Time coarse-graining of stochastic processes and the Transition State Theory

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Langevin dynamics is used in many scientific fields to model the evolution of molecular systems. Thanks to results from statistical physics, macroscopic quantities of interest can be obtained by sampling such dynamics at the atomistic level. One major issue for the sampling of trajectories of the overdamped Langevin dynamics is the possible metastable behaviour of this dynamics. Metastability refers to the case when the typical time to observe transitions between some regions of the configuration space (which are called metastable regions) is much longer than the typical timestep for the discretization of the dynamics. For some applications transition times could be of the order of microseconds while the timestep is typically of the order of a few femtoseconds. By integrating naively this dynamics, most of the computational time is wasted to simulate vibrations within metastable states. This is also related to a sampling problem for trajectorial averages which approximate erg odic averages since it is difficult to visit the whole configuration space.

To deal with this issue, the Transition State Theory is usually used in several computational algorithms in order to accelerate the trajectorial sampling. Transition State Theory draws connections between the original overdamped Langevin dynamics and an underlying jump process between metastable states. I will present preliminary results to measure the accuracy of the transition State Theory. This relies on tools from semi-classical analysis and on the notion of Quasi Stationary Distribution.

Références

[1] Auteur, *Titre*, Editeur, année.

[2] Auteur, *Titre*, Revue, références, année.

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