen, D. Weingarth, V. Presser and R. van Roij, *Energy Environ. Sci.* **8**, 2396 (2015). [5] T. Krupenkin, J.A. Taylor, *Nat. Commun.* **2**, 448 (2011). [6] M. Janssen, B. Werkhoven, R. van Roij, *RSC Adv.* **6**, 20485 (2016).

*Poster

Physics and social sciences : the dangerous liaisons

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Physics and social sciences have been exchanging ideas for centuries, giving rise for example to statistical physics. I present several approaches used by physicists to help understanding the social world. Firstly, simple models inspired from statistical physics, as Schelling's racial segregation model or opinion dynamics. Second, simple models derive from data, aiming at " uncovering the essential mechanisms at play ". But there are more 'complex' approaches that can be used to analyze real data, which acknowledge the complexity of social systems. Finally, I'll discuss the advantages and limits of these different approches, from a conceptual point of view and also in terms of knowledge gained about society. What are the politics of modeling and explanation, especially for social systems?

*Poster

Game theory for semifinalists' dilemma

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We consider tournament-style competitions and find optimal strategies for four evenly matched semifinalists. The participants must choose how much "stamina" to use in the semifinals, provided that the rest is available in the final and the third-place playoff. We present symmetric Nash equilibria for general payoff structures under a general condition that the winning probability is a non-decreasing function of stamina difference. There are three different phases of the Nash equilibria in the payoff space. First, in a winner-takes all format, in which the champion's payoff is much larger than the others, the optimal strategy is to copy what everyone else does. Any pure strategy can constitute a Nash equilibrium as long as all four players adopt it in common. Second, when the first two places are much more valuable than the other two, the only Nash equilibrium is such that everyone invests all stamina in the semifinal. Third, when the payoffs for the first three places are much larger than the last place, a Nash equilibrium is formed when everyone adopts a mixed strategy of using all or none of its stamina in the semifinals. We also study the evolution of strategies using replicator dynamics and show that the population evolves to the corresponding Nash equilibria.

*Poster

The transition point of the Chinese multilayer air transportation networks

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The air transportation network across a certain area, a typical multilayer complex system, is composed of a number of individual airlines, each of which forms a single layer. A central problem in airline merging is the minimal number of layers, denoted by n_{ml}, that needed for the merged network to function nearly as well as the fully aggregated network. For that purpose, we monitor several structural measures during the network aggregation process in which n_{ml} is gradually increased. For China air transportation network (CATN) we identify a universal, sharp transition point yielding $n_{ml} = 9$. Whereas for European Air Transportation Networks (EATN) there is no clear signal of such a transition point. The transition point of CATN is confirmed by means of the Wasserstein distance and the relative entropy. Our results indicate that there is still room in the optimization of CATN while EATN may have already been optimized in structure.

*Poster

Two-group conflict dynamics on networks

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We consider two disputing groups. Each individual i in each of the two groups has a preference si regarding the way in which the conflict should be resolved. The individual preferences span a range between -S (prone to settlement) to +S (prone to protracted conflict). Between these limits, we assume a number of intermediate discrete individual states. A pair of individuals i, j within group A contributes -JAsi*sj to the intra-group energy where JA is the strength of intra-group interaction. The same expression is used for group B with JA replaced by JB. The inter-group energy of individual i is taken to be proportional to the product between si and the mean value of the preferences from the other group's members. The inter-group interaction is not symmetric, namely JAB is not necessarily equal to JBA. The noise in this system is quantified by a ?social temperature? T. We consider an equivalent-neighbor (Renyi-Erdos) network where everyone interacts with everyone. Individuals interact within their group and with individuals of the other group. We explore effects of the network topology on the qualitative behavior of this model by doing Monte-Carlo simulations on finite size networks. Then we analyze situations where the strength of interactions diminishes with social or geographic distance between individuals. Time is incorporated in the models as follows: In the equivalent-neighbor network by allowing for a lag in the interactions between the current individual preference and the average preferences of individuals from the two groups at earlier time while in the simulations we use the Monte Carlo time as a proxy for the real time. We also define an order parameter which measure the intra-group stability. We analyze some macroscopic effects by averaging on all possible microscopic individual states generated at T. We show that the intra-group ordered state of each group depends on T and on the order stability of the other group. Effects of JA, JB, JAB and JBA are investigated. Discussions on social and political impacts of the model are provided.

*Poster

Understanding lifecycle of popularity using large-scale social data

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Analyzing and modeling for complex human behavior becomes a major target as a twenty-first century science, thanks to a development of computer technology[1][2]. The huge data of articles in cyber space written by humans such as blog and tweet is especially interesting database because the data directly reflects trends and topics in human society. For example, the number of blog entries including ?earthquake? have a clear peak when a large earthquake occurs. By using a huge Japanese blog data base with the author's ID, we can observe not only the number of entries per day for any words, but also personal dynamics of blog entries. In this presentation, we report statistical properties and modeling for three major categories of words. The First is ?ordinary words? which is used in our daily life, for example ?soon?. The number of entries of ?soon? has a steady fluctuation. The Second is ?News words?, for example ?Michael Jackson?. We can observe clear jump and power law decaying in the number of entries of ?Michael Jackson? after the news of which Michel Jackson died. It is remarkable that the function of decaying follows power law. We assume this decaying reflects a dropping interest in Michael Jackson. Additionally we can observe many examples of power law decaying in other words after big news[3]. The Third is ?Trending words?, for example ?Twitter?. The number of entries of ?Twitter? was increasing exponential from Oct. 2008 to Jun. 2010. Before 2008, most people didn't know the word Twitter, but now Twitter has become a very popular social networking tool. It is natural to consider that the time series implies the process. The fourth is "event words" which has growth and relaxation characterized by a power function around the peak day such as national holidays. We reproduced these dynamics by an agent-based model based on the SIR (Susceptible-Infected-Recovered) model which is well known in mathematical epidemiology to clarify the origin of these dynamics from the view point of bloggers interactions. In our social model, we introduce ?ground?,?excited? and?final?states respectively instead of susceptible, infected and recovered states. Agents move from the ground state to the excited state and from the excited state to the final state according to transition probabilities. In order to reproduce not only an exponential but also a power law growth and relaxation behaviors observed in trending words, we developed the base model by adding some effects to our model, for example an external shock effect, a deadline effect and an amorphous effect. The amorphous effect, inspired by solid physics studies, gives bloggers individual characteristics, in other words individual duration of interest for the specific word. As a result of adding these essential effects, our model reasonably reproduces the dynamics observed from our data. In addition we give master equation of our stochastic agent-based model and derive the equation of lifecycle of popularity as seen in the trending words. Our model can be applied to a prediction and control for spreading false rumors as seen in after the huge 2011 earthquake in Japan[4]. [1] Watts, D.J. A twenty-first century science. Nature 445, 489 (2007). [2] Lazer, D. et al. SOCIAL SCIENCE: Computational Social Science. Science 323, 721-723 (2009) [3] Y. Sano, K. Yamada, H. Watanabe, H. Takayasu, and M. Takayasu, Phys. Rev. E 87, 012805 (2013). [4]M. Takayasu, K. Sato, Y. Sano, K. Yamada, W. Miura, and H. Takayasu, PLoS ONE 10, e0121443 (2015).

*Poster

Finite-size effects in time-varying networks

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We provide the study of finite-size scaling (FSS) in temporal networks with and without the constraint of populations, where temporal-pattern coarsening is considered in several aspects. Dynamic scaling and structural properties in the time-varying networks are compared to those in the time-aggregated regime of quenched and annealed networks in the whole time window. Based on the early studies of random walkers [1] and epidemic processes [2] in generalized activity-driven network models with memory [3], we argue how the dynamical connectivity patterns play a role in FSS whether the limited temporal resolution exists or not. Finally, our arguments are also numerically tested. [1] N. Perra et al., Phys. Rev. Lett. 109, 238701 (2012); J. Saramaki and P. Holme, Eur. Phys. J. B 88, 334 (2015). [2] M. Gueuing, J.-C. Delvenne, and R. Lambiotte, Eur. Phys. J. B 88, 282 (2015); K. Sun, A. Baronchelli, N. Perra, ibid, 326 (2015); E. Valdano, C. Poletto, and V. Colizza, ibid, 341 (2015). [3] A.D. Medus, C.O. Dorso, J. Stat. Mech.: Theor. Exp. 2014, P09009 (2014); G.Laurent, J. Saramaki and M. Karsai, Eur. Phys. J. B 88, 301 (2015); H. Kim, M. Ha, and H. Jeong, ibid, 315 (2015).

*Poster

Percolation properties in spatial evolutionary prisoner's dilemma game

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We investigate percolation cluster properties of cooperator (C) and defector (D) in spatial evolutionary prisoner's dilemma game (SEPDG) on two-dimensional lattices. Percolation properties depend on both the lattice structure and the temptation factor b. On the hexagonal lattices, C (D) clusters undergo the percolation transition when 1.

*Poster

Collapse of Group Intimacy Network

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In formation of online communities, it is pointed out that effect of intimacy causes decline of the number of total users in communities. We assume that tightly connected groups of small number of intimate members can harm the further growth of the whole community, by making newcomers feel lonely, which eventually reduces the community size. In this paper, we propose a growing network model in which nodes interact with preferential probability with the strength of intimacy. This model contains eliminating process of nodes which fail to adapt to the network. We observe that the number of eliminated nodes is affected by the strength of the intimacy, and find the existence of a phase transition-like behavior in terms of the cumulative number of removed nodes.

*Poster

Dynamical analysis of four financial stock markets

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We study the network metrics in a time series of the S&P500, SSEC, Nikkei225, and KOSPI altering by the visibility algorithm. Data source is extracted the daily prices of all stocks that are exchanged on four financial stock markets during a period 1996–2010. These degree distributions adopting the visibility algorithm are proportional to a power law rather than the Poisson distribution. We mainly simulate and analyze several network metrics from the nodes and its links in financial networks. We are not able to find the universal and irregular properties of statistical quantities in financial networks, but it may be inferred that these topological properties improve by implementing the statistical method and technique from registered data of financial networks.

*Poster

Retarded Percolation Transition with the Second Source of Disorder

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The ranges of transmission of the mobiles in a Mobile Ad-hoc Network are not uniform in reality. They are affected by the temperature fluctuation in air, obstruction due to the solid objects, even the humidity difference in the environment, etc. How the varying range of transmission of the individual active elements affects the global connectivity in the network may be an important practical question to ask. Here a new model of percolation phenomena, with an additional source of disorder, has been introduced for a theoretical understanding of this problem. As in ordinary percolation, sites of a square lattice are occupied randomly with the probability p. Each occupied site is then assigned a circular disc of random value R for its radius. A bond is defined to be occupied if and only if the radii R1 and R2 of the discs at its end sites satisfy certain pre-defined condition. In a very general formulation, one divides the $R1 - R2$ plane into two regions by an arbitrary closed curve. One defines that a point within one region represents an occupied bond, otherwise it is a vacant bond. Study of three different rules under this general formulation, indicates that the percolation threshold is always retarded and varies continuously. This threshold has two limiting values, one is pc(sq), the percolation threshold for the ordinary site percolation on the square lattice and the other being unity. The variation of the thresholds are characterized by exponents, which are not known in the literature. In a special case, all lattice sites are occupied by discs of random radii $R \in \{0, R0\}$ and a percolation transition is observed with R0 as the control variable, similar to the site occupation probability.

*Poster

Markov State Modeling of Sliding Friction

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Markov State Modeling has recently emerged as one of the key techniques for analyzing rare events in molecular simulations. In particular in biochemistry this approach is successfully exploited to find the metastable states of complex systems in thermal equilibrium, such as a protein undergoing a folding event. We show here that this technique can be exported to the study of friction, where strongly non-equilibrium events and steady-state sliding are induced by an external force. The approach is benchmarked on a Frenkel-Kontorova model, used as a simple test system whose properties are well established. We demonstrate that our method allows the unprejudiced identification of the minimal basis of natural microscopic states necessary for describing the dynamics of sliding, including frictional dissipation and stick-slip events. We anticipate that the same technique will be applicable to the analysis of realistic frictional systems.

*Poster

Traffic dynamics with information flow

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Abstract for Topic 8: Interdisciplinary and complex systems (subtopics traffic flow, networks) Information and communication between vehicles is being promoted intensively by car and transportation manufacturers. V2X communication (V2V: vehicle to vehicle,V2S: vehicle to system and V2I: vehicle to infrastructure) is developing very fast. For instance VANET networks for traffic management are an object of fast developing research. The impact of this development must be considered at several scales. At the local scale V2V (vehicle to vehicle) communication impacts the car-following behavior [1] and traffic dynamics. Indeed with respect to classical inter-vehicular interaction, V2V is long range and instantaneous. V2V and V2I communication can also be included in cooperative traffic flow management of intersections. At a higher level still V2V communication can provide information on local network state in terms of traffic speed, density and travel times. At a larger scale still (urban network) V2X can provide the basis for routing and user information schemes [2]. These issues must be addressed by dynamic traffic assignment as in [4]. Dynamic assignment in this context must aim equity, Pareto-optimality (as closely as possible) and avoidance of Braess like adverse effects of competitive rerouting (in the case of several operators providing competing services). The object of the contribution is to propose a global framework for analysis of these issues based on GSOM traffic modeling [3] which integrates macroscopic traffic flow features (kinematic waves) and individual driver attributes and behavior. The contribution will also discuss some recent results.

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*Poster

A New Approach to the Kinetics of Diffusion-Influenced Reversible Bimolecular Reactions

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We propose a new approach to treat the kinetics of diffusion-influenced reversible bimolecular reactions, and apply it first to the reactions of the type A+B¡-¿C+B. For this type of reactions with some provisions, Gopich et al. showed that the relaxation kinetics can be described exactly in the same way as the reactant decay in an "equivalent" irreversible A+B-¿C+B reaction. In this article, we will show that the same relation can be derived in a very elementary way by using a new approach based on the hierarchical kinetic equations governing the reduced distribution functions of reactant molecules.

*Poster

Distribution of Power Supplies in Korean Power-Grid Network

Mi Jin Lee * [1], Eun Lee, Beom Jun Kim

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The emergence of synchronization in complex networks like power-grid systems has been a fascinating topic. Especially, the robust synchronization of phases and frequencies is essential for the stable operation of power grid. If the power generators fail to keep the phase- and frequency-locking, power outage could be caused on the whole grid. Proper power distribution for consumers is also important in order to avoid the blackout. In this paper, we focus on the power supply for stable operation. In Korean power-grid network structure, we check how generators supply the power with the assumption that power consumption is proportional to the local population. Our result may give some inference on adjustment of supply, preventing the power outage.

*Poster

Deviation-based spam filtering method in online ranking system

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Since the validity of ranking system is up to evaluator's sincerity,determining their sincerity is an important problem. As a way to measure sincerity, the group-based ranking(GR) method has been suggested to give each individual the reputation value which is determined by the majority of their evaluation. Extending this method, we focus on the fundamental statistical characteristics in the distribution of the reputation. By investigating various real evaluation data, we propose a null model of reputation distribution and successfully detect unreliable evaluators.

*Poster

Surface growth on diluted lattices by restricted curvature and conserved-noise restricted solid-on-solid models

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The surface growth by a restricted curvature (RC) model and a conserved-noise restricted solid-on-solid (CNRSOS) model was studied by numerical simulations on diluted lattices, i.e., on infinite percolation networks, embedded in two spatial dimensions. The growth exponent β and the roughness exponent α defined, respectively, by the mean-square surface width via $W^2(t) \sim t^{2\beta}$ and the mean-square saturated width via $W^2_{\rm sat}(L) \sim L^{2\alpha}$, were measured, and the results were compared with the power-counting predictions by the fractional Langevin equations, that were derived from the fourth-order Herring-Mullins equations with and without noise conservation by replacing $\nabla^2 \to \nabla^{z_{\rm rw}}$, where L is the system size and $z_{\rm rw}$ is the dynamic exponent of random walks. For the percolation probability p above the threshold, i.e., for $p_c < p \leq 1$, the lattice dilution did not influence the asymptotic growth for both models. For $p = p_c$, on the other hand, the critical exponents calculated on infinite networks and backbone networks were different from the results on a regular lattice. While the results for the RC model agreed well with the predictions, those for the CNRSOS model deviated by 8% – 12%. The deviation appeared to be distinct for the model for which the growth exponent β is small, and it is attributable to the discreteness of the simulation models. Thus, the fractional Langevin equations well describe the growth dynamics on random fractal lattices, unless the growth exponent is too small.

*Poster

Optimal Transport in Worldwide Metro Networks

Wei Li * [1], Jiao Gu, Shiping Liu, Yueying Zhu, Shengfeng Deng, Longfeng Zhao, Jihui Han,and Xu Cai

[1] Central China Normal University – China

Metro networks are crucial means of transportation on which most city inhabitants rely for daily mobility. The jam-free nature endows metro systems high degree of feasibility for analysis of transport properties. However, a systematic study of metro networks for understanding the intricate relations between geometric patterns and transport properties still lacks. Here we study and compare 28 world major metro networks in terms of the Wasserstein distance, the key metric for optimal transport, and measures geometry related, e.g. graph energy and fractal dimension. Our analysis leads to the following findings. First, there exists a scaling of the mean Wasserstein distance between any pair of directly connected stations versus the fractal dimension, which can be well approached by the theoretical treatment on homogeneous tree graphs. Second, the average graph energy per unit area decays with the fractal dimension as power-law, indicating lower mean energy costs for higher dimensioned metros. Third, the treelike structures of metro networks, shared by many natural transport systems, may facilitate the flow allocation, while the loops, especially those consisting of 3 or 4 nodes, are essential for achieving an economic transport cost. Furthermore, by ranking several key quantities transport concerned, we obtain corresponding ranking lists of three essential costs in which New York metro consistently tops the rest ones. All these insights may shed some light on the planning of metro systems, which could help achieve better overall performance at relatively low costs.

*Poster

Optimizing Synchronization Stability of Kuramoto Model

Bo Li * [1], K. Y. Michael Wong

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Maintaining the stability of synchronization state is crucial for the functioning of many natural and artificial systems, such as bird flocks and power grids. In this study, we develop methods to optimize the synchronization stability of Kuramoto model by minimizing the maximal Lyapunov exponent. With the help of the recently proposed cut-set space approximation of the steady states, we greatly simplify the objective function, and further derive its gradient and hessian with respect to natural frequencies, which leads to an efficient algorithm with quasi-Newton method. The optimized systems are demonstrated to achieve better synchronization stability for Kuramoto model with or without inertia in certain regimes, hence our method is applicable in improving stability of power grids. It is also viable to adjust the coupling strength of each link to improve the stability of the system. Various operational constraints can also be easily integrated into our scope by employing the interior point method in convex optimization. The properties of the optimized networks are also discussed.

*Poster

Stock Markets are Unpredictable, but Can be Exploitable

Sy-Sang Liaw * [1], Cheng-Yen Wang

[1] National Chung Hsing University – Taiwan

In 1900, Bachelier was the first to consider the variation of stock prices as a path of random walk. Subsequent researchers found, however, the ups and downs of the stock indices are different from randomness except for very long time scales. Clear evidence of this non-randomness is that the distribution of returns is not Gaussian but universally has a fat tail. Optimistic researchers quickly attempted to utilize the information gathered from these returns to predict the market. Others have used agent-based models to generate series with return distributions similar to the real ones. Here we have shown that the time sequences of some stock indices behave like the trajectory of a weakly-persistent random walk (WPRW). The trajectory of a WPRW is a crossover-fractal, a fractal which has one fractal dimension for short scales and another for large scales. We studied various pieces of stock index series from ten different countries and found that some of them were crossover-fractals with the crossovers at about 20 minutes. Beyond that time the fractal dimension was close to 1.5, much like a simple random walk. Since the long-range variance of the WPRW is larger than that of a random walk, the stock index is harder to predict than a random walk. On the other hand, because of this persistent feature, one can exploit the market at shorter scales than 20 minutes and always profit by high-frequency transactions.

*Poster

Agent-based modeling of heterogeneous traffic: Dealing with lane discipline breakdown and inhomogeneous driving behavior

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We use a modified Nagel-Schrekenberg cellular automata model for two vehicle types (cars and motorcycles) to study the interplay of lane discipline, lane changing, predictable/unpredictable slowdowns and vehicle density. Sans lane changing and with a fixed slowdown probability, the vehicle density delineating the free flow and congested states increases with the fraction of cars. When lane changing is allowed, the smaller motorcycles tend to fill in unused spaces, until the point when the wider cars effectively block their way at high vehicle densities. When lane discipline is allowed to break down, a further increase in throughput becomes possible at the cost of required driver attentiveness.
We catalog the various empirical causes of slowdowns and discuss their implications on our model.

*Poster

Air Traffic, Boarding of Passengers and Scaling Exponents

Reinhard Mahnke * [1], Jevgenijs Kaupuzs, Hans Weber, Martins Brics

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The growing need for mobility through the world shows no sign of slowing down. The air traffic is a very important part of the global transportation network. In distinction from vehicular traffic, the boarding of an airplane is a significant part of the whole transportation process. Here we study an airplane boarding model, introduced earlier by Frette and Hemmer, with the aim to determine precisely the asymptotic power–law scaling behavior of the mean boarding time $langlet_bangle$ and other related quantities for large number of passengers N. The power–law scaling $langlet_banglepropto N^{alpha}$ has been earlier stated with the exponent $alpha = 0.69pm0.01$ being evaluated from the data within $2leNle16$. Our analysis is based on Monte Carlo simulation data for very large system sizes up to $N = 2^{16} = 65,536$. In analogy with critical phenomena, we have used appropriate scaling ansatz, which includes the leading term as some power of N, as well as power–law corrections to scaling. Our analysis clearly shows that the true (asymptotic) exponent $alpha$ is $1/2$ ($alpha = 0.5001pm0.0001$). We have estimated also other exponents: $u = 1/2$ for the mean number of passengers taking seats simultaneously in one time step, $beta = 1$ for the second moment of $langlet_bangle$ and $gammaapprox1/3$ for its variance. The difference between the asymptotic exponents and the effective exponents, extracted from relatively small system sizes, is explained by corrections to scaling, which are described by the correction–to–scaling exponent $hetaapprox1/3$. In relation to critical phenomena, this model can serve as a toy example, clearly demonstrating the importance of corrections to scaling and the necessity to consider very large systems to obtain correct values of the exponents.

*Poster

Entropy reducing dynamics of a double daemon

Michael Maitland * [1], Ian Ford

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We study the reduction in total entropy, and associated conversion of environmental heat into work, that is made possible by the mechanical coupling and decoupling of two systems followed by separate processing under suitable mutual feedback. The scheme is an extension on recent considerations of the way in which Maxwell's demon might perform a measurement on a system and then exploit the knowledge gained. When this is carried out in a symmetric fashion, with one system informing the exploitation of the other, with both therefore acting as a demon, it may be shown that the second law can be broken. We contrast this with the preservation of the law when the exploitation is performed on one system only. The study illustrates the limits of the second law when confronted with system dynamics that have a self-sorting character.

*Poster

Statistical Mechanics of Continuous Spin Models and Application to Nonlinear Optics in Disordered Media

Alessia Marruzzo * [1], Luca Leuzzi

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We have studied the XY model and its discrete p-clock proxy on bipartite random graphs by means of the cavity method. Our interest on the nonlinear XY model needs to be mainly found in optics, i.e., to describe the nonlinear interactions among electromagnetic modes within a nonlinear response medium. In particular, we have in mind random lasers, in which the feedback is provided by the multiple scattering of light. In this case, modes may in general exhibit complicated spatial extensions that can more localized than in respect to ordinary Fabry-Perot cavity lasers. The network of interactions results then to be more diluted with quenched disordered couplings. Dilution among the possible interacting quadruplets has to be considered also if the frequencies of the modes are added in the description. Indeed, the frequencies of a mode quadruplet needs to satisfy a non-trivial matching condition, imposed by the non-linear interaction (see Refs. [1,2]). This effect is responsible of the Mode-Locking transition in lasers. As a first step, we have analyzed the effect of dilution induced by the frequencies. We have seen that, if the connectivity of the nodes and the coupling strength are high enough, when frequencies are added in the description, there appear a Phase-Locked solution characterized by high intense electromagnetic peaks. As a second step, we have analyzed, parallel to dilution, quenched disordered couplings. Through the 1-step Replica Symmetry Breaking Cavity Method, we have determined the phase diagrams of the system from the ordered case to the spin-glass case. Dynamic, spinodal and thermodynamic transition lines are identified by analyzing free energy, complexity and three recostruction function as temperature and disorder are changed. A great part of our works focus on the convergence of the p-clock model to the XY limit down to temperature low enough to determine all relevant transition points for different node connectivity. References: Alessia Marruzzo and Luca Leuzzi: Multi-body quenched disordered XY and p-clock models on random graphs Phys. Rev. B 93, 094206 (2016) DOI:10.1103/PhysRevB.93.094206 Alessia Marruzzo and Luca Leuzzi: Nonlinear XY and p-clock models on sparse random graphs: Mode-locking transition of localized waves Phys. Rev. B 91, 054201 (2015) DOI: 10.1103/PhysRevB.91.054201

*Poster

Synchronization and energy transfer between colloids using critical interactions.

Ignacio A. Martínez * [1], Clemence Devailly, Artyom Petrosyanm and Sergio Ciliberto

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We report the observation of a temperature controlled synchronization of two Brownian-particles which are inside a binary mixture close to the critical point of the mixing transition. The two beads are trapped by two optical tweezers whose distance is periodically modulated. We show that the motion synchronization of the two beads appears when the critical temperature is approached and that it is induced by the critical forces. Instead when the fluid is far away from its critical temperature the motions of the two beads are uncorrelated. Finally, the measured energy transfers inside the system produced by the critical interaction are also presented. Small changes in temperature can radically change the global dynamics and energetics of the system, opening new doors to control small machines in the mesoscale.

*Poster

Sparse modeling approach to the STM datasets analysis

Masamichi J. Miyama * [1], Koji Hukushima

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We propse the new framework of the real-space data analysis of the STM (Scanning Tunneling Microscope) topography image and STS (Scanning Tunneling Spectroscopy) by applying the recent developement of informational statistical physics, especially sparse modeling. With the improvements of measuring technique, it becomes difficult to extract the important physical information from the experimental datasets. For example, STM enables us to determine the surface structure at the atomic scale. However, the conventional data analysis technique is based on the Fourier analysis, so it is difficult to focus on the local phenomena, such as local (electric) strains, which is regarded as the key role of the origins of high-T_c superconductors and other interesting physical properties. Then, we take the strategy to utilize the data model estimation for the data analysis. The first example is to determine the positions of atoms to the degree where we can extract the locally strain of the atom's configuration from the noisy STM topography datasets. In our analysis, we utilize the relevant vector machine (RVM) as a data model, a 2D Gaussian function as a base function that corresponds to a position of a single atom peak, and LASSO as the prior information. We validated our scheme by applying to the dummy data and the real experimental datasets of a $SrVO_3$ surface. In our presentation, we show the our algorithm and the results obtained by our framework, and discuss the possibility of applications to other experimental datasets.

*Poster

Relation between Zipf 's law and the distribution of shared components in complex component systems.

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Several complex systems of diverse nature consist of realizations which can be broken into their elementary constitutive components, for example, books into words, genomes into genes, and technological systems into building blocks. The statistics of the components (e.g., word) across realizations (e.g., books) shows several quantitative laws, such ad the well-known example of the power-law distribution of component abundances, known as Zipf's law in the context of in the context of natural languages. Central to the current debate in evolutionary genomics is a different law, the "gene-frequency distribution", or "occurrence distribution", where a component occurrence is defined as the fraction of realizations in which the component is present. In genomes, the occurrence distribution shows a peculiar ?U-shape? due to a large number of rare (i.e. belonging to very few species) and common genes (present in almost all the species), compared to genes at intermediate occurrences. While several possible theoretical explanations of the U-shaped gene occurrence distribution have been proposed, its causes are still under debate. Here, we consider occurrence distributions in three datasets from genomics, linguistics (literary texts), and technology (LEGO toy constructions), showing that the U-shape is linked to the component frequency (i.e., the Zipf's law). By means of a theoretical model based on sampling, we establish an analytical relationship between these two laws, which allows us to identify the crucial parameters affecting the occurrence distribution power law decay and the size of the common component peak. The null model captures some relevant empirical features, as well as highlighting deviations that carry important information about the specificity of each system.

*Poster

Statistical mechanics of feedforward active noise control

Seiji Miyoshi * [1], Norihiro Ishibushi, Yoshinobu Kajikawa

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We apply a statistical-mechanical method to the field of signal processing. The behaviors of active noise control are analyzed using a statistical-mechanical method. Cross-correlations between the elements of a primary path and those of an adaptive filter and autocorrelations of the elements of the adaptive filter are treated as macroscopic variables. We obtain simultaneous differential equations that describe the dynamical behaviors of the macroscopic variables under conditions in which the tapped-delay line of the adaptive filter is sufficiently long. We show that there is an optimal step size owing to the trade-off between the noise misadjustment and the lag misadjustment when the primary path is time variant.

*Poster

Analysis of player interaction in football games based on tracking data

Takuma Narizuka * [1], Yoshihiro Yamazaki

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The present work aimes to characterize interpersonal interactions in football games based on player tracking data. The dataset is collected from the mathes in the Japan Professional Football League 2015. It includes positional coordinates of all players every 0.04 seconds. We focus on the angle $heta$ formed by velocity vectors of two players who belong to different teams. The angle distribution $f(heta, r)$ for different interpersonal distance r are investigated. The angle distribution with low circular variance corresponds to the strong tendency of players to align their moving directions. We find that the circular variance increases linearly with r for $r < 5$ (m), while it becomes almost constant value for $r > 5$ (m). In addition, $f(heta, r)$ follows the wrapped cauchy distribution function, which is defined on the circle. These results imply that there is a characteristic interaction region around each player in football, and the coordination behavior among players follow the simple statistical law.

*Poster

Revealing physical interaction networks from statistics of collective dynamics

Mor Nitzan * [1], Jose Casadiego, Marc Timme

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Revealing physical interactions in complex systems from observed collective dynamics constitutes a fundamental inverse problem in science. Current reconstruction methods require access to a system's model or dynamical data in a detail often not available. Here we exploit changes in invariant measures, in particular distributions of sampled states of the system, in response to driving signals, and employ compressed sensing to reveal physical interaction networks. Dynamical observations suffice to infer physical connectivity even if they are temporally disordered, acquired at large sampling intervals, and stem from different experiments. Testing various nonlinear dynamic processes emerging on artificial and real network topologies indicates high reconstruction quality for existence as well as type of interactions. These results advance our ability to reveal physical interaction networks in complex synthetic and natural systems.

*Poster

Statistical mechanics for variable selection in linear regression: Fast and reliable cross validation

Tomoyuki Obuchi * [1], Yoshiyuki Kabashima

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Approximation of a high-dimensional vector by a small combination of column vectors selected from a fixed matrix has been actively debated in several different disciplines. Variable selection is its key issue and causes computational difficulty. In this talk, three ways to treat this problem will be shown: Monte Carlo sampling, mean-field approximations, and L_1 relaxation. The performance of these ways will be manifested in a theoretical analysis and applications to some actual dataset. Especially, determination of the degrees of freedom (the number of used columns) by cross validation is focused on and tested.

*Poster

All particles are Different

Dino Osmanovic * [1], Yitzhak Rabin, Lenin Shagolsem

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We present results of systems where all particles are different(APD), by which we mean that the interaction energy between any pair in the system is different. We show that this leads to systems which are both fluid and organized. We then extend this work using heuristics and monte carlo and show that such systems are intimately related to spin glasses, and by extension differing fields like computational complexity and the traveling salesman problem.

*Poster

Hide and Seek Games

Shubham Pandey * [1]

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This study deals with a game called Hide-and-Seek, which involves competition between two agents, hider and seeker, where the seeker is trying to find the tokens hidden by the hider in a network. Previous studies have shown that the number of distinct sites, S(n), visited by a random walker (seeker), who is performing an unbiased random walk in a network, after n time steps, is equal to Bn, in the limit of large n, where B is a constant. We have generalised those previous findings and found B when a degree-correlated random walk is being performed. Various strategies followed by the seeker include both degree-correlated and degree-independent strategies, the simplest of them being an unbiased random walk. Similarly, the hider can follow both degree-independent and degree-correlated strategies. It turns out that the total number of tokens, T(n), found by the seeker in n time steps, is equal to Jn, with J being the prefactor. The prefactor J is a measure of efficiency of a search strategy, and we have been comparing different search strategies for a given hiding strategy or multiple hiding strategies based on the corresponding values of J. This problem potentially has multiple applications, including applications in cyber security since it is desirable to find the strategies that maximise or minimise the efficiency of a search in cyber security.

*Poster

Emergence of cooperation: Growing habitat with empty sites

Hye Jin Park * [1], Beom Jun Kim, Hyeong-Chai Jeong, Christian Hilbe, and Martin A. Nowak

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In prisoner's dilemma game all individuals defect each other in the end according to Nash-equilibrium even if mutual cooperation maximizes total profit. Many theoretical and experimental researches have been performed in various aspects to reveal mechanisms for emergence of cooperation. However, there is a lack of understanding for population growth effect on emergence of cooperation. Here, we investigate growing effects on emergence of cooperation allowing empty sites. Population grows through death and birth: If a randomly chosen site is empty, neighboring site's offspring occupies this site. Otherwise the individual in the chosen site dies at the probability depending on his(her) payoff which comes from the game with neighboring sites. When the population is homogeneous we find the cooperator population can be more endurable than defector population to survive. Moreover, cooperators can dominate defectors in the mixed population because the empty site generated from the death of a cooperator in the domain boundary between defectors and cooperators protect cooperators from the invasion of defectors.

*Poster

Effects Of Non-Uniform Occupancy On Selective Transport Through Nanochannels

Luis A. Perez * [1], Heinrich Terborg

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By using an exclusion model, we address how the non-uniform occupancy of a nanochannel, for a limited set of conditions, is related to the transport of specific molecules through it. The results show that the shape of a channel greatly influences its transporting behavior and therefore, it can be used as a tunable parameter to achieve a desired set of transporting conditions. In particular, we have found that for applications which require a highly selective channel that is able to handle large input fluxes of specific particles in both directions, a double-funnel architecture is the best suited. As the obtained results mainly arise from the competition of particles for limited space, we expect them to be applicable to a great variety of transporting phenomena where the channel has a limited number of interacting sites with the transported particles.

*Poster

Linking entropy with self-affinity in time series

Zhi Qiao * [1], Zeyu Zheng

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In order to predict the complex state and quantify the complexity of a system, one of the most useful ways is to examine the dynamical fluctuations of the output signals (time series) and use the quantity "entropy" originated from thermodynamics to quantify the regularity (orderliness) of a system. Following the understanding that complexity is associated with "meaningful structural richness", the entropy rate and Kolmogorov complexity have been raised up. When applied in the analysis of short and noisy time series, approximate entropy (ApEn) and later modified algorithm sample entropy (SampEn) have been proposed. On the other hand, complex systems are often characterized by periodic or nearly periodic behavior extended over a wide spectrum that fluctuates on many time scales with broad distribution of the values. This dynamics can be characterized by scaling laws valid over a wide range of time scales or frequencies, which are denoted as fractal or multifractal. Up to date, numerous work has been done in the above two areas of complex system, but few people have realized the importance of linking self-affinity or fractal, a more mathematical property, with entropy, a quantity originated from physics describing the rate of information production. This paper aims to link up these two quantities not only in time series, but also goes back to the definition of entropy to reveal the underlying dynamics of this relationship, providing a deeper understanding of complex pattern formation. At the same time, we will provide a much better method to quantify different scales of entropy for the complex signals. Several applications in natural and social systems will be demonstrated at the end of the paper.

*Poster

Large deviations in complex systems: simulation of extreme heatwaves in climate models using genealogical algorithms

Francesco Ragone * [1], Freddy Bouchet, Jeroen Wouters

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The climate system is an outstanding example of a complex system, constituted by several subsystems (atmosphere, ocean, biosphere, etc.) interacting on a wide range of spatial and temporal scales. A key issue involving many groups worldwide is to understand if tools borrowed from statistical physics or complex systems could be useful for improving our understanding of climate dynamics. We consider here the specific issue of extreme events, approached through large deviation theory and importance sampling. For some aspects of climate dynamics, rare dynamical events may play a key role. A first class of problems are extreme events that have huge impacts, for instance exceptionally intense precipitations, droughts, or heat waves. A second class of problems are rare trajectories that suddenly drive the complex dynamical system from one attractor to a completely different one, for instance abrupt climate changes. One of the goals of climate science is to characterize the statistics of these extreme, potentially dangerous events in the present and future climate. In the recent past, new theoretical and numerical tools have been developed in the statistical mechanics community, in order to specifically study such rare events. Those approaches are based on large deviation theory for complex dynamical systems, and their application to observational datasets and/or climate numerical simulations could help to determine accurately the probability of these events and to study the dynamical processes responsible for their formation. We consider here the probability of extreme heatwaves, characterized by large values of time and space averages of the surface temperature, for instance for about six weeks and over western Europe, in a simple but comprehensive general circulation model of the atmosphere. The dynamics of events with return times ranging from decades to hundreds of years can not be studied using brute force simulations, because the computational cost required for getting a robust statistics would be prohibitively large. We show that that large deviation algorithms (the Giardina-Kurchan algorithm in our specific case) allow to sample extremely efficiently extreme heatwaves, opening the door to the study of their dynamics, precursor and fluctuation paths, in a way that can not be foreseen using conventional tools based on direct numerical simulations. The number of extreme heatwaves obtained with this importance sampling algorithm is about a factor one hundred larger than what obtained with direct numerical simulations for the same computational cost. We also address fundamental questions about non-equilibrium statistical mechanics and large deviation theory related to extreme heatwaves: for instance we show that for surface temperature six weeks averages are at the margin of validity of the Donsker-Varadhan regime of large time large deviations, and we discuss the interest of this result for predicting probability of even longer lasting and rarer heatwaves.

*Poster

On the criticality and predictability of scale-invariant avalanches

Osvanny Ramos * [1]

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Earthquakes, granular avalanches, solar flares, and even stock markets have been reported to evolve through events with power-law distributions of sizes. During decades, the formalism of equilibrium phase transitions has classified these phenomena as critical, which compromises the predictability of their catastrophic (system-size spanning) events. This work revises these ideas and uses earthquakes to show that slowly driven systems evolving through uncorrelated and power-law distributed avalanches (UPLA) are not necessarily critical systems, and therefore not necessarily unpredictable. By linking the correlation length of the system to the distribution of avalanche sizes, and comparing it with the one obtained at a critical point, a new condition of criticality is introduced. It indicates how far is the system from a critical situation through the analysis of the correlation length, which decreases exponentially as the exponent of the distribution moves away from its critical value. Simulations in the Olami-Feder-Christensen (OFC) earthquake model confirm the findings.

*Poster

Nonequilibrium Thermodynamics of Chemical Reaction Networks

Riccardo Rao * [1], Massimiliano Esposito

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Driven Open chemical networks (DOCN) are large sets of coupled chemical reactions where some of the species are externally controlled. Cell metabolism and biochemical signal transduction networks are notable examples of DOCN. We present a rigorous nonequilibrium thermodynamic description of DOCN in terms of deterministic rate equations. Our description is inspired by Stochastic Thermodynamics and is based on Chemical Reaction Network Theory. The energy and entropy balances of DOCN are derived and a nonequilibrium Gibbs free energy is introduced. This latter is related to the chemical work necessary to control the network far from equilibrium. The relationship between the thermodynamics and the topology of DOCN is illustrated by considering detailed-balanced networks as well as complex- balanced networks. An application to oligosaccharides exchange dynamics performed by so-called D-enzymes is provided. References R. Rao and M. Esposito, "Nonequilibrium Thermodynamics of Chemical Reaction Networks: Wisdom from Stochastic Thermodynamics", arXiv:1602.07257. R. Rao, D. Lacoste and M. Esposito, "Glucans monomer-exchange dynamics as an open chemical network", J. Chem. Phys. (2015) 143, 244903.

*Poster

Communities' detection and evolution: Estonian economic network of payments

Stephanie Rendón de la Torre * [1], Robert Kitt Jaan Kalda

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We study an Estonian economic network of payments, identify its community structure and analyze the evolution of the communities found. In this network the nodes are Estonian companies and the edges are the payments done between the companies. This data set is unique in its kind because around 80% of Estonia's bank transactions are completed through Swedbank, hence, the economic structure of the country can be reconstructed. The detection of community structures in networks helps to comprehend more about the local organization of the components of networks. In this work, we identify the communities in the Estonian economic network and study some aspects of their evolution through time. Our results reveal that the relationship between the nodes' classifications found through a community detection algorithm and the real economic groups' classifications is high. We found that investigating the time dependence of overlapping communities in our network helps to uncover hidden relationships with economic events. Also, we found that through the study of economic communities' structure and their evolution it is possible to understand some aspects of the economy.

*Poster

Hybrid method for construction of earthquakes network: active and passive points

Soghra Rezaei * [1]

[1] University of Zanjan – Iran

Complex network theory is the way to study the complexity of earthquakes. It is so essential for these studies to construct an appropriate network. To construct our network, we combine Abe - Suzuki method [1] and Telesca - Lovallo method [2]. We divide a geographical region into small square cells that these cells cover the entire region without any overlapping. If an earthquake with any value of magnitude occurs in a cell, we identify it as a vertex of a network. Two events are connected to each other if visibility condition holds true between them. For Iran, California and Italy-Greece earthquakes we divide the longitudinal and latitudinal ranges into cells (cell sizes changes from 4km- 220km). We show that the constructed networks are scale free and theirs degree distribution obey the q-exponential function which is used in non-extensive statistical mechanics [3]. Also we find the universal behavior of links and nodes number with time for same areas and same resolution of Iran, California and Italy-Greece earthquakes. This behavior is power law and similar to Omori law but there are differences between them. Furthermore, analogy to Darooneh- Lotfi [4] by using the concept of PageRank, we find the passive and active points in the geographical region of Iran. [1] S. Abe, N. Suzuki, Scale-free network of earthquakes, Europhys. Lett. (2004). [2] L. Telesca, M. Lovallo, Analysis of seismic sequences by using the method of visibility graph, Europhys. Lett. (2012). [3] C.Tsallis, Introduction to Nonextensive Statistical Mechanics, Springer.(2009), [4] A.H.Darooneh, N.Lotfi, Active and passive faults detection by using the PageRank algorithm, EPL, 107 (2014) 49001

*Poster

Observation of a crossover in kinetic aggregation of Palladium colloids

Shahin Rouhani * [1], M Ghafari, M Ranjbar, S Rouhani

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We use field emission scanning electron microscope (FE-SEM) to investigate the growth of palladium colloids over the surface of thin films of WO3/glass. The film is prepared by Pulsed Laser Deposition (PLD) at different temperatures. A PdCl2(aq) droplet is injected on the surface and in the presence of steam hydrogen the droplet is dried through a reduction reaction process. Two distinct aggregation regimes of palladium colloids are observed over the substrates. We argue that the change in aggregation dynamics emerges when the measured water drop Contact Angel (CA) for the WO3/glass thin films passes a certain threshold value, namely $CA \approx 46^0$, where a crossover in kinetic aggregation of palladium colloids occurs. Our results suggest that the mass fractal dimension of palladium aggregates follows a power law behavior. The fractal dimension (Df) in the fast aggregation regime, where the measured CA values vary from 27^0 up to 46^0 according to different substrate deposition temperatures, is (Df 1.75 ± 0.02). The value of Df is in excellent agreement with kinetic aggregation of other colloidal systems in fast aggregation regime. Whereas for the slow aggregation regime, with $CA = 58^0$, the fractal dimension changes abruptly to $Df = 1.92(\pm 0.03)$. We have also used a modified Box Counting method to calculate fractal dimension of gray-level images and observe that the crossover at around $CA = 46^0$ remains unchanged

*Poster

A Pairwise Maximum Entropy Model Able to Learn and Imitate Melodic Styles

Jason Sakellariou * [1], Francesca Tria, Vittorio Loreto, Francois Pachet

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We introduce a Maximum Entropy model able to capture the statistics of melodies in music. The model can be used to generate new melodies that emulate the style of the musical corpus which was used to train it. Instead of using the n-body interactions of (n-1)-order Markov models, traditionally used in automatic music generation, we use a k-nearest neighbour model with pairwise interactions only. In that way, we keep the number of parameters low and avoid over- fitting problems typical of Markov models. We show that long-range musical phrases don't need to be explicitly enforced using high-order Markov interactions, but can instead emerge from multiple, competing, pairwise interactions. We validate our Maximum Entropy model by contrasting how much the generated sequences capture the style of the original corpus without plagiarizing it. To this end we use a data-compression approach to discriminate the levels of borrowing and innovation featured by the artificial sequences. The results show that our modeling scheme outperforms both fixed-order and variable-order Markov models. This shows that, despite being based only on pairwise interactions, this Maximum Entropy scheme opens the possibility to generate musically sensible alterations of the original phrases, providing a way to generate innovation.

*Poster

The role of wind power production in power-grid outages: does intermittency matter?

Christoph Schiel * [1], Pedro Lind, Philipp Maass

[1] Universität Osnabrück – Germany

The role of wind power production in power-grid outages: does intermittency matter? Christoph Schiel, Pedro Lind, Philipp Maass University of Osnabrueck, Germany We investigate the stability of power grids in terms of transmission line capacity with integrated wind generators based in empirical data of wind velocity measures. The power grid is modelled as a quasi static lossless DC grid, being in a balanced state of demand and generation. Assuming this state, the most probable outages in the grid, primarily line overloads, are calculated with an exact algorithm [1]. From empirical statistical features of wind data, we then compare two different stochastic distributions modeling wind velocity measurements: the Gaussian distribution and the more realistic Weibull distribution. Parameterized with the same mean and standard deviations, all differences observed in outage scenarios when using the Weibull model results from the non-Gaussian character of this distribution, namely the intermittency of large wind velocity fluctuations. Finally, we discuss the optimal embedding of a wind generator in a specific test grid. [1] Michael Chertkov, Mikhail G. Stepanov, Feng Pan, and Ross Baldick. Exact and efficient algorithm to discover extreme stochastic events in wind generation over transmission power grids. CoRR, abs/1104.0183, 2011.

*Poster

Language Dynamics approach to the study of Mazatec dialects

Kiran Sharma * [1], Anirban Chakraborti, Marco Patriarca, Els Heinsalu, Jean Léo Léonard

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The Mazatec dialects [1], belonging to the family of Oto-Manguean languages (Mexico), represent an emblematic example of linguistic diversity. We carry out an interdisciplinary study of Mazatec dialects by using a complex systems approach. The study consists of two parts: phenomenological and theoretical, which are carried out in parallel, and eventually matched and combined with each other in a global comprehensive picture of the Mazatec linguistic system. The phenomenological side of the work is based on the analysis of some available linguistic databases. We carry out a complex network analysis of a database of grammatical taxonomy [2], that we analyze in terms of their mutual Levenshtein distances, and one obtained from a series of mutual dialect intelligibility tests [3]. The results of these analyses provide an overall picture of the relatedness between the various dialects and are able to recover the known sub-families of Mazatec dialects. Then we construct a reaction-diffusion model of language dynamics [4,5] which can also take into account the evolution of a language into dialects [5], mimicking the expansion and differentiation of the Mazatec linguistic community. We study the model by performing extended numerical simulations and comparing the results with the constrains from the known data. It turns out that in order to reproduce the observed distribution and diversity of the dialects, described by the databases, it is essential to take into account both the local physical and economic geography, as well as the road connections and other ecological factors.
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*Poster

Synchronization of parallel simulations on the small-world network

Liudmila Shchur * [1], Lilya Ziganurova, Lev Shchur

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We model conservative algorithm of parallel discrete event simulation (PDES) class on the small-world network. It is know that conservative algorithm on the regular lattice belongs to the universality class of Karzad-Parazi-Zhang (KPZ) equation. Small-world network is a way to have two limiting cases, KPZ universality with the vanishing concentration of random links and mean-field universality with high enough concentration of random links. We present results of simulations and discuss universality issue.

*Poster

Statistical-mechanical analysis of Boolean compressed sensing for noiseless group testing

Satoshi Takabe * [1], Koji Hukushima

[1] The University of Tokyo – Japan

Detecting a small number of defects among many items is a traditional but essential issue in statistical inference. Given the number of items N and defects $K(llN)$, $O(N)$ tests are naively required for complete detection. If some of items are tested at once by pooling them, however, the number of tests reduces to $O(KlogN)$. This technique is called the group testing and is applied to the DNA cloning library screening, for example. Recently, focusing on the sparsity of defects, Boolean compressed sensing (BCS) is proposed to improve detection performance of the group testing. In this presentation, we report its implementation based on the Max-Sum algorithm and analysis of its typical behavior for noiseless cases averaged over random pools. Our analysis successfully estimates its detection ratio even in the case of a finite number of items. It also shows that our method based on BCS asymptotically needs less number of tests than other greedy methods; a half of the combinatorial matching pursuit and a quarter of the combinatorial basis pursuit.

*Poster

Retrieval capabilities of generalized Boltzmann machines

Daniele Tantari * [1], lena Agliari, Alessia Annibale, Adriano Barra, A.C.C Coolen, Francesco Guerra, Peter Sollich

[1] Centro E. De Giorgi, Scuola Normale Superiore, Pisa – Italy

In the framework of the equivalence between feedback statistical networks with hidden layers and generalized Hopfield models, I will investigate the robustness of the retrieval capabilities of the system in the presence of analog (or noisy) units and analog (or noisy) patterns of informations. Then I will analyze the case of patterns with diluted entries, where the network acquires the ability to process in parallel under appropriate conditions of load and sparsity.

*Poster

Non-deterministic self-assembly of two tile types on a lattice

Salvatore Tesoro * [1], S. Tesoro, K. Göpfrich, T. Kartanas, U. F. Keyser, S. E. Ahnert

[1] University of Cambridge – United Kingdom

I will present a complex behaviour that is both interesting from a statistical and complex systems point of view and from a more abstract point of view on complexity and evolutionary theory. I will introduce simple a theoretical framework to predict and describe all possible growth behaviours that self-assembly of two tile types can produce on a 2D lattice, given binary interaction rules between the faces of the tiles in the system. Such simple set up can give rise to critical transitions between bound and unbound growth regimes and other non-critical behaviours. I will illustrate how this work completes efforts conducted by Ahnert et Al. in the field of Complexity and Evolution, whereby deterministic self-assembly pathways have been exploited as a useful tool in addressing questions on complexity and modularity in nature. I will further show how this theoretical framework can be experimentally verified using DNA-tiles as a building material and providing experimental validation of the theoretical predictions made

*Poster

Correspondence between Phase Oscillator Network and Classical XY model with the Same Interaction

Tatsuya Uezu * [1]

[1] Nara Women's University – Japan

We study phase oscillator networks with distributed natural frequencies and classical XY models, both of which have interactions in common. We study several interactions and study the correspondence between two models.

*Poster

Structural origin of mean field behaviour in neuronal avalanches

Michiels van Kessenich * [1], L. de Arcangelis, H. J. Herrmann

[1]ETH Zurich – Switzerland

Neuronal avalanches measured *in vitro* and *in vivo* in different cortical networks consistently exhibit power law behaviour for the size and duration distributions with exponents typical for a mean field self-organized branching process. These exponents are also recovered in neuronal network simulations implementing various neuronal dynamics on different network topologies. They can therefore be considered a very robust feature of spontaneous neuronal activity. Interestingly, this scaling behaviour is also observed on regular lattices in finite dimensions, which raises the question about the origin of the mean field behaviour observed experimentally. In this study we provide an answer to this open question by investigating the effect of activity dependent plasticity in combination with the neuronal refractory time in a neuronal network. Results show that the refractory time hinders backward avalanches forcing a directed propagation. Hebbian plastic adaptation plays the role of sculpting these directed avalanche patterns into the topology of the network, slowly changing it into a branched structure where loops are marginal.

*Poster

Transmission of a signal through a neural network

Bertha Vázquez-Rodríguez * [1], Hernán Larradle Ridaura, Andrea Avena-Koenigsberger, Olaf Sporns

[1] Institute of Physical Sciences, Universidad Nacional Autónoma de México – Mexico

The study of the spreading dynamics of a signal through a network is relevant in different contexts, from infectious diseases to information in social networks. With the increasing acquisition of neural data, it is possible nowadays to analyze the spreading of activity in the brain. Besides studying the organizational principles that shape the communication within the brain, we are also interested in the role that the noise has on it. It has been found experimentally, that the presence of a nonzero level of noise may enhance the ability to detect weak stimuli. For example, Gaussian noise applied to the index finger can help improve performance of some mechanical tasks. In this phenomenon, which is similar to stochastic resonance, noise appears to aid in the detection and transmission of a signal through the nervous system. In order to study these effects, we analyze the transmission of a signal through an anatomical brain network, that is derived from a high resolution diffusion spectrum imaging, using a discrete dynamic model of integrate and fire neural regions.

*Poster

Interacting dynamics of opinion and disease on multiplex networks

Fatima Velasquez Rojas * [1], Federico Vazquez

[1]CONICET - UNLP – Argentina

We study the effects on the interaction between two different processes, the formation of opinions and the propagation of a disease in a population of individuals. This is modeled using a bilayer network, where the nodes (people) are the same for both networks, which are superposed through a fraction q ($0 \leq q \leq 1$) of pairs of nodes connected by the two types of links (opinion and disease). The frequency of interaction between two nodes depends on their states of disease and opinion. Sick people avoid leaving home and reduce their influence on the opinion of their peers, at least physically; on the other hand, people who think differently, do not meet frequently, thus reducing the possibility of infecting others. To model the dynamics of opinion we use the Voter Model (Holley & Liggett), where each person or agent takes one of two possible positions before a public issue. When a person has to decide for any of these options, they simply adopt the opinion of one of his neighbors chosen at random. We also use the Contact Process (Marro & Dickman) to model the spread of a disease. Every ill person tries to infect a susceptible neighbor with a probability of infection β or becomes susceptible with a probability of recovery $1 - \beta$. We explore how the formation of opinions affects the spread of diseases and vice versa: we analyze the dependence of the mean consensus time of opinions (τ) with the coupling. The mean consensus time is larger compared to the case of uncoupled networks and their behavior can increase monotonically or even, not monotonous. We also found that for finite systems, the density of infected individuals presents an abrupt jump with the coupling (q) and the infection probability (β), while for infinite systems the phase transition between endemic and healthy phase is continuous. Similarly, as the coupling increases, the effective infection probability decreases, reducing the size of the infected phase.

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*Poster

Variability recognition by means of a tunable algorithm based on information theory: application to wind energy

Eugenio E. Vogel * [1], G. Saravia, S. Kobe, R. Schumann, R. Schuster

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An algorithm based on data recognition in any sequence has been proposed and successfully applied to different fields [1-4]. It has been named ?word length zipper? or wlzip for short. It is based on recognition of meaningful information along any chain of sequential data; specific chains on precise digital places for a numerical basis are recognized by exact or tunable approximate matching. Length of the chains and size of the window within the data bases are among the possible tunable parameters to optimize wlzip. The information content is characterized by two parameters: a) mutability, which is the ratio in bytes of the size of the file with the map with respect to the size of the original file; b) diversity, which is a measure of the number of different words used by the map file. High values of mutability are reached when a phase transition or period of rapidly changing indicators approaches. Applications have been done to magnetic transitions [1], stock markets [2], pension funds [3], blood pressure variations [4], and current investigation is to anticipate good periods for wind energy generation which is the emphasis of this presentation.

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*Poster

When does inequality freeze an economy?

Valerio Volpati * [1], Joao Pedro Jerico, Francois Landes, Matteo Marsili, Isaac Perez Castillo

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Inequality and its impact and consequences are the the subject of intense recent debate. We address the relation between inequality and liquidity, i.e. the frequency of economic exchanges in the economy. We do that within an intentionally simplified model of the economy, where all exchanges that are compatible with agents' budget constraints are possible. Assuming a Pareto distribution of capital for the agents, that is consistent with empirical findings, we find an inverse relation between inequality and liquidity. By quantifying the amount of inequality in the system by the exponent of the Pareto distribution, we show that an increase in inequality of capital results in an even sharper concentration of financial resources, leading to congestion of the flow of goods and the arrest of the economy when the Pareto exponent reaches one.

*Poster

Dissipation in noisy chemical systems: The role of deficiency

Artur Wachtel * [1], Matteo Polettini, Massimiliano Esposito

[1] University of Luxembourg – Luxembourg

We study the effect of intrinsic noise on the thermodynamic balance of complex chemical networks subtending cellular metabolism and gene regulation. A topological network property called *deficiency*, known to determine the possibility of complex behavior such as multistability and oscillations, is shown to also characterize the entropic balance. In particular, when deficiency is zero the average stochastic dissipation rate equals that of the corresponding deterministic model, where correlations are disregarded. In fact, dissipation can be reduced by the effect of noise, as occurs in a toy model of metabolism that we employ to illustrate our findings. This phenomenon highlights that there is a close interplay between deficiency and the activation of new dissipative pathways at low molecule numbers.

*Poster

Asymmetric dynamics in networks of coupled oscillators

Stefan Wieland * [1], Sebastien Aumaître, Hervé Bercegol

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Many real-world systems can be considered networks of coupled oscillators, with frequency synchronization often being the dynamical regime of interest. For mathematical convenience, the distribution of the oscillators' natural frequencies is frequently assumed to be unimodal and symmetric, whereas in systems like electrical grids, it is bimodal and asymmetric. We describe the influence of such distributions on the onset of synchronization and on the spread of stationary phase angles. Several standard network topologies are considered, and the coexistence of stable phase-locked regimes is discussed.

*Poster

Impact of power fluctuations on stability measures of electric power grids

Matthias Wolff * [1], Pedro Lind, Philipp Maass

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With the ever increasing share of renewable sources in electric power production, the problem of keeping electric grids stable against fluctuating power input becomes increasingly important. Here we report on simulations of the time-dependent ac power flow in grids, where power input from a fraction of the generator nodes is fluctuating and follows a continuous stochastic dynamics. The results of our simulations provide insights into the problem how strongly power input fluctuations affect different measures of the grid stability, as, for example, frequency stability, phase synchrony, and probabilities of transmission line failures. In particular we address the role of intermittency in the stochastic dynamics of the input power.

*Poster

What Drives Commodity Prices to Rise Sharply at Turning Points?

K. Y. Michael Wong * [1], Bin Li, Amos H. M. Chan, Tsz Yan So, Hermanni Heimonen, and David Saad

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Commodity prices have profound effects on both economies and individuals. They are determined through their complex interdependencies with supply and demand, reserves and accessibility. Understanding the drivers of tipping points in prices is of broad interest, both academically and commercially, and is a considerable challenge. We investigate trading networks by employing an agent-based model to identify conditions that give rise to the onset of turning points and validate the new understanding using real data. In previous studies, few attempts have been made to gain insights into the phenomena through modelling and principled analyses. We devised a model consisting of a network of traders that is amenable to analysis. The major components of the model are identified to be the uneven distribution of resources, the market interactions that lead to states that maximize the utility of agents, and the role played by inventory kept by each agent to guarantee the smooth running of their business. Prices rise sharply at a turning point when producers with excess resources disappear. This establishes the link between macroscopic price behaviors and underlying resource distributions among the agents, reminiscent of phase transitions in statistical physics. By reducing noises in market data of commodities, we revealed evidence of turning points for essential commodities, as well as yield points for non-essential ones. The new approach helps explain the driving forces behind sharp price rises and will potentially lead to forecasting tools through further modelling and new insights in other trading network models.

*Poster

The asymptotic, near-equilibrium sensory response

Willy Wong * [1]

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An approach reminiscent of statistical physics can be used to quantify the asymptotic near-equilibrium sensory response. An equation can be derived which is compatible with data recorded from many sensory modalities and animal species. This approach provides an exact method for calculating the peripheral neural response to sensory signals. The theoretical approach involves the use of information theory as well as concepts of Bayesian statistics and complex systems.

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*Poster

Political inclination and opinion spread on presidential elections in South Korea

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The voter model has been studied in various systems to understand how opinions spread. Recently, several studies showed that election results can be addressed by applying the voter model with commuter flow. However, political opinions of individuals can be strongly affected by their birthplaces as well as where they are. We apply the voter model to presidential election in South Korea from 1971 to 2012, considering the annual inter-province flow of migration. Keeping information of birthplace, agents change their political opinions with given probability which is assigned by birthplace. We optimize the probability of changing opinions, comparing the outcome from real elections with simulation results. From several presidential elections, traces of the probability show the evolution of political bias based on a province. In addition, results are robust on fluctuation of population growth. We expect that the long-term evolution of the probability may show the changes in province-wise political opinions.

*Poster

Flat Band Generators in One Dimension

Maimaiti Wulayimu * [1], Alexei Andreanov, Hee Chul Park, Oleg Gendelman, Sergej Flach

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The band structure of certain Hamiltonian tight binding periodic lattices contains flat bands (FB), which are dispersionless and imply macroscopic degeneracy. FBs are accompanied by compact localized states (CLS) - eigenstates to the FB energy that spread over a finite number U of unit cells and have strictly vanishing amplitudes elsewhere. The absence of dispersion in flat band networks makes these systems highly sensitive to interactions, disorder or other perturbations. We propose a local flat band generator which constructs all tight-binding Hamiltonians for fixed U, hopping range, and total number of bands.The generator can be also used as a systematic local test of whether a given Hamiltonian has a flat band or not, circumventing the usual band structure calculation.

*Poster

Superstatistical analysis of surface temperature and precipitation statistics

G. Cigdem Yalcin * [1], Pau Rabassa, Christian Beck

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Superstatistical techniques are powerful tools to describe general classes of complex systems [1]. Important applications are in turbulence, defect turbulence, share price dynamics, random matrix theory, models of the metastatic cascade in cancerous systems, scattering processes in high-energy physics and complex systems of solid state physics [2].More recently we have shown that superstatistical techniques could be also successfully applied to environmental aspects of surface temperature and rainfall amounts distributions [3-4]. In this talk, we will discuss that superstatistical distributions f(?) of surface temperature and rainfall amounts are very different at different geographic locations on the Earth.For surface temperature, they typically exhibit a double-peak structure for long-term data. For some of our data sets we also find a systematic drift due to global warming. On the other hand, we will discuss the extreme value statistics for extreme daily rainfall, which can potentially lead to flooding, and the waiting time distribution between rainfall events.

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*Poster

Statistical mechanics and data-driven information technogy - Theory and Practice -

Yohei Saika * [1]

[1] Natioanal Institute of Technology, Gunma College – Japan

On the basis of statistical mechanics of the Ising model, we construct an information prediction system, such as for power consumption and environmental data, both using the Bayesian inference and data-driven information technoogy, such as the principal component analysis. We find that the Bayesian inference succeeds in the prediction usins multiple data similar to the target one by some methods, such as the PCA, if we control fluctuations around the MAP solution appropriately by making use of the EM algorithm.

*Poster

Theoretical test and application of the method based on variance decomposition for uncertainty and sensitivity analysis

Yueying Zhu * [1], Qiuping Alexandre Wang, Wei Li, Xu Cai

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*Poster

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- Brunnet Leonardo
- Bruot Nicolas
- Buca Berislav
- Budrikis Zoe
- Bukman Dirk Jan
- Bunin Guy
- Burioni Raffaella
- Busiello Daniel Maria
- Calero Carles
- Cammarota Chiara
- Canosa Norma
- Carlu Mallory
- Carnaffan Sean

- Carvente Osvaldo
- Casademunt Jaume
- Caselle Michele
- Casetti Lapo
- Caupin Frédéric
- Cavallaro Massimo
- Cepas Olivier
- Cha Minryeong
- Chakrabarti Dwaipayan
- Chakraborti Anirban
- Chamberlin Ralph
- Chang Yunfeng
- Chang Cheng-Hung
- Chang Shang-Yuan
- Charbonneau Patrick
- Chaté Hugues
- Chatelain Christophe
- Chatterjee Sayani
- Chattopadhyay Surajit
- Chaudhuri Debasish
- Chavanis Pierre-Henri
- Chen Yeng-Long
- Chen Hsiang-Ying
- Chen Nan-Yow
- Chen Yiing-Rei
- Chen Wei
- Chen Kaun-Peng
- Chen Hsuan-Yi
- Chepizhko Oleksandr
- Chevillard Laurent
- Chi Liping
- Chiacchiera Silvia

- Chiang Kuan-Hsun
- Chibbaro Sergio
- Chmiel Anna
- Choi Jeehye
- Choi Wonjun
- Choquard Philippe
- Chou Tom
- Chremos Alexandros
- Christou Christos
- Chu Dominique
- Chuang Yao-Li
- Chung Myung-Hoon
- Chung Kihong
- Ciccotti Giovanni
- Ciliberto Sergio
- Cividini Julien
- Clement Colin
- Clément Jean-Emmanuel
- Clervaux Nadine
- Cleuren Bart
- Coghi Francesco
- Cohen Ezechiel
- Cohen Ohad
- Colabrese Simona
- Cole Milton
- Colliva Alberto
- Concetti Francesco
- Constantin Doru
- Conti Daniele
- Cornu Françoise
- Corral Alvaro
- Corwin Eric

- Coslovich Daniele
- Costa Antonio
- Costantini Giulio
- Couder Yves
- Crampe Nicolas
- Crauste-Thibierge Caroline
- Cristelli Matthieu
- Cuerno Rodolfo
- Cugliandolo Leticia
- Cui Xiaohua
- Curatolo Agnese
- Czaplicka Agnieszka
- Da Luz Marcos
- Daisuke Tsuji
- Daivis Peter
- Dalibard Jean
- Dallas Vassilios
- Damart Tanguy
- Damart Tanguy
- Dandekar Rahul Sunil
- Dang Yiteng
- Daniels Karen
- Darsheshdar Elnaz
- Das Rakesh
- Das Subir
- Dauchot Olivier
- Dauxois Thierry
- David-Rus Diana
- Davis Géraldine
- De Lillo Silvana
- De Almeida Alexandre
- De Arcangelis Lucilla

- De Bacco Caterina
- De Buyl Pierre
- De Castro Caio
- De Forges De Parny Laurent
- De Los Santos Francisco
- De Magistris Giulio
- De Mulatier Clélia
- De Nigris Sarah
- De Oliveira Jr. Zolacir
- De Pietro Massimo
- De Rosis Alessandro
- De Santis Francesco
- De Zotti Vincent
- Debra Audus
- Decamp Jean
- Decelle Aurélien
- Degiovanni Pascal
- Degiuli Eric
- Delfau Jean-Baptiste
- Demery Vincent
- Denet Bruno
- Deng Weibing
- Deokjae Lee
- Dequidt Alain
- Derivaux Jean-François
- Deroulers Christophe
- Derrida Bernard
- Derzhko Oleg
- Dessup Tommy
- Detcheverry François
- Devailly Clémence
- Deviri Dan

- Dhar Abhishek
- Dhiman Isha
- Díaz-Méndez Rogelio
- Dickman Ronald
- Dickman Adriana
- Diehl Hans-Werner
- Dobnikar Jure
- Doebele Victor
- Doering Charles
- Dolai Pritha
- Dombre Thierry
- Domínguez-García Pablo
- Dong Wei
- Douglass Ian
- Driscoll Robin
- Driscoll Robin
- Du Roure Olivia
- Dubinin Nikolai
- Dukan Sasha
- Dumazel Laure
- Duplantier Bertrand
- Durand Marc
- Durang Xavier
- During Gustavo
- Ebrahimnazhad Rahbari S. H.
- Ehlinger Quentin
- Eiser Erika
- Ejtehadi Mohammad Reza
- El Mekkaoui Najlae
- Elci Eren
- Elskens Yves
- Erdem Riza

- Evans Martin
- Everaers Ralf
- Faggian Marco
- Falasco Gianmaria
- Family Fereydoon
- Fan Ying
- Fauve Stephan
- Fedorenko Andrei
- Feigel Alexander
- Feigenbaum Mitchell
- Feltgen Quentin
- Fernandez-Castellanos David
- Ferrand Jérémy
- Ferrari Franco
- Ferraz Mariana
- Ferreira Fernando
- Ferreira Silvio
- Ferrero Ezequiel
- Fierling Julien
- Filoche Marcel
- Filoche Marcel
- Filoux Boris
- Finn Caley
- Flottat Thibaut
- Fodor Etienne
- Fogedby Hans
- Foglino Martina
- Foini Laura
- Fomin Sergei
- Fomin Yury
- Font-Clos Francesc
- Ford Ian

- Fort Emmanuel
- Foulaadvand Ebrahim
- Fourcade Bertrand
- Fouts Stephanie
- Frahm Holger
- Franosch Thomas
- Franz Silvio
- Fredrich Thierry
- Frenkel Daan
- Frerot Irénée
- Frette Vidar
- Frey Erwin
- Fröhner Christoph
- Fuchizaki Kazuhiro
- Fuchs Matthias
- Fukai Yosuke
- Furlan Alexandre
- Furtlehner Cyril
- Furtmaier Oliver
- Furukawa Akira
- Gabrielli Andrea
- Gagliardi Alessio
- Gagliardi Luca
- Galimzyanov Bulat
- Gallego Rafael
- Ganapathy Rajesh
- Gandica Yerali
- Ganiev Orifjon
- Garcia De Soria Maria Isabel
- García-García Reinaldo
- Garoni Tim
- Gaspard Pierre

- Gauthier Georges
- Gawedzki Krzysztof
- Geffert Paul
- Geminard Jean-Christophe
- Gerstman Bernard
- Géza ódor
- Ghodrat Malihe
- Giacometti Achille
- Gianchandani Kaushal
- Giardina Irene
- Gibaud Thomas
- Gibby William
- Ginelli Francesco
- Ginot Félix
- Giri Debaprasad
- Gironella Marta
- Giuliani Alessandro
- Glavatskiy Kirill
- Gleria Iram
- Gnan Nicoletta
- Gnan Nicoletta
- Gobron Thierry
- Golden Kenneth
- Goldstein Raymond
- Golushko Ivan
- Gomez-Solano Juan-Ruben
- Gonzalez Diego
- Gonzalez Narvaez Ruth
- Gordillo Maria
- Goree John
- Goswami Partha
- Goyal Sidhartha

- Gradenigo Giacomo
- Grafke Tobias
- Granek Rony
- Granero Belinchón Carlos
- Gray Callum
- Grebenkov Denis
- Grégoire Guillaume
- Grimm Jens
- Grosjean Galien
- Gross Markus
- Gruenwald Michael
- Guevara Esteban
- Guichardaz Robin
- Guioth Jules
- Gunaratne Gemunu
- Gupta Shamik
- Gupta Arvind
- Gupta Mayanak
- Gupte Neelima
- Gutierrez Ricardo
- Guttmann Tony
- Gwak Sang-Hwan
- Ha Meesoon
- Habdas Piotr
- Haddad Noelle
- Hafner Anne
- Haga Taiki
- Hagita Katsumi
- Hakim Vincent
- Hammond Andrew
- Hannam Stephen
- Hannam Ryan

- Hansen Alex
- Haralson Zach
- Haroche Marianne
- Harris Rosemary
- Harrowell Peter
- Hartich David
- Hartmann Alexander
- Hasegawa Masahiro
- Hashizume Yoichiro
- Hassan Ahmed
- Hatakeyama Tetsuhiro
- Haug Nina
- Hayakawa Hisao
- Hayden Lorien
- He Dahai
- Hébert Frédéric
- Heinonen Vili
- Helden Laurent
- Henkes Silke
- Hentschel Hilary
- Herbert Corentin
- Hernandez Laura
- Hernandez-Garcia Anier
- Hernandez-Zapata Sergio
- Herrera-Pacheco Jose
- Herrmann Hans
- Hervy Jordan
- Hilfer R.
- Hilhorst Henk
- Hobrecht Hendrik
- Holdsworth Peter
- Höll Marc

- Holm Christian
- Honda Ryojiro
- Horňák Ivan
- Horsch Martin
- Horsley Eric
- Hoshiya Yushi
- Huang Wenwen
- Huang Ding-Wei
- Hubert Maxime
- Hucht Fred
- Hukushima Koji
- Hurtado Pablo
- Hwang Dong-Uk
- Hwang Sungmin
- Hwang Dong-Uk
- Hyeon-Deuk Kim
- Iacovacci Jacopo
- Ibrahim Yahaya
- Ichou Hamza
- Ignacio Maxime
- Iikawa Naoki
- Ikeda Harukuni
- Ilg Patrick
- Imparato Alberto
- Indekeu Joseph
- Inoue Yasuhiro
- Ishihara Shuji
- Ishii Takashi
- Isobe Masaharu
- Ispolatov Yaroslav
- Issenmann Bruno
- Itami Masato

- Ithier Gregoire
- Ito Shin-Ichi
- Ito Sosuke
- Itoh Satoru
- Iyoda Eiki
- Izmailyan Nikolay
- Izumida Yuki
- Jabbari Farouji Sara
- Jack Robert
- Jafari Rouhollah
- Jafarizadeh Arash
- Jaiswal-Nagar Deepshikha
- Janke Wolfhard
- Janssen Mathijs
- Janssen Liesbeth
- Jaramillo Diego
- Jaubert Ludovic
- Javarone Marco
- Jensen Pablo
- Jeon Euijin
- Jeong Hyeong-Chai
- Jeong Hawoong
- Jepps Owen
- Jian Jiang
- Jin Fengping
- Johal Ramandeep
- Johnston Desmond
- Jonathan Ron
- Josserand Christophe
- Jost Daniel
- Joubaud Sylvain
- Juknevicius Vaidas

- Jung Youngkyun
- Jørgensen Loren
- Kabakcioglu Alkan
- Kahng Byungnam
- Kaiser Vojtech
- Kalda Jaan
- Kallel Nabil
- Kallus Yoav
- Kalogeropoulos Nikolaos
- Kamimura Atsushi
- Kaminishi Eriko
- Kancharla Sarma
- Kang Kyongok
- Kantor Yacov
- Kapfer Sebastian
- Kappler Julian
- Karanouskaya Yuliya
- Karasawa Naoyuki
- Kardar Mehran
- Karsai Marton
- Kastner Michael
- Kato Masanari
- Kato Takeo
- Katori Makoto
- Katzav Eytan
- Kaufman Miron
- Kav Batuhan
- Kenna Ralph
- Kent-Dobias Jaron
- Kenta Yamada
- Kertész János
- Kervil Ronan

- Khomeriki Ramaz
- Khoshyaran Mahkame
- Khudayberdiev Zafar
- Kieffer John
- Kim Beom Jun
- Kim Jaeup
- Kim Jin Min
- Kim Ji-Hyun
- Kim Dong-Hee
- Kim Kibum
- Kim Doochul
- Kim Heesuk
- Kim Seongjin
- Kim Yong Woon
- Kim Purin
- Kim Lae
- Kim Yup
- Kim Jin-Hyeon
- Kim Hyewon
- Kiyohide Nomura
- Kleiner T
- Kluemper Andreas
- Kobayashi Tetsuya
- Kobayashi Michikazu
- Kocillari Loren
- Koizumi Takashi
- Kolb Max
- Konevtsova Olga
- Konincks Thomas
- Koss Xeniya
- Kosterlitz John
- Kosterlitz Berit

- Kovaleva Agnessa
- Kozlowski Karol
- Kraemer Isabella
- Krakoviack Vincent
- Kranz Till
- Krasnytska Mariana
- Kree Reiner
- Kreplak Laurent
- Krug Joachim
- Kruger Matthias
- Kumar Chandan
- Kumar Pradeep
- Kumar Sanjay
- Kundu Sumanta
- Kurzhals Jan
- Kwon Chulan
- Kyungsik Kim
- Labidi Malika
- Labousse Matthieu
- Lacoste David
- Ladieu François
- Lagarde Francois
- Lajko Peter
- Laleman Michiel
- Lam Julien
- Landes Francois
- Lang Guillaume
- Langlois Vincent
- Lanoiselée Yann
- Lapas Luciano
- Larralde Hernán
- Lathrop Daniel

- Laurson Lasse
- Laut Ingo
- Lazarescu Alexandre
- Le Cunuder Anne
- Le Goff Thomas
- Le Merrer Marie
- Lebacque Jean-Patrick
- Lecomte Charles-Edouard
- Lecomte Vivien
- Lee Daekyung
- Lee Sangyoub
- Lee Hyun Keun
- Lee Mi Jin
- Lee Byunghwee
- Lee Sang
- Lee Edward
- Lee Nam-Kyung
- Lee Sangyun
- Lee Sang Hoon
- Lee Chi-Lun
- Lee Wen-Jay
- Lee Ji Oon
- Leishangthem Premkumar
- Leitão Jorge
- Lemaître Anaël
- Lemoy Rémi
- Lenz Martin
- Leocmach Mathieu
- Leos Zamorategui Arturo
- Lerner Edan
- Lestang Thibault
- Leuzzi Luca

- Levernier Nicolas
- Levin Yan
- Levis Demian
- Leyton Ortega Vicente
- Leyvraz Francois
- Lherminier Sébastien
- Li Yao
- Li Ruiqi
- Li Bo
- Li Wei
- Li Yunyun
- Li Ming
- Liang Luo
- Liarte Danilo
- Liaw Sy-Sang
- Lidon Pierre
- Lim May
- Lin Jyun-Ting
- Lin Chang-You
- Lin Po-Cheng
- Lin Yu-Cheng
- Lin Jung-Hsin
- Lingua Fabio
- Lips Dominik
- Liu Fei
- Liu Chen
- Lohse Detlef
- Lokhov Andrey
- Lomholt Michael
- Lopes Cardozo David
- López Juan
- López De Haro Mariano

- Louvet Thibaud
- Loverdo Claude
- Lozano Celia
- Lu Xiancong
- Lubensky Tom
- Lucas Maxime
- Lucibello Carlo
- Lukovic Mirko
- Lupo Cosimo
- Lupo Cosimo
- Machta Benjamin
- Machta Jonathan
- Maciolek Ania
- Maggs Anthony
- Mahault Benoit
- Mahnke Reinhard
- Maillet Jean Michel
- Maimbourg Thibaud
- Maiti Moumita
- Maitland Michael
- Maitra Ananyo
- Majee Arghya
- Majumder Rupamanjari
- Malatesta Enrico
- Maleki-Jirsaraei Nahid
- Maloney Craig
- Mamasakhlisov Yevgeni
- Manghi Manoel
- Manjunath Naren
- Manneville Sébastien
- Manning Mary
- Marbach Sophie

- Marconi Verónica
- Marcozzi Matteo
- Marcq Philippe
- Marcuzzi Matteo
- Marino Raffaele
- Marino Ricardo
- Marruzzo Alessia
- Marsili Matteo
- Martens Kirsten
- Martin Philippe
- Martin-Mayor Victor
- Martinez Ignacio A.
- Martinez Alvaro
- Martinez-Mekler Gustavo
- Martiniani Stefano
- Masamichi J
- Masrour Rachid
- Mateos Jose
- Mateos Jose
- Mathey Steven
- Matoz-Fernandez Daniel
- Matsui Chihiro
- Matyushov Dmitry
- Mauduit Laurence
- Max Ursula
- Maynar Pablo
- Mazars Martial
- Mazzolini Andrea
- Meerson Baruch
- Melillo Stefania
- Melkikh Aleksei
- Melkikh Ekaterina

- Menon Gautam
- Menzel Adrian
- Merikoski Juha
- Merminod Simon
- Messina René
- Messio Laura
- Métivier David
- Meyer Erich
- Meyer-Ortmanns Hildegard
- Mezard Marc
- Michel Manon
- Michiels Van Kessenich Laurens
- Middleton A. Alan
- Mila Frederic
- Mindlin Gabriel
- Miracle-Sole Salvador
- Mitran Tudor
- Mixteco Sanchez Juan
- Miyahara Shin
- Miyazaki Takashi
- Miyoshi Seiji
- Mizuguchi Tomoko
- Mizuguchi Tsuyoshi
- Mobilia Mauro
- Moessner Roderich
- Mohamad Alhamad
- Mohebbi Mehran
- Mokshin Anatolii
- Mól Lucas
- Molina Daniel
- Mollgaard Anders
- Monceau Pascal

- Monchaux Romain
- Monnai Takaaki
- Montel Fabien
- Mora Serge
- Morand Jules
- Morfu Saverio
- Mori Takashi
- Mori Shintaro
- Morigi Giovanna
- Morikawa Masahiro
- Morikuni Yohei
- Morillo García Juan
- Morin Alexandre
- Moritz Clemens
- Mossa Stefano
- Mouhanna Dominique
- Mounkachi Omar
- Movassagh Ramis
- Mueller Marcus
- Mujica Nicolas
- Mukamel David
- Mungan Muhittin
- Munoz Jose
- Murashita Yuto
- Musacchio Stefano
- Mussardo Giuseppe
- Mussardo Giuseppe
- Mutabazi Innocent
- Muzdalo Anja
- Nadah Amine
- Nadal Jean-Pierre
- Naert Antoine

- Nagao Taro
- Nagar Apoorva
- Nagler Jan
- Nair Niketh
- Najafi Amin
- Najafi Saeed
- Nakagawa Yuya
- Nandi Saroj
- Napiorkowski Marek
- Nardini Cesare
- Nariaki Sakaï
- Narizuka Takuma
- Naserzare Felora
- Nasri Yasmina
- Navas Víctor
- Néel Marie-Christine
- Nemoto Takahiro
- Niccoli Giuliano
- Nicholls Joel
- Nicolas Alexandre
- Nicole Robin
- Nielsen Ole
- Nieva José
- Nili Hossein
- Ninarello Andrea
- Nishiguchi Daiki
- Nishikawa Yoshihiko
- Nissinen Jaakko
- Nitzan Mor
- Niven Robert
- Noh Jae Dong
- Noirhomme Martial

- Nomidis Stefanos Konstantinos
- Novotny Mark
- Nunzi François
- Nyberg Markus
- Oakes Tom
- Obuchi Tomoyuki
- Odier Céleste
- Ogunjo Samuel
- Oh Se-Wook
- Ohta Hiroki
- Okumura Ko
- Okumura Keiji
- Okumura Hisashi
- Oliveira João
- Onorato Miguel
- Opsomer Eric
- Orlandini Enzo
- Ortiz De Zarate Jose
- Osmanovic Dino
- Oswald Patrick
- Ozawa Misaki
- Ozeki Yukiyasu
- Pagonabarraga Ignacio
- Pak Hyuk Kyu
- Pakpour Maryam
- Pandey Shubham
- Pandey Toplal
- Pandit Rahul
- Parisen Toldin Francesco
- Parisi Giorgio
- Park Sojung
- Park Jinha

- Park Jeong-Man
- Park Hee Chul
- Park Seong Jun
- Park Hyunggyu
- Park Su-Chan
- Park Hyejin
- Parmar Anshul
- Parra-Rojas César
- Parrondo Juan
- Pastore Giorgio
- Patelli Aurelio
- Paterson Chay
- Patinet Sylvain
- Paul Wolfgang
- Pazó Diego
- Pekola Jukka
- Pelizzola Alessandro
- Peña Rosselló Julián
- Pennetta Cecilia
- Peredo-Ortiz Ricardo
- Pereira Emmanuel
- Pereira Rodrigo
- Perelló Josep
- Perera Aurélien
- Perez Luis
- Perez-Gaviro Sergio
- Perk Jacques
- Perugini Gabriele
- Petrelis Francois
- Petrov Oleg
- Peyrard Michel
- Pezelier Baptiste

- Pietracaprina Francesca
- Pietzonka Patrick
- Pires Antonio
- Piscitelli Antonio
- Pittorino Fabrizio
- Plihon Nicolas
- Poincloux Samuel
- Polettini Matteo
- Polewczak Jacek
- Pollack Yoav
- Pomeau Yves
- Ponce Dawson Silvina
- Poncet Alexis
- Popescu Mihail
- Portesi Mariela
- Poryles Raphael
- Posch Ingeborg
- Posch Harald
- Potters Marc
- Poty Martin
- Pouliquen Olivier
- Poy Guilhem
- Požar Martina
- Pretti Marco
- Procacci Aldo
- Procaccia Itamar
- Proesmans Karel
- Prolhac Sylvain
- Prosen Tomaz
- Prudnikov Vladimir
- Prudnikov Pavel
- Puga-Cital Enrique

- Puisto Antti
- Pumir Alain
- Qi Wanming
- Qiao Zhi
- Qiao Chongzhi
- Qin Pinquan
- Qiu Haibo
- Quan Haitao
- Quinn Katherine
- Raban Valentin
- Radisson Basile
- Radons Guenter
- Djelti Radouan
- Ragone Francesco
- Rahman Shafiqur
- Rainone Corrado
- Rajabi Sayeh
- Raju Archishman
- Ramaswamy Sriram
- Ramirez Rosa
- Ramola Kabir
- Ramos Osvanny
- Rancon Adam
- Rao Riccardo
- Rapaport Dennis
- Rasmussen Jorgen
- Rasuli Seyyed Nader
- Rasulova Mukhayo
- Ray Somrita
- Razin Nitzan
- Redondo Juan
- Reichl Linda

- Renaud Antoine
- Rendón De La Torre Stephanie
- Rens Robbie
- Reuveni Shlomi
- Reygner Julien
- Rezaei Soghra
- Rica Sergio
- Ricateau Hugo
- Rico Marc
- Rizzo Tommaso
- Ro Sunghan
- Roa Oppliger Luis
- Robinson Joshua
- Robles Miguel
- Rocchi Jacopo
- Rodríguez Miguel
- Rodriguez Arias Ines
- Rohwer Christian
- Roichman Yael
- Rolland Joran
- Romero-Bastida Mauricio
- Ronceray Pierre
- Ronellenfitsch Henrik
- Ronti Michela
- Roosen-Runge Felix
- Rosa Angelo
- Rosales Pablo
- Rosanova Antonio
- Roscilde Tommaso
- Rossi Paulo
- Rouhani Shahin
- Roussel Benjamin

- Roy Ushasi
- Roy Sutapa
- Roy Subhadeep
- Roy Analabha
- Royall C. Patrick
- Ruffo Stefano.
- Ruiz Jean
- Ruiz Chavarria Gerardo
- Rulquin Charlotte
- Ruppeiner George
- Ruscher Céline
- Rusek Pawel
- Rutkevich Sergei
- Ryu Jung-Wan
- Ryzhov Valentin
- Sabbagh Ali
- Sachdeva Himani
- Sadeghi Sina
- Sadhu Tridib
- Sahbi El Hog
- Saint-Michel Brice
- Saint-Raymond Laure
- Saito Nen
- Sakai Toru
- Sakellariou Jason
- Sakumichi Naoyuki
- Salazar Robert
- Salbreux Guillaume
- Salgado-Garcia Raul
- Labidi Salima
- Salinas Silvio
- Salort Julien

- San Miguel Maxi
- Sanchez Pedro
- Sanchez Ruiz Jorge
- Sanchez-Salas Norma
- Sanders David
- Sano Masaki
- Santos Fernando
- Santos Andres
- Santucci Stéphane
- Sarkar Niladri
- Sarkar Debarati
- Sarman Sten
- Sasa Shin-Ichi
- Sasaki Kazuo
- Sastry Srikanth
- Satoshi Natori
- Savenko Ivan
- Savvidy George
- Saw Shibu
- Sawai Satoshi
- Sbailo Luigi
- Scalliet Camille
- Schadschneider Andreas
- Schertzer Daniel
- Schiel Christoph
- Schmidt Christian
- Schmidt Michael
- Schmidt Johannes
- Schmiedeberg Michael
- Schmitt Regina
- Schockmel Julien
- Schram Raoul

- Schreiber Nir
- Schroeder-Turk Gerd
- Schulz Robert
- Schwarz Jen
- Sean David
- Segall Nimrod
- Seguin Antoine
- Seifert Udo
- Seki Yuya
- Seoane Beatriz
- Serrao Shannon
- Serres Marion
- Sethna James
- Sevier Stuart
- Sevilla Francisco J
- Seyboldt Rabea
- Shakirov Timur
- Shannon Nic
- Sharapova Iryna
- Sharma Auditya
- Sharma Kiran
- Shchur Liudmila
- Shchur Lev
- Sheng Nan
- Shimizu Akira
- Shimokawa Michiko
- Shin Jaeoh
- Shinagawa Ryota
- Shirai Tatsuhiko
- Shiraishi Naoto
- Shiri Somayeh
- Shor Carmel

- Shukla Pragya
- Shukla Vishwanath
- Shulga Sergiy
- Sibani Paolo
- Sicuro Gabriele
- Sienkiewicz Julian
- Simini Filippo
- Simonnet Eric
- Singh Murari
- Singh Navin
- Skaugen Audun
- Skrbic Tatjana
- Slater Gary
- Slowman Alexander
- Smerald Andrew
- Soh Hyungjoon
- Solon Alexandre
- Somsikov Vyacheslav
- Song Juyong
- Sood Ajay
- Sorokin Michael
- Soto Rodrigo
- Spagnolo Bernardo
- Spathis Panayotis
- Speck Thomas
- Spiechowicz Jakub
- Spigler Stefano
- Spohn Herbert
- Squarcini Alessio
- Stäger Dominik
- Steffenoni Stefano
- Steinberger Audrey

- Steinle R
- Straka Peter
- Sughiyama Yuki
- Sugiura Sho
- Sulc Petr
- Sumedha Sumedha
- Sun Meng
- Suñé Simon Marc
- Sung Myung
- Sung Jaeyoung
- Sung Bong June
- Sung Wokyung
- Suzuki Masuo
- Suzuki Takafumi
- Suzuki Takafumi
- Szamel Grzegorz
- Taberlet Nicolas
- Tacchella Andrea
- Tajima Hiroyasu
- Takabe Satoshi
- Takagi Hiroyoshi
- Takahashi Masahiro
- Takahasi Hiroki
- Takahiro Tanabe
- Takano Hiroshi
- Takenaka Hikaru
- Takeuchi Hiromitsu
- Takeuchi Kazumasa
- Talon Laurent
- Tamai Keiichi
- Tamm Mikhail
- Tamura Ryo

- Tanaka Hajime
- Tanaka Shu
- Tang Lei-Han
- Tang Chao
- Tang Kai-Hsiang
- Tani Marie
- Tanis Ioannis
- Tantari Daniele
- Tapias Diego
- Tarama Mitsusuke
- Tarasevich Yuri
- Tarazona Pedro
- Tarbiat Andisheh
- Tarpin Malo
- Tarquini Elena
- Tatsumi Soichi
- Tauber Clément
- Tauber Uwe
- Tellez Gabriel
- Telo Da Gama Margarida
- Teomy Eial
- Tesoro Salvatore
- Thalabard Simon
- Theurkauff Isaac
- Thibaut Jérôme
- Tian Jing
- Timonin Pavel
- Tiribocchi Adriano
- To Tung
- Todo Synge
- Tokuda Satoru
- Toledo-Marin Javier

- Tong Hua
- Toral Raul
- Toyabe Shoichi
- Tria Francesca
- Tripathi Ashwani
- Trovato Antonio
- Tschirhart Hugo
- Tsironis George
- Tsobgni Nyawo Pelerine
- Tu Meihsien
- Tuncer Aslı
- Tyukodi Botond
- Ucar Mehmet
- Ueda Masahiko
- Uezu Tatsuya
- Um Jaegon
- Urbic Tomaz
- Urrutia Efraín
- Usatenko Zoryana
- Vadakke Veettil Prasad
- Van De Put Maarten
- Van Saarloos Wim
- Van Tiggelen Bart
- Vandebroek Hans
- Vandembroucq Damien
- Vandewalle Nicolas
- Vanel Loïc
- Vanicat Matthieu
- Vasin Mikhail
- Vázquez Federico
- Vazquez Federico
- Vázquez-Rodríguez Bertha

- Velasquez Rojas Fatima
- Venaille Antoine
- Verderosa Antonella
- Verley Gatien
- Verma Mahendra
- Verma Atul
- Viader Godoy Xavier
- Vidal Valerie
- Villada-Balbuena Alejandro
- Villain-Guillot Simon
- Vilone Daniele
- Vinutha H. A.
- Vogel Eugenio
- Volpati Valerio
- Von Der Heydt Alice
- Vroylandt Hadrien
- Wachtel Artur
- Wakita Jun-Ichi
- Wald Sascha
- Wan Rongzheng
- Wang Xipeng
- Wang Ting
- Wang Yan
- Wang Shou-Wen
- Watt Graeme
- Weigel Martin
- Weijs Joost
- Wesfreid Jose Eduardo
- Wettstein Marcus
- Weyer Floriane
- Whitfield Carl
- Wieland Stefan

- Wiese Kay
- Wiesner Karoline
- Wio Horacio
- Woillez Eric
- Wolf Pierre-Etienne
- Wolff Matthias
- Wong Chun-Shang
- Wong Willy
- Wong Michael
- Woo Seong Jo
- Wright Katherine
- Wu Ming-Chya
- Wu Ten-Ming
- Wu Kuan-Ting
- Wulayimu Maimaiti
- Xi Jingyi
- Xu Limei
- Xu Song
- Yalcin Gulistan Cigdem
- Yamaguchi Hiroki
- Yamamoto Takaki
- Yamamoto Takaki
- Yamamoto Kaoru
- Yamanaka Sadato
- Yang An-Cheng
- Yeomans Julia
- Yi Juyeon
- Yi-Teng Hsiao
- Yin Lan
- Yizhou Tan
- Yizhou Tan
- Yohei Saika

- Yong Daeseong
- Yoshihiko Nonomura
- Yoshimori Akira
- Yun Jinhyuk
- Zaccarelli Emanuela
- Zaccaria Andrea
- Zakharov Anatoly
- Zamponi Francesco
- Zapperi Stefano
- Zeng An
- Zeraati Somayeh
- Zeravcic Zorana
- Zezyulin Dmitry
- Zhang Yong
- Zhang Ben-Wei
- Zhang Chuanbiao
- Zheng Wen
- Zhitomirsky Mike
- Zhou Yujie
- Zhou Xin
- Zhu Yueying
- Zhukova Aleksandra
- Ziff Robert
- Zippelius Annette
- Znidaric Marko
- Zu Mengjie
- Zwanikken Jos
- Zwicker David
- žukovič Milan