A simple approach to reconstruct free energy, friction and mass profiles from short molecular dynamics trajectories

Fabio Pietrucci – Sorbonne Université, IMPMC, Paris

The dynamics of many-particle systems projected on one degree of freedom can be accurately modeled by Langevin equations. Despite of this, Langevin models of rare events are mostly invoked as conceptual or benchmark tools, with only a limited number of applications to specific systems in physics, chemistry or biology. The main reason is that existing model-optimization methods typically exploit very long ergodic MD trajectories, available only in small-barrier cases [1]. I will present numerical evidence indicating that a simple approach based on direct comparison of probability histograms can reconstruct an optimal Langevin model of a high-barrier process based only on ~100 short MD trajectories relaxing from the barrier top [2]. Free energy, friction, and mass profiles as a function of a collective variable can thus be recovered in a conceptually simple and computationally efficient way. The method is not limited to Markovian cases but it includes generalized Langevin equations, hence it could be applied to a broad range of processes going from conformational changes of biomolecules to crystal nucleation to chemical reactions in solution [3]. Furthermore, the possibility to obtain optimal Langevin models for different collective variables starting from the same set of MD data could be exploited in reaction coordinate optimization algorithms.

[1] C. Camilloni and F. Pietrucci, *Adv. Phys. X* 3, 1477531 (2018)
[2] A. Pérez-Villa and F. Pietrucci, *arXiv* 1810.00713 (2018)
[3] F. Pietrucci, *Rev. Phys.* 2, 32 (2017)