Ecole Doctorale des Sciences Fondamentales

Title of the thesis: Metastable and active systems through a piecewise deterministic Markov process prism

Supervisor : Arnaud Guillin and Manon Michel
Laboratory : Laboratoire de Mathématiques Blaise Pascal
University : Université Clermont-Auvergne
Email and Phone : arnaud.guillin@uca.fr (04 73 40 70 90) manon.michel@uca.fr (04 73 40 70 88) Possible co-supervisor :
Laboratory :

Summary :

Motivation: Complete understanding of the vast majority of physical, chemical and biological processes requires a fine knowledge of the underlying dynamics. At equilibrium, a complex system is described at the mesoscopic level by the probability distribution to find it into one of its numerous microscopic configurations. It then exhibits a stochastics dynamics which comes down to a random walk over an energetic landscape. In the context of high-dimensional multimodal distributions, these stochastic dynamics are however difficult to simulate as they remain trapped in certain areas of the phase space over a long time before exhibiting a transition to another metastable mode, corresponding to a different macroscopic state (e.g. protein conformation, polymer melting). Methods to accelerate these simulations or to infer directly from the energy landscape the dynamics, or important dynamics quantities as transition times, need to be improved or developed [1, 2], which requires a robust theoretical framework [3, 4]. On another hand, outside of equilibrium, as under an external driving, an atomistic description at equilibrium will not even be sufficient to characterize the full properties of a given system, as for example transport coefficients or thermal conductivity. These out-of-equilibrium behaviors can not be a priori framed into the usual static equilibrium description based on stationary probability distributions, while the number of involved degrees of freedom makes it intractable to derive the exact equations ruling those complex systems. The theoretical understanding of these stochastic dynamics then remains far from complete and constitutes a current active field of research in mathematics and physics [5, 6]. This theoretical work is also strongly intertwined with numerical explorations [7], which have recently known important developments thanks to both a robust mathematical characterisation of commonly used heuristics and accelerations stemming from the introduction of the most recent methods used in statistical inference and machine learning [8].

Goal: This PhD thesis aims to use piecewise deterministic Markov processes (PDMP) to build a theoretical and numerical framework to describe metastable dynamics, quasistationarity, and active systems and, therefore, to potentially better characterize them. PDMP are processes described by ballistic trajectories whose directions are changed according to a Poisson process [9]. Simulation methods based on PDMP have been under a growing interest since their first appearance in physics and applications in Bayesian inference [10, 11]. In spite of the numerically-observed acceleration they bring [12], these novel simulation algorithms are still poorly theoretically understood and characterized [13]. This theoretical understanding is all the more crucial as these methods, based on dynamics which break the local equilibrium, could lead to new perspectives into the sampling of outof-equilibrium systems and their dynamics.

We then propose three research axes:

- Simulating metastable and active systems with PDMP: How to bias the non-reversible dynamics in PMDP to produce efficient metastable state sampling? How to exploit directly the out-of-equilibrium nature of the PMDP dynamics to study the system at hand? Which new theoretical tools (as in [14]) to develop to study metastability and quasistationarity for PDMP?
- Modeling active systems as PDMP: What are the conditions on the systems to admit a PDMP characterisation? What are the required properties of the dynamics to have a stationary distribution? How to infer dynamical quantities, as transition rates, in this framework?
- Enhancing equilibrium PDMP simulation: could the results obtained on out-of-equilibrium dynamics be used to accelerate PDMP simulations in a broader context, as in Bayesian inference? How to use topological information to adapt the dynamics on the fly?

Directeur : Pr Yanick HEURTEAUX
tél. 04.73.40.50.64
E-mail : yanick.heurteaux@uca.fr

Secrétariat : Lucie NAUD
tél. 04.73.40.53.76
E-mail : edsf.drv@uca.fr

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