Effective dynamics for non-reversible stochastic differential equations
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Coarse-graining is central to reducing dimensionality in molecular dynamics, and is typically characterized by a mapping which projects the full state of the system to a smaller class of variables. While extensive literature has been devoted to coarse-graining starting from reversible systems, not much is known in the non-reversible setting. Starting with a non-reversible dynamics, we study an effective dynamics which approximates the (non-closed) projected dynamics. Under fairly weak conditions on the system, we prove error bounds on the trajectorial error between the projected and the effective dynamics. In addition to extending existing results to the non-reversible setting, our error estimates also indicate that the notion of mean force motivated by this effective dynamics is a good one.
Joint work with T. Lelièvre and U. Sharma (ENPC).