Workshop Program

26 mai 2023

Wednesday 31st May

13h-13h30 : Registration and welcome
13h30-14h30 : Pierre Monmarché
14h30-15h30 : Martin Slowik
15h30-16h : coffee break
16h-17h : Benjamin Jourdain
17h-18h : Simone Baldassarri

Thursday 1st June

9h-10h : Boris Nectoux
10h-11h : Michela Ottobre
11h-11h30 : coffee break
11h30-12h30 : Giovanni Conforti
12h30-14h : Lunch
14h-15h : Freddy Bouchet
15h-16h : Ashot Aleksian
16h-16h30 : coffee break
16h30-17h30 : Tony Lelièvre
19h30 : Dinner at "Grand Café Foy", place Stanislas (Nancy)

Friday 2nd June

9h-10h : Fabien Panloup
10h-11h : Hong Duong
11h-11h30 : coffee break
11h30-12h30 : Julien Reygnier
12h30 : Closure of the workshop and lunch

Titles and abstract

Ashot Aleksian : Exit-time for Self-interacting and other non-linear diffusions.

In this talk, we discuss the exit-time of a Self-interacting diffusion from an open domain G in R^d. We focus on the behavior of the exit-time from the domain of attraction of potentials as the noise level, σ, tends to zero. The main process of interest, so-called Self-interacting diffusion (SID), is defined by the SDE

$$dX_t = -(\nabla V(X_t) + 1/t \int_0^t \nabla F(X_t - X_s) ds) dt + \sigma dW_t$$

and does not possess a Markov property, which makes it impossible to use the standard methods to resolve the exit-time problem in this case. We present the Large Deviation Principle for Self-Interacting Diffusions with generalized initial conditions and how this property aids in controlling non-linearity and non-Markovianity up until the exit-time. The main result of the study is the establishment of Kramers' type law for the exit-time, given rather weak assumptions on potentials V and F and domain G. In the end of the talk, we will discuss how the techniques developed in this work, which are an adaptation of the Freidlin-Wentzell theory for SID, can be used to solve exit-time problems for other non-Markov and/or non-linear processes. This is the joint work with A. Kurtzmann and J. Tugaut.

Simone Baldassarri : Droplet dynamics in a two-dimensional rarefied gas under Kawasaki dynamics

We study a lattice gas subject to Kawasaki dynamics at inverse temperature $\beta > 0$ in a large finite box $\Lambda_\beta \subset \mathbb{Z}^2$. Each pair of neighbouring particles has a negative binding energy $-U < 0$, while each particle has a positive activation energy $\Delta > 0$. The initial configuration is drawn from the grand-canonical ensemble restricted to the set of configurations where all the droplets are subcritical. Our goal is to describe, in the metastable regime $\Delta \in (U, 2U)$ and in the limit as $\beta \to \infty$, how subcritical droplets form and dissolve when the volume is moderately large, namely $|\Lambda_\beta| = e^{\theta\beta}$ with $\Delta < \theta < 2\Delta - U$. We will see that the evolution of the gas consists of droplets wandering around on multiple space-time scales in a way that can be captured by a coarse-grained Markov chain on a space of droplets.

This is a joint work with Alexandre Gaudillière, Frank den Hollander, Francesca Romana Nardi, Enzo Olivieri and Elisabetta Scoppola.

Freddy Bouchet

Giovanni Conforti : On the exponential convergence of Sinkhorn algorithm

Over the last decade, the entropic optimal transport (EOT) problem has emerged as a computationally more tractable proxy for the classical optimal transport problem. The successful applications of EOT in statistical machine learning is in large part due to the fact that optimisers can be computed by means of Sinkhorn's algorithm, whose convergence is expected to be exponential in the number of iterations. The aim of this talk is to give an introduction to the EOT problem and Sinkhorn's algorithm and to present a probabilistic approach based on coupling arguments and stochastic control to prove its convergence that allows to obtain the first exponential convergence results for quadratic costs.

Joint work with Alain Durmus and Giacomo Greco.

Hong Duong : Asymptotic analysis for the generalized Langevin equation with singular potentials

We consider a system of interacting particles governed by the generalized Langevin equation (GLE) in the presence of external confining potentials, singular repulsive forces, as well as memory kernels. Using a Mori-Zwanzig approach, we represent the system by a class of Markovian dynamics. Under a general set of conditions on the nonlinearities, we study the large-time asymptotics of the multi-particle Markovian GLEs. We show that the system is always exponentially attractive toward the unique invariant Gibbs probability measure. The proof relies on a novel construction of Lyapunov functions. We then establish the validity of the small mass approximation for the solutions by an appropriate equation on any finite-time window. Important examples of singular potentials in our results include the Lennard-Jones and Coulomb functions.

This talk is based on a joint work with D. H. Nguyen (UCLA).

Benjamin Jourdain : Central limit theorem for nonlinear functionals of empirical measures and fluctuations of mean-field interacting particle systems

In this work, we prove a generalised version of the central limit theorem for nonlinear functionals of the empirical measure of i.i.d. random variables, provided that the functional satisfies some regularity assumptions for the associated linear functional derivative. We use this result to deal with the contribution of the initialisation in the convergence of the fluctuations between the empirical measure of interacting diffusions and their mean-field limiting measure, when the dependence on measure is nonlinear. A complementary contribution related to the time evolution is treated using the master equation, a parabolic PDE involving L-derivatives with respect to the measure component, which is a stronger notion of derivative that is nonetheless related to the linear functional derivative.

This is a joint work with Alvin Tse.

Tony Lelièvre : From Langevin dynamics to kinetic Monte Carlo : mathematical foundations of accelerated dynamics algorithms

We will discuss models used in classical molecular dynamics, and some mathematical questions raised by their simulations. In particular, we will present recent results on the connection between a metastable Markov process with values in a continuous state space (satisfying e.g. the Langevin or overdamped Langevin equation) and a jump Markov process with values in a discrete state space. This is useful to analyze and justify numerical methods which use the jump Markov process underlying a metastable dynamics as a support to efficiently sample the state-to-state dynamics (accelerated dynamics techniques à la A.F. Voter). It also provides a mathematical framework to justify the use of transition state theory and the Eyring-Kramers formula to build kinetic Monte Carlo or Markov state models.

References :

- G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux, Jump Markov models and transition state theory : the Quasi-Stationary Distribution approach, Faraday Discussion, 195, 2016.
- G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux, Sharp asymptotics of the first exit point density, Annals of PDE, 5(1), 2019.
- T. Lelièvre, Mathematical foundations of Accelerated Molecular Dynamics methods, In : W. Andreoni and S. Yip (Eds), Handbook of Materials Modeling, Springer, 2018.
- T. Lelièvre, D. Le Peutrec, and B. Nectoux, Eyring-Kramers exit rates for the overdamped Langevin dynamics : the case with saddle points on the boundary, https ://hal.archives-ouvertes.fr/hal-03728053.
- T. Lelièvre, M. Ramil, and J. Reygner, Quasi-stationary distribution for the Langevin process in cylindrical domains, part I : existence, uniqueness and long-time convergence, Stochastic Processes and their Applications, 144, 176-201, (2022).

Pierre Monmarché : Mean Field kinetic processes and numerical schemes

We consider the question of sampling Gibbs measure with mean-field potential using numerical scheme of Hamiltonian Monte Carlo or Langevin type. We will present non-asymptotic bounds in relative entropy with the correct linear scaling in the number of particles and a second-order accuracy in the step size (this is a joint work with Evan Camrud, Alain Durmus and Arnaud Guillin). We will also discuss on toy models the effect of the mini-batching method on phase transitions.

This is a joint work with Arnaud Guillin and Pierre Le Bris.

Boris Nectoux : Metastable behavior of some non-reversible diffusions in a bounded domain

In this talk, we provide sharp asymptotic equivalents of the mean exit time from a bounded domain for some non reversible elliptic diffusions in the zero white noise limit. The precise asymptotic behaviors of the law of the exit time and of the principal eigenvalue are also derived. The main novelty follows from the fact that, simultaneously, the diffusion is non reversible and the associated deterministic flow has equilibrium points on the boundary of the metastable domain.

This is a joint work with D. Le Peutrec (Orléans) and L. Michel (Bordeaux).

Michela Ottobre : Non mean-field Vicsek type models for collective behaviour

We consider Interacting Particle dynamics with Vicsek type interactions, and their macropscopic PDE limit, in the non-mean-field regime ; that is, we consider the case in which each particle/agent in the system interacts only with a prescribed subset of the particles in the system (for example, those within a certain distance). It was observed by Motsch and Tadmore that in this non-mean-field regime the influence between agents (i.e. the interaction term) can be scaled either by the total number of agents in the system (global scaling) or by the number of agents with which the particle is effectively interacting at time t (local scaling). We compare the behaviour of the globally scaled and the locally scaled system in many respects ; in particular we observe that, while both models exhibit multiple stationary states, such equilibria are unstable (for certain parameter regimes) for the globally scaled model, with the instability leading to travelling wave solutions, while they are always stable for the locally scaled one.

Based on work with with P. Butta, B. Goddard, T. Hodgson, K.Painter.

Fabien Panloup : Asymptotically unbiased approximation of the QSD of diffusion processes

We build and study a recursive algorithm based on the occupation measure of an Euler scheme with decreasing step for the numerical approximation of the quasistationary distribution (QSD) of an elliptic diffusion in a bounded domain. We prove the almost sure convergence of the procedure for a family of redistributions and show that we can also recover the approximation of the rate of survival and the convergence in distribution of the algorithm. This last point follows from some new bounds on the weak error related to diffusion dynamics with renewal.

This is a joint work with Julien Reygner.

Julien Reygnier : Estimation of statistics of transitions and Hill relation for Langevin dynamics

In molecular dynamics, statistics of transitions, such as the mean transition time, are macroscopic observables which provide important dynamical information on the underlying microscopic stochastic process. They can, for example, describe conformational changes in proteins. A direct estimation using simulations of microscopic trajectories over long time scales is typically computationally intractable in metastable situations.

The first part of the presentation will introduce an identity that allows to express reaction statistics in terms of quantities that can be easily sampled using existing rare event algorithms. This identity is sometimes attributed to Hill in the physical literature. From a mathematical perspective, it can be seen as a result of potential theory.

In the second part, the specific case of systems modelled by Langevin dynamics will be examined. In particular, it will be shown how this model enables the explicit computation of the measure under which to initialise the simulation of rare events, providing a complete numerical method that is relatively simple and hopefully efficient for computing reaction statistics.

This is a joint work with T. Lelièvre and M. Ramil.

Martin Slowik : Metastability of Glauber dynamics with inhomogeneous coupling disorder

Metastability is a phenomenon that occurs in the dynamics of a multi-stable non-linear system subject to noise. It is characterised by the existence of multiple, well separated time scales. The talk will be focused on the metastable behaviour of a general class of mean-field-like spin systems with random couplings that evolve according to a Glauber dynamics at fixed temperature. This class of systems comprises both the Ising model on inhomogeneous dense random graphs and the randomly diluted Hopfield model. Assuming that the corresponding system in which the random couplings are replaced by their averages is metastable I will explain how the metastability of the random system is implied with high probability. In particular, I will discuss the tail behaviour of the relevant metastable hitting times of the two systems and the moments of their ratio.

This is joint work with A. Bovier, F. Den Hollander, S. Marello and E. Pulvirenti.