Weighted-Ensemble Brownian Dynamics Simulation

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It is difficult to determine high-energy conformations of proteins, because they are dynamic molecules that exist in high energy states for too short of a time to acquire laboratory data. The alternative for determining high-energy protein conformations outside the laboratory is through a dynamics simulation. Most algorithms for dynamics simulations are incapable of simulating a protein long enough to identify a protein's high energy conformation. However, Huber and Kim's weighted-ensemble Brownian (WEB) dynamics simulation surpasses its contemporary algorithms.

The WEB method makes such an improvement on the standard Brownian algorithm that it can produce the same length of real-time simulation as the standard Brownian method, but at a fraction of the computing time. In order to fully appreciate the advantage the WEB method provides over the standard Brownian algorithm, we wrote a small-scale WEB dynamics simulation in Perl that assessed particle movement in an one-dimensional, double-welled energy coordinate and compared our results to the theoretical data and the standard Brownian algorithm.