Computation of transition trajectories and rare events in non-equilibrium systems

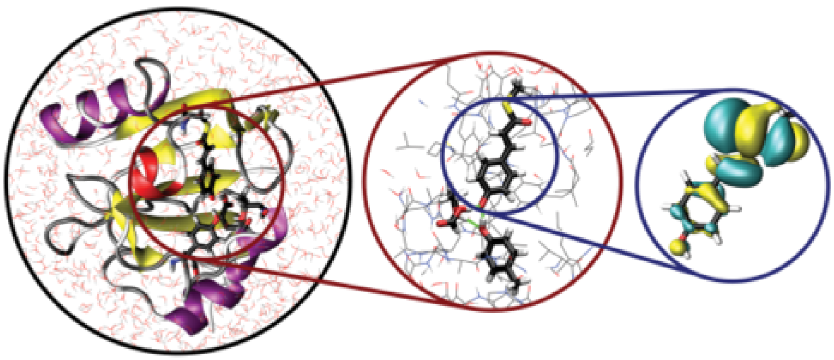
Applications in Turbulence, Chemistry, Physics, Biophysics

June 11–15, 2012

Lyon, France

Booklet of Abstracts

Centre Blaise Pascal, École normale supérieure de Lyon



Chemical reactions inside proteins, by Bolhuis group

http://www.cbp.ens-lyon.fr/RareEventsWorkshop/

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1 Practical information

If you need Internet access, use the wireless network named '**invites**':

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2 Organizing committee

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3 Programme

See document '**Programme.pdf**'.

4 Abstracts

4.1 Monday

Applications of rare-event sampling to study supercooled liquid dynamics and non-equilibrium amorphous solids

David Chandler
University of California, Berkeley, USA

Transition path sampling (i.e., Monte Carlo of trajectory space) provides a means to study the statistical properties of ensembles of trajectories. These ensembles can be characterized in various ways. For example, in rare-event sampling, ensembles of interest are those with trajectories connecting two meta-stable basins. For cases where glassy dynamics is of interest, these rare events can refer to elementary excitations in an otherwise static system. Control parameters can move between ensembles of trajectories exhibiting different amounts of dynamical activity (i.e., differing concentrations of elementary excitations). The dynamical partition function (i.e., sum over histories) is sometimes a singular function of these control parameters, and evidence for the singularities can be found numerically. In this way, it is possible to detect the presence of inactive (i.e., glass-like) basins in a complex system, even when these basins have no significant statistical weight in the active (i.e., liquid) equilibrium phase. In one illustration, I will focus on yet-to-be published results considering the behavior of supercooled water. This system exhibits polyamorphism (i.e., more than one distinct non-equilibrium amorphous solid phase). Connections with experiment and juxtaposition with some old ideas about water will be discussed.

Minimizing extinction risk by migration

Leonard M. Sander
Physics & Complex Systems, University of Michigan, USA

Many populations in nature are fragmented: they consist of local populations occupying separate patches. A local population is prone to extinction due to the shot noise of birth and death processes. If the steady-state population is large, this is a rare event.

A migrating population from another patch can dramatically delay extinction. What is the optimal migration rate that minimizes the extinction risk of the whole population? We answer this question for a connected network of model habitat patches with different carrying capacities. We use WKB methods to find the exit paths, and supplement them with numerics.

(Collaboration with M. Khasin, B. Meerson, and E. Khain)

Biased sampling of unbiased dynamical trajectories in complex systems

Peter Bolhuis
University of Amsterdam, The Netherlands

The transition path sampling (TPS) methodology has enabled the sampling of rare events in complex systems using unbiased dynamical trajectories. The method works by restricting the trajectory space to paths that visit specific stable states. Of the many applications that TPS has, I will discuss one on rare events occurring in the relaxation process of a signaling protein. In the last few years the TPS framework has been extended in various ways. On the one hand by the transition interface approach (TIS) (related to the forward flux method) to sample kinetic properties more efficiently. On the other hand by allowing transitions between the multiple (meta) stable states that often are present in complex systems. I will discuss these approaches. Finally, I will introduce a novel scheme that combines the multiple state TIS approach with a single replica exchange method, that, in principle, is able to explore the entire trajectory space starting from a single stable minimum.

Heterogeneities in a 2-dimensional driven glassy model: Current fluctuations and finite-size effects

Estelle Pitard
Université Montpellier 2, France

We report in detail on the fluctuations of current and their spatial consequences in a two-dimensional glassy system which is brought out-of-equilibrium by an external field. This system lies in the class of Kinetically Constrained Models (KCMs) which have been widely studied in the context of glassy dynamics. The dynamical constraints lead to a dramatic slowing down of the dynamics of the macroscopic system. In these models without forcing, it has been shown using the thermodynamic formalism for histories, that there is a coexistence between an active and an inactive phase. This coexistence can be described by a first-order transition, and a related discontinuity in the derivative of the large deviation function for the activity [1]. Later, it has been found that adding a driving field to a KCM model leads to a singularity in the large deviation function of the current at large fields. According to the initial condition, the system can flow easily or be almost blocked [2]. Here, we study in detail the relation between the current and microscopic features, in particular the heterogeneous, intermittent dynamics of the particles, transient shear-banding and blocking walls. We study the distribution of wall sizes and the distribution of velocities. The study of the system in finite sizes gives access to the dynamical correlation length, both in the shear-thinning and the shear-thickening regimes. The distribution of current in a confined system is investigated as well.

[1] Garrahan J. P., Jack R. L., Lecomte V., Pitard E., van Duijvendijk K., and van Wijland F., Phys. Rev. Lett. 98 (2007) 195702.

J. Phys. A 42 (2009) 075007.

[2] Turci F., Pitard E., Europhys. Lett., 94 (2011) 10003.

Large deviations of the density and of the current in non-equilibrium steady states

Bernard Derrida
Ecole normale supérieure, Paris, France

This talk will review some results obtained over the last decade on the large deviations of the density and of the current in non-equilibrium steady states of diffusive systems. It will also discuss some open questions on non steady state situations and on non diffusive systems.

Diffusion with stochastic resetting

Martin Evans
University of Edinburgh, UK

'Stochastic resetting' is a rather common process in everyday life. Consider searching for some target such as, for example, a face in a crowd or one's misplaced keys at home. A natural tendency is, on having searched unsuccessfully for a while, to return to the starting point and recommence the search. In this talk I explore the consequences of such resetting on perhaps the most simple and common process in nature, namely, the diffusion of a single or a multi-particle system. It turns out that a nonzero rate of resetting has a rather rich and dramatic effect on the diffusion process, strongly affecting the behaviour of mean first passage times and survival probabilities.

Long-range correlations in driven, non-equilibrium systems

David Mukamel
Weizmann Institute of Science, Rehovot, Israel

Systems driven out of thermal equilibrium often reach a steady state which under generic conditions exhibits long-range correlations. As a result these systems sometimes share some common features with equilibrium systems with long-range interactions, such as the existence of long range-order and spontaneous symmetry breaking in one dimension, ensemble inequivalence and other properties. Some models of driven systems will be presented, and features resulting from the existence of long-range correlations will be discussed.

Dynamical phase transition in a two-dimensional diffusive system

Carlos Perez-Espigares
Departamento de Electromagnetismo y Fisica de la Materia, Universidad de Granada, Spain

In this work we study the large deviations of the time-averaged current in the periodic two-dimensional (2D) Kipnis-Marchioro-Presutti model of energy transport. Unlike the 2D-KMP model subject to a boundary gradient, where an appropriate generalization of the additivity principle can be made [1,2], we observe here that the optimal profile associated to a given current fluctuation becomes time dependent. This time dependence emerges for currents above a critical threshold and was first observed in one dimension [3]. This suggests that rare events are generically associated with coherent, self-organized patterns which enhance their probability.

[1] P.I. Hurtado, C. Perez-Espigares, J.J. del Pozo and P.L.Garrido (2011) Symmetries in fluctuations far from equilibrium. Proc. Natl. Acad. Sci. USA 108:7704-7709

[2] Perez-Espigares C, del Pozo JJ, Garrido PL, Hurtado PI (2011) Current large deviations in a two-dimensional diffusive system. AIP Conf Proc 1332:204–213.

[3] P.I. Hurtado and P.L. Garrido (2011) Spontaneous Symmetry Breaking at the Fluctuating Level. Phys. Rev. Lett. 107:180601

4.2 Tuesday

Transition path theory for the modeling and simulation of reactive events

Eric VANDEN-EIJNDEN
New York University, USA

Reactive events such as conformation change of macromolecules, chemical reactions in solution, nucleation events during phase transitions, regime changes in climate, etc. pose challenges both for computations and modeling. At the simplest level, these events can be characterized as the hopping over a free energy barrier associated with the motion of the system along some reaction coordinate. Indeed this is the picture underlying classical tools such as transition state theory or Kramers reaction rate theory, and it has been successful to explain reactive events in a wide variety of context. However this picture presupposes that we know or can guess beforehand what the reaction coordinate of the event is. In many systems of interest arising from molecular biology, material science, atmosphere-ocean science, etc. making such educated guesses is hard if not impossible. The question then arises whether we can develop a more general framework to describe reactive events, elucidate their pathway and mechanism, and give a precise meaning to a concept such as the reaction coordinate. In this talk I will discuss an attempt at such a framework, termed transition path theory (TPT), and indicate how it can be used to develop efficient algorithms to accelerate brute-force numerical simulations or to interpret the data generated by such simulations.

Sampling methods in molecular dynamics: Efficient sampling of metastable trajectories

Tony LELIÈVRE
Ecole des Ponts ParisTech, France

We will present some mathematical results on numerical methods for efficient sampling in molecular dynamics, with an emphasis on techniques used to sample trajectories between metastable states. This presentation is based on the following papers: [1] F. Cérou, A. Guyader, T. Lelièvre and D. Pommier, A multiple replica approach to simulate reactive trajectories, Journal of Chemical Physics 134, 054108, 2011. [2] C. Le Bris, T. Lelièvre, M. Luskin and D. Perez, A mathematical formalization of the parallel replica dynamics, http://arxiv.org/abs/1105.4636, to appear in Monte Carlo Methods and Applications.

Non-classical large deviations in the AB model

Hugo TOUCHETTE
Queen Mary, University of London, UK

I will discuss the large deviation properties of a two-dimensional dynamical system perturbed by noise, referred to as the AB model. Unlike previous models studied in large deviation theory, this model does not have an isolated attractor. Instead, it has a line of stable steady states connected to a line of unstable steady states. I will show how this property gives rise to a nonequilibrium stationary current and to fluctuation paths of zero action. The latter are important from the point of view of large deviation theory as they themselves give rise to a non-classical scaling of the stationary distribution, which cannot be obtained from the Freidlin-Wentzell theory. Connections with more general models will be discussed.

DMRG-approach to large deviations

Carlo Vanderzande
Hasselt University, Belgium

It is his shown how the density matrix renormalisation group (DMRG) originally introduced to study quantum chains can be adapted to calculate the properties of systems far from equilibrium. We explain how to determine the cumulant generating function and density profiles associated with atypical currents for exclusion processes. The method is used to verify the additivity principle in weakly asymmetric models and to determine the first four cumulants of the current in the asymmetric exclusion process.

[1] M. Gorissen and C. Vanderzande, Finite size scaling of current fluctuations in the totally asymmetric exclusion process, J. Phys. A 44, 115005 (2011).

[2] J. Hooyberghs and C. Vanderzande, Thermodynamics of histories for the one-dimensional contact process, J. Stat. Mech. P02017 (2010).

Large deviations in boundary-driven systems: Numerical evaluation and effective large-scale behavior

Guy Bunin
Technion, Haifa, Israel

We study rare events in systems of diffusive fields driven out of equilibrium by the boundaries. We present a numerical technique and use it to calculate the probabilities of rare events in one and two dimensions. Using this technique, we show that the time evolution leading to a configuration which slowly varies in space can be captured with a small number of long wave-length modes. For a configuration which varies rapidly in space this description can be complemented by a local equilibrium assumption.

[1] Guy Bunin, Yariv Kafri, and Daniel Podolsky, Large deviations in boundary-driven systems: Numerical evaluation and effective large-scale behavior, arXiv:1202.0286

Finite time stochastic thermodynamics and optimal mass transport

Krzysztof Gawedzki
Ecole normale supérieure de Lyon, France

I shall discuss the problem of minimizing entropy production and heat release in finite time stochastic processes. The results shed new light on the Landauer principle about memory erasure.

Information and thermodynamics: Experimental verification of Landauer's erasure principle

Sergio Ciliberto
Ecole normale supérieure de Lyon, France

Rolf Landauer argued that the erasure of information is a dissipative process. A minimal quantity of heat, proportional to the thermal energy, is necessarily produced when a classical bit of information is deleted. A direct consequence of this logically irreversible transformation is that the entropy of the environment increases unavoidably by a finite amount. We experimentally show the existence of the Landauer bound in a generic model of a one-bit memory. Using a system of a single colloidal particle trapped in a modulated double-well potential, we establish that the mean dissipated heat saturates at the Landauer bound in the limit of long erasure cycles. This result demonstrates the intimate link between information theory and thermodynamics.

How slow instanton is renormalized by fluctuations

Gregory FALKOVICH
Weizmann Institute of Science, Rehovot, Israel

I describe an optimal fluctuation that determines the statistics of strong vorticity fluctuations in the direct cascade of 2d turbulence.

Sampling microcanonical measures of the 2D Euler and Shallow Water equations with Creutz's algorithm

Max POTTERS
Technical University Delft, The Netherlands

The 2D Euler model is the basic example of fluid models for which a microcanical measure can be built from first principles. Such measures are defined through finite-dimensional approximations and a limiting procedure. We use Creutz's algorithm, a microcanonical generalization of the Metropolis-Hasting algorithm (to sample Gibbs measures, in the canonical ensemble), to sample finite-dimensional approximations of the 2D Euler microcanonical measures (incorporating fixed energy and other invariants). Making use of Creutz's algorithm is essential as microcanonical and canonical measures are known to be inequivalent at some values of energy and vorticity distribution of the 2D Euler equations. Creutz's algorithm is applied to check predictions from the mean-field statistical mechanics theory of the 2D Euler equations (Robert-Sommeria-Miller theory). We found full agreement with these predictions. Also, three different ways to compute the temperature gave consistent results. Furthermore, a phase transition for the 2D Euler statistical equilibrium and a situation of statistical ensemble inequivalence are found and studied. Generalization of this algorithm to other models, for which a mean-field theory does not yet exist, is discussed. Some preliminary results for the Shallow Water equations are addressed.

4.3 Wednesday

Dynamics with selection, large deviations and metastability

Jorge Kurchan
PMMH-ESPCI / IHP, Paris, France

I will discuss the formal relation between i) extremal trajectories and large deviation functions , ii) metastability and dynamical phase transitions. iii) dynamics in a complex landscape with superimposed selection based on an independent fitness function, Extremal trajectories are of general interest in subjects as diverse as meteorology (storms, rougue waves) an planetary systems (stable planets). Dynamical phase transitions as a method to encapsulate metastability has been proposed as an approach to glassiness, but may have more general applications. Finally, dynamics in the presence of natural selection finds a natural application in the case of cells whose fitness is a function of their transcriptional state.

Transition trajectory for equilibrium droplet formation

Wolfhard Janke
Institut für Theoretische Physik and Centre for Theoretical Sciences (NTZ), Universität Leipzig, Germany

Within the Ising lattice-gas model, large-scale Monte Carlo computer simulations of the formation of equilibrium droplets are presented and compared with analytical predictions. Universal aspects of the formation-dissolution transition in two dimensions are high-lighted: Three different lattice discretizations yield very similar results when presented in properly scaled variables. Particular emphasis is placed on the free-energy barrier governing the transition trajectory for droplet formation and its implication for multicanonical simulations.

[1] A. Nußbaumer, E. Bittner, and W. Janke, *Monte Carlo study of droplet formation-dissolution transition on different two-dimensional lattices*, Phys. Rev. E **77**, 42 041109 (2008).

[2] A. Nußbaumer, E. Bittner, and W. Janke, *Free-energy barrier at droplet condensation*, Prog. Theor. Phys. Suppl. **184**, 400 (2010).

Rare current events in non-equilibrium systems with long-range memory

Rosemary Harris
Queen Mary, University of London, UK

I will discuss recent work to characterize, analytically and numerically, the most probable paths leading to given current fluctuations in interacting particle systems with history-dependent rates. In particular, I will demonstrate how long-range memory dependence can modify the current large deviation principle, resulting for example in a superdiffusive regime in the phase diagram of the well-known asymmetric simple exclusion process.

[1] Current fluctuations in stochastic systems with long-range memory, R. J. Harris and H. Touchette, J. Phys. A: Math. Theor. 42, 342001 (2009)

Bistability and transitions induced by topography in a laboratory model of a geostrophic jet

Manikandan Mathur
Laboratoire des Ecoulements Géophysiques et Industriels, Grenoble, France

Equilibrium statistical mechanics predicts a phase transition between two different states (their difference being characterized by the topology of the vorticity distribution) for the two dimensional Navier Stokes equations without forcing and dissipation. Introducing weak forcing and dissipation takes the system away from equilibrium, and Bouchet & Simmonet (2009) have observed a first order transition between states that are qualitatively similar to the steady states predicted by equilibrium statistical mechanics. The first order phase transition allows for bistable behaviour, a striking property of some climate features like the atmospheric jet stream and the oceanic Kuroshio current. In this talk, we report results from laboratory experiments reproducing geostrophic jets in an annular rotating tank. The jet is influenced by a non-axisymmetric bottom topography interfering with the natural wavy pattern of the jet. Varying the system parameters, we identify three different states - the (i) “blocked”, (ii) “propagating” and (iii) “mixed” states. The “blocked” and “propagating” states are observed over an overlapping range of the system parameters, thus pointing to bistability in the system. The blocked and the propagating states, once achieved, persist for long times in spite of the strong turbulent fluctuations; transitions from one state to another are induced by an abrupt change in the system parameters within the bistable regime. The “mixed” state exhibits step-like features in the phase propagation of different modes in the azimuthal direction, thus suggesting indeterministic switches between the “blocked” and the “propagating” states. The statistics of the time spent on each step in the phase evolution will be discussed.

Optimal control of molecular dynamics using Markov state models

Christof Schuette
Freie Universitaet Berlin and DFG Research Center MATHEON, Germany

The effective dynamics of molecular system can be characterized by the switching behavior between several metastable states, the so-called conformations of the system that determine its functionality. Steering a molecular system from one conformation into another one on the one hand is a means to controlling its functionality while on the other hand it can be used to gather information about transition trajectories. This talk considers optimal control problems that appear relevant in steered molecular dynamics (MD). It will be demonstrated how the associated Hamilton-Jacobi-Bellman (HJB) equation can be solved. The main idea is to first approximate the dominant modes of the MD transfer operator by a low-dimensional Markov state model (MSM), and then solve the HJB for the MSM rather than the full MD. We then will discuss whether the resulting optimal control process may help to characterize the ensemble of transition trajectories. The resulting method will be illustrated in application to the maximization of the population of alpha-helices in an ensemble of peptides.

Universality of large deviations in diffusive systems

Frédéric van Wijland
Université Paris Diderot, France

After having characterized, on the basis of canonical examples, diffusive systems described by fluctuating hydrodynamics, I will show that the large deviation properties of several quantities, in these systems, display universal features. Universality extends, in some cases, to nonequilibrium settings. Finally, it will appear that diffusive systems may exhibit dynamical phase transitions between homogeneous realizations and heterogeneous ones. I will spend the remaining time discussing such phase transitions.

This presentation results from collaborations with: C. Appert, B. Derrida, J.P. Garrahan, A. Imparato, and V. Lecomte.

Simulating rare events in dynamical processes

Julien Tailleur
CNRS – Université Paris-Diderot, France

Atypical trajectories often play a crucial role in dynamical systems. For instance, resonances and separatrices determine the fate of planetary systems, and localized objects like solitons and breathers provide mechanisms of energy transport in nonlinear systems such as Bose-Einstein condensates and biological molecules. I will present simulation methods that can be used to simulate such rare trajectories in an efficient, accelerate way and show how these methods give access to central quantities in non-equilibrium statistical mechanics: the large deviation functions.

The first part of my talk will focus on applications in the field of dynamical systems whereas the second part will deal with standard problems of non-equilibrium statistical mechanics, such as exclusion processes and absorbing phase transitions.

A large deviation approach to computing rare transitions in multi-stable stochastic turbulent flows

Jason Laurie
Ecole normale supérieure de Lyon, France

Many turbulent flows undergo sporadic random transitions, after long periods of apparent statistical stationarity. For instance, paths of the Kuroshio [1], atmospheric flows [2], the Earth's magnetic field reversal and MHD experiments [3], 2D turbulence experiments [4,5], and 3D flows [6] show this kind of behavior. The understanding of this phenomenon is extremely difficult due to the complexity, the large number of degrees of freedom, and the non-equilibrium nature of these turbulent flows.

A straightforward study of these transitions, through direct numerical simulation of the governing equations is nearly always impracticable. This is mainly a complexity problem, due to the large number of degrees of freedom involved for genuine turbulent flows, and the extremely long time between two transitions.

In this talk, we consider two-dimensional and geostrophic turbulence models with stochastic forces. We consider regimes where two or more attractors coexist. As an alternative to direct numerical simulation, we propose a non-equilibrium statistical mechanics approach to the computation of this phenomenon. Our strategy is based on large deviation theory for stochastic dynamical systems (Freidlin–Wentzell theory) [7], derived from a path integral representation of the stochastic process. We discuss in which cases one can generalize Freidlin–Wentzell theory to turbulent flows and when one cannot.

Interestingly, we prove that in the class of models we consider, a mechanism exists for diffusion over sets of connected attractors [8]. For the type of stochastic forces that allow for this diffusion, the transition between attractors is not a rare event, and then it is very difficult to characterize the flow as bistable. However, for another class of stochastic forces, this diffusion mechanism is prevented, and genuine bistability or multi-stability is observed. Finally, we discuss how these results are probably connected to the long debated existence of multi-stability in the atmosphere and oceans.

[1] M. J. Schmeits and H. A. Dijkstra, Bimodal behavior of the Kuroshio and the Gulf stream. J. Phys. Oceanogr. 31, 12, 3435–3456, (2001).

[2] E. R. Weeks, Y. Tian, J. S. Urbach, K. Ide, H. L. Swinney and M. Ghil, Transitions between blocked and zonal flows in a rotating annulus with topography, Science, 278, 5354, 1598–1601, (1997).

[3]M. Berhanu et al., Magnetic field reversals in an experimental turbulent dynamo, Europhys. Lett. 77, 59001, (2007).

[4] J. Sommeria, Experimental study of the two-dimensional inverse energy cascade in a square box, J. Fluid Mech. 170, 139–168, (1986).

[5] S. R. Maassen, H. J. H. Clercx and G. J. F. van Heijst, Self-organization of decaying quasi-two-dimensional turbulence in stratified fluid in rectangular containers, J. Fluid Mech. 495, 19–33, (2003).

[6] F. Ravelet, L. Marié, A. Chiffaudel and F. Daviaud, Multistability and memory effect in a highly turbulent flow: experimental evidence for a global bifurcation, Phys. Rev. Lett. 93, 164501, (2004).

[7] M. I. Freidlin and A. D. Wentzell, Random perturbations of dynamical systems, 2nd ed. Springer, New York, (1998).

[8] F. Bouchet and H. Touchette, Non-classical large deviations for a noisy system with non-isolated attractors, J. Stat. Mech. P05028, (2012).

4.4 Thursday

An introduction to particle rare event simulation

Pierre Del Moral
Inria Bordeaux Sud-Ouest, France

The many faces of percolation

Peter Grassberger
University of Calgary, Canada

A few years ago, percolation theory was considered a mature subject holding few surprises, but recent progress has changed this radically. While "classical" or "ordinary" percolation is a second order phase transition between long range connectivity and disconnectedness on diluted regular lattices or random graphs, examples have now been found where this transition can range from infinite order to first order. The latter is of particular importance in social sciences, where first order percolation transitions show up as a consequence of synergistic effects, and I will point out their close relationship with rough interfaces in condensed matter physics. Another case where first order percolation transitions show up is interdependent networks, although first claims about this have to be substantially modified – in some cases of interdependent networks the transition is second order but in a new universality class. The very notion of universality classes has been questioned for "Achleoptas processes", and blatant violations of universality has been observed in "agglomerative percolation", where it can be related to a symmetry breaking transition coinciding with the percolation transition.

Non-Stationary FFS: Simulating rare events in non-stationary systems

Pieter Rein ten Wolde
FOM Institute AMOLF, The Netherlands

We present a method, Non-Stationary Forward Flux Sampling, that allows efficient simulation of rare events in both stationary and non-stationary stochastic systems. The method uses stochastic branching and pruning to achieve uniform sampling of trajectories in phase space and time, leading to accurate estimates for time-dependent switching propensities and time-dependent phase space probability densities. It is suitable for equilibrium or non-equilibrium systems, in or out of stationary state, including non-Markovian or externally driven systems. We demonstrate the validity of the technique by applying it to a one-dimensional barrier crossing problem that can be solved exactly, and show its usefulness by applying it to the time-dependent switching of a genetic toggle switch.

Emergence of long range order in the XY model on diluted Small World Networks

Sarah De Nigris
Centre de Physique Theorique, Marseille, France

We study the XY model on diluted Small World networks, i.e Small World networks whose number of links scales with the system size $N_{links} \sim N^{\gamma}$ $1 < \gamma < 2$. Starting from the regular lattice topology, we first concentrate on the behaviour varying the dilution parameter γ: for low values, the system doesn't exhibit a phase transition; while for γ approaching 2 a second order transition of the magnetisation arises since the system is near the HMF regime. Hence $\gamma_c = 1.5$ appears to be a critical value: an energy range is observed in which the magnetisation shows important fluctuations and doesn't not seem reaching the equilibrium state. We then take in account the model on a Small World network: for the latter, we have chosen the Watts-Strogatz model, whose topology is parametrized by the rewiring probability p, 0<p<1. We performed microcanonical simulations of the dynamics and we highlight the presence of a second order phase transition appearing even for very low p values, when the topology is still near the regular lattice one. Moreover we observe a dependence of the critical temperature T_c on the rewiring probability.

[1] Dynamical processes on Complex Networks, A.Barrat, M.Barthelemy, A.Vespignani, Cambridge University Press, 2008

[2] Long-range Interactions and Diluted Networks, A.Ciani, D.Fanelli and S.Ruffo, Nonlinear Physical Science, Volume 0, Springer, 2011

Reconstructing free energy profiles from force spectroscopy experiments

Jasna Brujic
New York University, USA

Reconstructing free energy profiles is an important problem in bimolecular reactions, protein folding or allosteric conformational changes. Nonequilibrium trajectories are readily measured experimentally, but their statistical significance and relation to equilibrium system properties still call for rigorous methods of assessment and interpretation. Here we show protein folding trajectories of tandem ubiquitin molecules obtained using single molecule force-clamp spectroscopy. A calibrated constant force is applied to a single protein and its end-to-end length is monitored over time. Exposing a me- chanically stable protein to a high pulling force leads to the unfolding and extension of the polypeptide chain. Quenching the force to a lower value triggers the collapse of the protein from a fully extended state back to a collapsed state with the same end-to-end length as the folded extended length. We then reconstruct the free energy of the end-to-end length at the low force from recordings of these collapsing traces. More generally, we address the question of how to calculate the free energy in situations where the data available is a set of nonequilibrium trajectories that, after initiation, evolve freely until they reach a specific location where they are terminated.

Fluctuations and response in sensory systems

Massimo Vergassola
Institut Pasteur, Paris, France

The statistics of fluctuations in biological sensing pathways and its relation to the response to environmental stimuli will be discussed. We shall specifically focus on bacterial chemotaxis, where detailed experiments and reliable models are available. A novel non-invasive experimental method to measure the chemotaxis response will first be presented. By using fluctuation relations, we then relate appropriate steady-state correlations to the response of the system to step and ramp stimuli of arbitrary amplitudes. That provides a systematic explanation for the observed relation between fluctuations and response, which strikingly combines linearity of the response with strong amplification gains as well as out-of-equilibrium with the apparently standard form of the fluctuation-dissipation relation.

Extreme value statistics: a renormalization group approach

Eric Bertin
Ecole normale supérieure de Lyon, France

The renormalization group transformation for extreme value statistics of independent, identically distributed variables, recently introduced to describe finite size effects, is presented here in terms of a partial differential equation (PDE). This yields a flow in function space and gives rise to the known family of Fisher-Tippett limit distributions as fixed points, together with the universal eigenfunctions around them. The PDE turns out to handle correctly distributions even having discontinuities. Remarkably, the PDE admits exact solutions in terms of eigenfunctions even farther from the fixed points. In particular, such are unstable manifolds emanating from and returning to the Gumbel fixed point, when the running eigenvalue and the perturbation strength parameter obey a pair of coupled ordinary differential equations. Exact renormalization trajectories corresponding to linear combinations of eigenfunctions can also be given, and it is shown that such are all solutions of the PDE. Explicit formulas for some invariant manifolds in the Fréchet and Weibull cases are also presented. Finally, the similarity between renormalization flows for extreme value statistics and the central limit problem is stressed, whence follows the equivalence of the formulas for Weibull distributions and the moment generating function of symmetric Lévy stable distributions.

[1] "Renormalization flow in extreme value statistics" E. Bertin, G. Györgyi, J. Stat. Mech. P08022 (2010)

[2] "Renormalization flow for extreme value statistics of random variables raised to a varying power" F. Angeletti, E. Bertin, P. Abry, J. Phys. A: Math. Theor. 45, 115004 (2012)

Stochastic thermodynamics of non-equilibrium steady states

Udo Seifert
University of Stuttgart, Germany

Stochastic thermodynamics provides a framework for describing small systems embedded in a heat bath that are externally driven to non-equilibrium. Examples are colloidal particles in time-dependent optical traps, single biomolecules manipulated by optical tweezers or AFM tips, and motor proteins driven by ATP excess. After briefly recalling the main established results of this approach for non-equilibrium steady states (NESSs) [1,2], I will report our recent progress for such systems concerning both a transparent general form of the fluctuation-dissipation theorem [3] and a fluctuation theorem for feedback-driven processes [4]. In a joint experimental-theoretical study, we have investigated the role of hidden slow degrees of freedom in the fluctuation theorem [5].

[1] U.S., Eur. Phys. J. B, 64, 423, 2008.
[2] U.S., Phys. Rev. Lett. 95, 040602, 2005.
[3] U.S. and T. Speck, EPL 89, 10007, 2010.
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Large deviations and amorphous order in glassy systems

Christopher Fullerton
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We investigate how large deviations of the dynamical activity are linked to dynamical phase transitions in a glass-forming binary mixture. We generate trajectories with low activity, which tend to occupy deep basins on the energy landscape. We use point-to-set correlations to characterise the amorphous order associated with these configurations, and discuss its relation to the stability of the inactive state.

[1] "Dynamic Order-Disorder in Atomistic Models of Structural Glass Formers" - L.O. Hedges, R.L. Jack, J.P. Garrahan, D. Chandler - Science 323 (5919) 1309-1313
[2] "Preparation and relaxation of very stable glassy states of a simulated liquid" - R.L. Jack, L.O. Hedges, J.P. Garrahan, D. Chandler - Phys. Rev. Lett. 107 (27) 275702

4.5 Friday

Reversals of a large-scale field generated over a turbulent background

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I consider systems in which a large scale field is generated in a turbulent flow. Several experimental examples are presented (in two-dimensional turbulence, in highly supercritical Rayleigh Benard convection or in magnetohydrodynamics) where the large scale field switches randomly between opposite states. These events amount to a reversal of the large scale field and are rare trajectories in the sense that the mean duration between reversals is very long compared to the characteristic time of velocity fluctuations. The involved mechanisms (excitability in the vicinity of a saddle-node bifurcation and crisis induced intermittency) are identified and presented.

Instantons in aggregation kinetics

Oleg ZABORONSKI
University of Warwick, UK

Large deviations analysis turns out to be a useful tool for studying non-equilibrium dynamics of systems of aggregating particles. In particular, for some classical aggregation kernels it is possible to solve the instanton equations exactly, and thus obtain a detailed description of fast gelation events.

Second-law like inequalities for transitions between non-stationary states

David LACOSTE
ESPCI, France

We discuss some consequences of a variant of the Hatano-Sasa relation in which a non-stationary distribution is used in place of the usual stationary one. We first show that this non-stationary distribution is related to a difference of traffic between the direct and dual dynamics. With this formalism, we extend the definition of the adiabatic and non-adiabatic entropies introduced by M. Esposito and C. Van den Broeck in Phys. Rev. Lett. 104, 090601 (2010) for the stationary case. We also obtain interesting second-law like inequalities for transitions between non-stationary states.

Inequalities generalizing the second law of thermodynamics for transitions between non-stationary states, G. Verley, R. Chétrite and D. Lacoste, Phys. Rev. Lett. in press (2012); http://arxiv.org/abs/1202.1161

Modified fluctuation-dissipation theorem for general non-stationary states and application to the Glauber-Ising chain, J. Stat. Mech. (2011) P10025

Level 2.9999... for a continuous-time Markov chain in 19.9999... minutes

Raphaël Chétrite

Laboratoire Jean Alexandre Dieudonné, Université de Nice Sophia-Antipolis, France

I will speak of an emerging project to go beyond Current (or Activity) in the large daviation analysis of physical systems. This results of a collaboration with Lorenzo Bertini, Alessandra Faggionato and Davide Gabrielli.

A justification and test for the statistical mechanics of trajectories

Mike Evans

University of Leeds, UK

This presentation reports the derivation of a far-from-equilibrium statistical-mechanical theory and its application to a nontrivial system with Newtonian interactions in continuous boundary-driven flow. Transition rates in continuously driven steady states (relevant to sheared complex fluids) can be derived by demanding that no information be used to describe it, other than the microscopic laws of motion and the macroscopic observables of the system. This implies that the non-equilibrium reservoir, to which the system is weakly coupled, is fully characterized by its mean energy and mean flux. This idea allows us to derive an ensemble of phase-space trajectories, and hence study the statistical mechanics of histories of the system.

Simulations of homopolymer collapse using forward-flux sampling

David Quigley

University of Warwick, UK

Simulations of crystallisation present a significant challenge to rare-event sampling methods. The free energy landscape can be extremely rugged, and the choice of reaction coordinate is fraught with potential pitfalls. In order to quantitatively explore some of the these issues, we have studied the globule to crystal transition in a minimalist model of a single homopolymer chain [1]. For certain parameter ranges, the free energy barrier to crystallisation is small and we are able to compute crystallisation rates via brute-force simualtions. For large barriers we employ the Forward-Flux sampling method of Allen et al [2], computing both the forward and backward rate as a function of temperature. In both cases we observe a systematic discrepancy between the temperature at which the two rates balance, and the thermodynamic transition temperature. We attribute this to a breakdown of the two state model implicit in such simulations, due to large barriers between the many possible realisations of the crystal state. Finally, our sampled transition trajectories lead us to propose an alternative reaction coordinate for this system based on eigenvalues of the contact matrix.

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5 Posters

Current fluctuations in the two-dimensional zero-range process

Rodrigo Villavicencio-Sanchez
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We study the zero-range process on a diamond lattice and show it allows the formation of current loops. These have been related to the breakdown of the Gallavotti-Cohen fluctuation relation. Additionally, we study a two-dimensional square lattice with open boundaries in the x-direction and periodic boundary conditions in the y-direction. We use both a microscopic and a hydrodynamic approach to calculate the rate function of particle current fluctuations. For large system sizes, our analysis lets us test the convergence to the recently proposed isometric fluctuation relation [Hurtado et al., PNAS 108, 7704 (2011)].

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The calcium-induced chain-chain association in the polyuronate systems: a transition path sampling study

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The calcium-induced formation of strong, hydrophilic gels is the important feature of polyuronates, connected with most of their practical applications [1,2]. The molecular details of gelling process dynamics were studied by the transition path sampling method and the standard molecular dynamics simulations [2]. The focus was on the poly(α-L-guluronate) systems, treated as the representative for all polyuronate-containing systems. The results allowed for identifying several distinct local minima of the free energy lying on the transition paths and visited by the system during the process of chain-chain association. These minima usually correspond to the intermediate structures in which the water molecules bridge calcium ion and carboxyl groups ('loose', i.e. solvent-separated binding of calcium ions). The crossing of the highest free energy barriers is associated with the significant perturbation of the water molecules arrangement within the first coordination sphere of the calcium ion.

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Towards order parameter prediction from molecular dynamics simulations in proteins

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A molecular understanding of how protein function is related to protein structure will require an ability to understand large conformational changes between multiple states. Unfortunately these states are often separated by high free energy barriers and within a complex energy landscape. This makes it very difficult to reliably connect, for example by all-atom molecular dynamics calculations, the states, their energies and the pathways between them. A major issue needed to improve sampling on the intermediate states is an order parameter – a reduced descriptor for the major subset of degrees of freedom – that can be used to aid sampling for the large conformational change. We present a novel way to combine information from molecular dynamics using non-linear time series and dimensionality reduction, in order to quantitatively determine an order parameter connecting two large-scale conformationally distinct protein states. This new method suggests an implementation for molecular dynamics calculations that may dramatically enhance sampling of intermediate states.

Keywords: order parameter, transfer entropy, protein conformational change

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