

Quantification of coarse-graining error in overdamped/non-overdamped Langevin dynamics

Upanshu Sharma (Eindhoven University of Technology, The Netherlands)

Coarse-graining or dimension reduction is the procedure of approximating a large and complex system by a simpler and lower dimensional one. A key feature that allows for such an approximation is a choice to consider only part of information by means of a coarse-graining map ξ . Assuming that the configuration of the large system is governed by a stochastic differential equation, say random variable X_t (representing for instance the position of particles in the system), one can easily construct coarse-grained version $\xi(X_t)$ (e.g. a particular angle between some atoms of the molecule). However in practice this coarse-grained version is cumbersome to work with.

Starting from an overdamped/non-overdamped Langevin equation, an effective closed dynamics which approximates the coarse-grained dynamics $\xi(X_t)$ (under time-scale separation assumptions) will be presented. In addition estimates on the accuracy of the effective dynamics will be provided. This is joint work with A. Lamacz, M.H. Duong, M.A. Peletier and A. Schlichting.