Rencontre « calcul des événements rares", au laboratoire de physique de l'ENS-Lyon, le jeudi 23 juin 2011.

Meeting « Computation of rare events », Laboratoire de Physique-ENS-Lyon, Thursday, June, 23rd 2011.

Cette rencontre se déroulera au Centre Blaise Pascal et est soutenue par le GDR Phénix.

But de la rencontre:

La dynamique des systèmes complexes, comme par exemple ceux rencontrés en mécanique des fluides, en physique du solide, en chimie, en océanographie, dans les sciences du climat ou dans de nombreuses autres sciences de la nature, mettent souvent en jeu plusieurs échelles, à la fois temporelles et spatiales. Dans ces systèmes, il est commun que de nombreux phénomènes microscopiques désordonnés et de faible intensité se conjuguent pour produire des événement observables à une échelle macroscopique. Une telle conjugaison est souvent très rare à l'échelle de temps microscopique où se situe la simulation numérique. Elle est donc très peu probable à cette échelle. Elle produit cependant des effets qui sont les phénomènes fondamentaux du ce système à l'échelle macroscopique. Citons comme exemples les changement de conformation (état de transition, transition) d'une molécule complexe ou d'un polymère, les passage d'une phase à une autre dans une situation de transition de phase (physique du solide, magnétisme, …), les transitions d'un attracteur à un autre pour un système turbulent (changement de polarité du champ magnétique terrestre, changement de régime en météorologie ou pour le climat, bistabilité du courant océanique Kuroshio, etc …).

Observer et comprendre ces phénomènes est donc essentiel. Cependant, étant donné la hiérarchie d'échelles de temps, ceci demeure en général impossible par une simulation numérique directe ou une simulation de dynamique moléculaire. Le but de ce groupe de travail est de discuter les méthodes théoriques ou numériques dont le but est spécifiquement le calcul de trajectoires rares. Des méthodes classiques ont récemment été remise au gout du jour et de nombreuses nouvelles méthodes sont apparues (méthodes "go with the winner", multilevel splitting, méthodes Monte Carlo, calcul d'instantons, minimum d'action, transition path sampling, etc).

Le but général de ce groupe de travail informel est d'essayer de comparer différentes méthodes, leurs intérêts et limitations respectifs. Les discussions seront nourries par les expériences de chacun.

Ce groupe de travail était initialement prévu pour une audience limitée, mais nous avons été encouragés à en faire la publicité. Ceci explique cette annonce tardive. Nous serions heureux d'accueillir toute personne intéressée. Si vous êtes intéressés par la thématique mais si cette annonce arrive trop tard, nous vous proposons de nous le faire savoir pour de futures rencontres.

Program:

Talks: 40 minutes + questions

9h45-10h00 Welcome, coffee and tee at « cafétéria du LR6 », ENS-Lyon

10h00-10h05 Introduction (Freddy Bouchet)

10h05-10h50 *Hugo Touchette.*
Recent results and open problems in large deviation theory.

10h50-11h35 *Julien Tailleur.*
Probing rare trajectories with Lyapunov weighted dynamic.

11h35-12h20 *Arnaud Guyader.*
Rare Event Simulation for Digital Watermarking and Molecular Dynamics.

12h20-13h20 Lunch

13h20-14h05 *Paul Maneville*
Growth/decay of turbulent bands in transitional plane Couette flow: a Large-Deviations problem?

14h05-14h50 *Oleg Zaboronsky*
Gelation in Aggregation as a Large Deviations phenomenon

14h50-15h20 *Laurent Chevillard.*
Rare events and non Gaussian fluctuations in fluid turbulence.

15h20-15h30 Break

15h30-16h15 *Jorge Kurchan.*
TBA.

16h15-17h00 *Jason Laurie, Mani Mathur and Freddy Bouchet.*
Bistability in turbulent flows: experimental results and theory using instanton and large deviation theory.

17h00 Discussion and end.

ABSTRACTS

Laurent Chevillard (ENS-Lyon)

Title: Rare events and non Gaussian fluctuations in fluid turbulence.

Arnaud Guyader (INRIA et université de Rennes)

Title: Rare Event Simulation for Digital Watermarking and Molecular Dynamics

Abstract: This work is divided in two parts. The first part is devoted to the presentation of a new algorithm in a static case. Namely, let X be a random vector with distribution μ on $\R^d$ and Φ be a mapping from $\R^d$ to $\R$. That mapping acts as a black box, e.g., the result from some computer experiments for which no analytical expression is available. In this framework, we propose an efficient algorithm to estimate a tail probability given a quantile or a quantile given a tail probability. It proceeds by successive elementary steps, each one being based on Metropolis-Hastings algorithm. The algorithm improves upon existing multilevel splitting methods and can be analyzed using Poisson process tools that lead to exact description of the distribution of the estimated probabilities and quantiles. The performance of the algorithm is demonstrated on a problem related to digital watermarking. This is a joint work with Nick Hengartner and Eric Matzner-Lober.

The second part focuses on the application of this algorithm in a dynamical case, more precisely in a molecular dynamics context. We will consider $\R^d$ as the space of configurations for a chemical system, where the probability of a configuration x is given by the Gibbs measure $\mu(dx)=\frac{1}{Z}\exp(-\beta V(x))dx$, where Z is the normalizing constant, β a temperature parameter, and V a known potential. The dynamics of the system is given by an overdamped Langevin (or gradient) equation. The problem is to find how the system can evolve from a local minimum of V to another, following the above dynamics. We will show on an example how our proposed adaptive splitting technique can be used in this setting not only to compute the rare event occurring rate, but also how the sampled paths, as they follow the true distribution of the rare paths, can be used to derive fine properties of the system. This is a joint work with Frédéric Cérou, Tony Lelièvre and David Pommier.

Jason Laurie (ENS-Lyon), Manikandan Mathur (LEGI Grenoble) and Freddy Bouchet (ENS-Lyon)

Title: Bistability in turbulent flows: experimental results and theory using instanton and large deviation theory

Abstract: Many examples of turbulent flows exhibit bistability behavior: the flow switches randomly from one attractor to the other. Examples range from geophysical flows (change of the Earth Magnetic field polarity, Milankovich cycles, Kuroshio bistability, …), experiments (Rayleigh-Besnard, Couette flows, rotating tank experiments, and so on …).

We will present recent theoretical prediction together with experimental and numerical study of such bistability phenomena in two dimensionnal and rotating tank experiments (Coriolis turntable).

We will present ongoing theoretical works using path integral representation (Onsager-Machlup formalism) and instanton theory, in order to compute the rare trajectories that lead from one of these states to the other, and the related transition probabilities.

Paul Maneville (LADHYX, Ecole Polytechnique)

Title: Growth/decay of turbulent bands in transitional plane Couette flow: a Large-Deviations problem?

Abstract: Plane Couette flow experience a subcritical transition to turbulence characterized with the coexistence of turbulent and laminar flow in a whole range of Reynolds numbers [Rg;Rt]. Above Rt, turbulence is uniform in space. Below Rg, turbulence decay within a nite time.
I shall present my on-going work in wide aspect-ratio systems using Direct Numerical Simulations of the Navier{Stokes equations. I shall focus on the decay of bands for R . Rg and the growth of bands from a turbulent germ of limited extension. It will be observed that the decay involves two main processes, (i) band breaking which corresponds to the nucleation of a wide enough laminar gap, and (ii) continuous band-segment withdrawal. On the other hand, growth from a germ for R & Rg result from (i) the nucleation of oppositely-oriented turbulent band segments and (ii) continuous band-segment growth.
All these processes are guessed to stem from the fact that, for R < Rt, local chaotic dynamics is vigorous enough to establish itself during su"ciently long periods of time and be able to contaminate the system (Pomeau's idea of percolation), while subcriticality implies a nucleation step (Pomeau's analogy with rst order thermodynamic phase transition). Nucleation of either the laminar gaps of the turbulent segments, depending on whether decay or growth is studied, appears to result from the accumulation of small scale (local) chaotic processes, while large scale flows around turbulent areas somehow come and complicate the analysis.

Hugo Touchette (Queen Mary College – London)

Title: Recent results and open problems in large deviation theory

Abstract: The goal of this informal talk is to encourage an exchange of ideas between statistical mechanics and large deviation theory. In the first part of the talk, I will give a quick overview of some recent results obtained in the statistical mechanics of equilibrium long-range systems and driven nonequilibrium systems, which have been inspired by large deviation techniques. In the second part, I will then discuss a number of open problems in statistical mechanics which, in my opinion, would benefit from being tackled from a large deviation point of view. I will also discuss an important problem in large deviation theory, namely that of numerically estimating large deviation rate functions, and will argue that statistical mechanics has a lot to offer in this problem in terms of techniques and ideas.

Julien Tailleur (Paris)

Title: Probing rare trajectories with Lyapunov weighted dynamics

Abstract: Along the transition from order to chaos, atypical structures like the first chaotic regions to appear, or the last regular islands to survive, play a crucial role in many physical situations. For instance, resonances and separatrices determine the fate of planetary systems, and localised objects like solitons and breathers provide mechanisms of energy transport in nonlinear systems. Unfortunately, most of the numerical methods to locate these 'rare' trajectories are confined to low-dimensional or toy models, while the realms of statistical physics, chemical reactions, or astronomy are still hard to reach. I will present a method, based on large deviation theory, that allows one to work in higher dimensions by selecting trajectories with unusual chaoticity. As an example, I will show that, for the Fermi-Pasta-Ulam nonlinear chain in equilibrium, the algorithm rapidly singles out the soliton solutions when searching for trajectories with low level of chaoticity, and chaotic-breathers in the opposite situation .

Oleg Zaboronsky (Warwick University)

Title: Gelation in Aggregation as a Large Deviations phenomenon

Abstract: We show how to calculate the probabilities of extremely slow or fast complete gelation events for the system of aggregating particles by solving the instanton equations.