

## Parallel Replica algorithm for Langevin dynamics and Adaptative Metadynamics

*vendredi 8 septembre 2023 12:30 (30 minutes)*

This talk will be divided into two independent parts. The first part shall focus on the extension of the formalization of an algorithm (Parallel Replica) to the case of the Langevin dynamics. Parallel Replica is used in material science to sample rare-events and consists in a parallelization in time of the sampling. It can be formalized using the notion of quasi-stationary distributions which can be seen as the local equilibrium reached by a dynamics when it remains trapped in a state for a long time. Due to the degeneracy of the Langevin dynamics, its existence was an open question until recently. In this talk we will provide an explicit control of the density of the Langevin process which allows us to obtain the existence of a QSD using well-known spectral results.

The second part of this talk shall focus on the sampling of the minimum energy path (MEP) between metastable states in a case where the MEP is locally orthogonal to the dynamics. In order to do that we will introduce Adaptative Metadynamics method with an augmented loss which takes into account the initial, final configuration as well as a penalization term for high energetic configurations.

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**Classification de Session:** Result Communication