Weighted-ensemble Brownian dynamics simulation: Sampling of rare events in non-equilibrium systems

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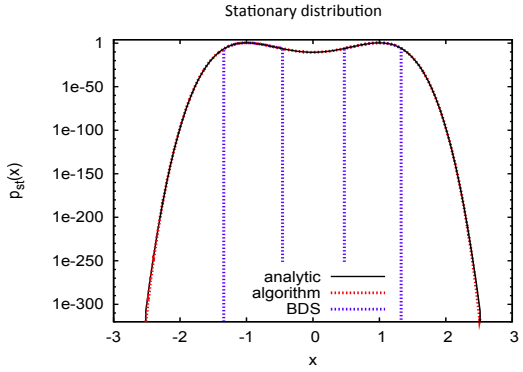
Rare events are ubiquitous in many biological, chemical and physical processes. Whereas the density of states is known in systems at thermal equilibrium, interesting phenomena often occur in non-equilibrium systems. Unfortunately, many such problems are inaccessible to analytic methods. Therefore computer simulations are a widely used tool to estimate the density of states or transition rates between them. Since standard Brownian dynamic simulation provides computational costs that are inversely proportional to the state's probability, specialized methods have to be used to adequately sample rare events, i.e. states with low probability or low transition rates.

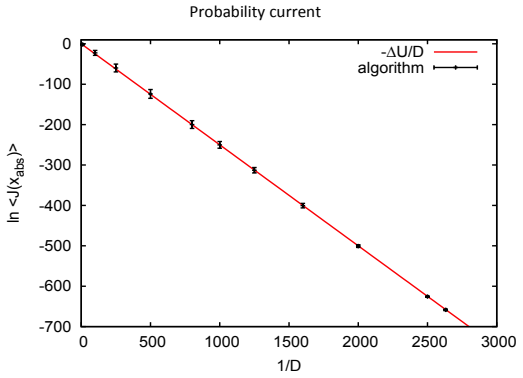
We have developed an algorithm[1], based on the previously developed weighted-ensemble (WE) Brownian dynamics simulations that allows one to calculate the stationary probability density function (SPDF) as well as transition rates between particular states. Like in WE simulations the space of interest is divided into several subregions and the probability for finding the system in them is calculated by generating equally weighted walkers in each region. By moving to the underlying dynamics, the walkers transport probability between the subregions. Thus, WE methods are usually applied to systems of Brownian particles moving in a potential landscape[2,3]. Our algorithm is based on WE Brownian dynamic simulations, but uses a uniform distribution of walkers within each subregion. In general the algorithm can be applied to arbitrary dynamical systems of the form:

$$\dot{x}_n = f_n(\mathbf{x}) + g_n(\mathbf{x})\xi_n(t),\ n = 1, ..., d, \qquad (1)$$

where d is the number of stochastic time-dependent degrees of freedom. We are interested in high precision sampling of the stationary probability current $J_{st}(\mathbf{x})$ and the SPDF $p_{st}(\mathbf{x})$ of finding the system in the d-dimensional cube $[x_1, x_1 + dx_1], \ldots, [x_d, x_d + dx_d]$.

Our method outperforms Brownian dynamics simulation by several orders of magnitude and its efficiency is comparable to weighted-ensemble Brownian dynamic simulations in all studied systems and lead to impressive results in regions of low probability and small rates. As an example, we show in the first figure the pdf computed for the classic double well potential $U(x) = -\frac{1}{2}x^2 + \frac{1}{4}x^4$ as well as, in the second figure, the verification of Kramers law for the probability current. Note that the vertical scale in both cases shows the high efficiency of the method in sampling low-probability events, as we are able to sample correctly events with probability of the order of 10^{-300} and currents of the order of 10^{-300}.





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