

Metastable and active systems through a piecewise deterministic Markov process prism (Funded Master internship and PhD project via selective funding)

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 stochastic 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 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]. Simulations 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 out-of-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 PDMP to produce efficient metastable state sampling? How to exploit directly the out-of-equilibrium nature of the PDMP dynamics to study the system at hand?
- 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?

Environment: The PhD candidate will work at the Université Clermont-Auvergne and will be part of the interdisciplinary ANR project *Su.Sa*. This thesis lies in the interface between physics,

mathematics and computer science, will be supervised by Arnaud Guillin and Manon Michel from Laboratoire de Mathématiques Blaise Pascal (UMR 6620) and will join a local dynamics revolving around stochastic and learning algorithms for physics (high energy physics, cosmology, statistical and chemical physics) and stochastic process analysis (mean-field approach, metastability, optimal transport, functional inequalities).

Profile: We are looking for an enthusiastic individual with a clear interest in interdisciplinary research and a strong background either in probability and/or theoretical, computational and/or statistical physics to apply. The PhD position will be funded through the competitive selection of the École doctorale Sciences fondamentales (<https://sf.ed.uca.fr/>), will start in 2021 and remains open until filled. Interested candidates can contact Manon Michel (manon.michel@uca.fr) for more details. A funded internship taking place in the beginning of 2021 can precede the PhD and is encouraged.

Webpages:

Manon Michel's webpage: <http://manon-michel.perso.math.cnrs.fr>

Arnaud Guillin's webpage: <http://math.univ-bpclermont.fr/~guillin>

SuSa project's webpage: <https://anr-susa.math.cnrs.fr>

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