Metastability: a journey from stochastic processes to semi-classical analysis.

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The simulation of materials at the atomistic scale is widely employed in various scientific fields, including biology, chemistry, and material science. Full atomistic models, however, are computationally expensive as they require simulating a large number of atoms over extended time scales. A common approach to bridging the gap between full atomistic models and more coarse-grained descriptions is the use of Markov State Models parameterized by the Eyring-Kramers formulas. These formulas determine the hopping rates between local minima of the potential energy function, resulting in a Markov jump process that is significantly more efficient to simulate.
In this presentation, we will demonstrate how quasi-stationary distributions can provide a rigorous connection between full atomistic models and Markov jump processes between metastable states. Our analysis is grounded in spectral techniques and the semi-classical analysis of Witten Laplacians. Additionally, we will illustrate how these methods can be leveraged to develop efficient simulation algorithms for full atomistic models.
This is a joint work with G. Di Gesù, B. Nectoux and D. Le Peutrec.

References

[1] G. Di Gesù, TL, D. Le Peutrec, and B. Nectoux, Jump Markov models and transition state theory : the Quasi-Stationary Distribution approach, Faraday Discussion, 195, 469-495, (2016). TL, D. Le Peutrec, and B. Nectoux, Eyring-Kramers exit rates for the overdamped Langevin dynamics : the case with saddle points on the boundary, https ://arxiv.org/abs/2207.09284.

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