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Reconstruction of free energy profiles from fast non-equilibrium processes

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Often, gaining insight into the functioning of biomolecular systems requires to follow their dynamics along a microscopic reaction coordinate (RC) on a macroscopic time scale, which is beyond the reach of current all atom molecular dynamics (MD) simulations. A practical approach to this inherently multiscale problem is to model the system as a fictitious overdamped Brownian particle that diffuses along the RC in the presence of an effective potential of mean force (PMF) due to the rest of the system. By employing a small number of fast nonequilibrium MD simulations in both forward and time reversed directions we reconstruct the PMF: (1) of deca-alanine as a function of its end-to-end distance, and (2) that guides the motion of potassium ions through the gramicidin A channel. In both cases the computed PMFs are found to be in very good agreement with previous results obtained by different methods. Compared to these PMF calculation methods our approach is about one order of magnitude faster and, in addition, also provides the position dependent diffusion coefficient along the RC. Thus, by employing the computed PMF and diffusion coefficient in a suitable stochastic model we could estimate important characteristics of the studied systems, e.g., the mean folding time of the stretched deca-alanine and the mean diffusion time of the potassium ion through gramicidin A.