

The Adaptive Biasing Force algorithm with non-conservative forces

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The aim of molecular dynamics is to study the time-evolution of a microscopic system of N particles in order to deduce various of its macroscopic properties. To do so, one needs to sample the *Boltzmann-Gibbs measure* $\mu_V \propto \exp(-\beta V)$ where V is the system's potential energy and β is the thermodynamic beta. A classical process used in this scope is the overdamped Langevin dynamics:

$$dX_t = -\nabla V(X_t)dt + \sqrt{2\beta^{-1}}dW_t,$$

where $(W_t)_{t \geq 0}$ is a classical d -dimensional Brownian motion, and $\mathcal{F} = -\nabla V$ is the interaction force. A force which is the gradient of a potential energy V is said to be *conservative*. Note that from a PDE point of view, the law of the process $(X_t)_{t \geq 0}$ satisfies a nonlinear *Fokker-Planck* equation.

Such a process has good theoretical properties, but one practical issue arises, that of *metastability*: the system may remain trapped in potential wells for long periods of time, and the system's law's relaxation towards the equilibrium can be far too slow. In order to avoid metastability, one relies on a *reaction coordinate*, namely a function ξ of the position which gives a low-dimensional representation of the system. One can then consider the *Adaptive Biasing Force* (ABF) method [1,2], which consists in biasing the force \mathcal{F} in the direction of ξ , and prove the longtime convergence of the algorithm [3]. A nice property of the method is the *flat histogram property*: the energy landscape is flattened in the direction of ξ . In this talk, we will present a study of the ABF method's robustness with generic -possibly non-conservative- forces. We first ensure the flat histogram property still holds, then prove the existence of a stationary state, relying on generic bounds on the invariant probability measures of homogeneous diffusions [4]. Using classical entropy techniques [5], we eventually prove the longtime convergence of the algorithm.

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