Coarse - Graining of stochastic system

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Coarse-graining or model reduction techniques are widely used to extend the time scale of molecular and stochastic simulations by reducing the number of degrees of freedom. In molecular dynamics, standard coarse-graining methods approximate the potential of mean force to construct effective Markovian models. To gain insight into the accuracy and limitations of such reduced models, we firstly investigate the simple case of quadratic and perturbed harmonic energy landscapes in an overdamped Langevin setting. We derive and analyze a hierarchy of reduced stochastic models, demonstrating that while classical approaches capture equilibrium statistics accurately, they introduce systematic errors in dynamical quantities such as mean-squared displacement, even under large time-scale separation. The results can also be extended to the case of weakly nonlinear potentials with similar techniques used in the linear case.

This is joint work with Dr. Thomas Hudson, University of Warwick, UK.