

PUSHING BACK THE FRONTIERS OF MOLECULAR DYNAMICS SIMULATIONS

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The free energy surface of a complex system is often characterized by the presence of deep minima separated by large barriers. Such minima correspond to distinct states of the system, and transitions among these minima reflect important changes such as phase transitions, chemical reactions and conformational modifications. Direct simulation of these processes is frustrated by the exponential dependence of the rate on the barrier height, and simulations often do not leave the free energy minimum from which they were started. In order to solve this problem we introduce a coarse-grained non-Markovian dynamics or metadynamics that can reconstruct the free energy dependence on a set of suitably defined collective coordinates. The metadynamics makes it possible to overcome large energy barriers in a modest amount of computer time. We illustrate the power of the method and demonstrate its ability to tackle a large variety of problems, from complex chemical reactions to structural phase transitions, and from the search for the lowest-lying minima to phase diagram calculations.