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 be able 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 :

$$\mathrm{d}X_t = -\nabla V(X_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}W_t,$$

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 can rely on a *reaction coordinate*, namely a function ξ of the position which gives a low-dimensional representation of the system. Given this coordinate, one can then consider the *Adaptive Biasing Force* (ABF) method [3, 4], which consists in biasing the force $\mathcal{F}$ in the direction of ξ, with an adaptive bias B_t, and prove the longtime convergence –in a sense to be precised– of the algorithm [5]. One can also consider the *Projected Adaptive Biasing Force* (PABF) method, whose convergence has been proven in [1]. A good property of both methods 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 under generic –possibly non-conservative– forces. We first ensure the flat histogram property is satisfied in all cases. We then introduce a fixed point problem yielding the existence of a stationary state for both the ABF and PABF algorithms, relying on generic bounds on the invariant probability measures of homogeneous diffusions [2]. Using classical entropy techniques [6], we prove the exponential convergence of both biasing force and law of the process as time goes to infinity, for the two considered algorithms. We will eventually quickly present the work in progress regarding the implementation of the ABF method within the Tinker–HP software.

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