Protein folding simulations by enhanced sampling techniques

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The ultimate goal of the present work is to predict protein tertiary structures solely from the amino-acid sequence information by computer simulations of all-atom models.
It is widely believed impossible to achieve this with the conventional simulation methods. The difficulty in protein folding simulations comes from the fact that there exist an astronomically large number of local minima in the energy function of the protein systems, forcing any simulation to get trapped in one of the energy local minima. Novel algorithms that can alleviate the multiple-minima problem are thus in urgent demand. We have been advocating the uses of generalized-ensemble algorithms. With these algorithms we can explore wide range of the configurational space. The advantage of generalized-ensemble algorithms such as multicanonical algorithm and replica-exchange method lies in the fact that from only one simulation run, one can obtain not only the global-minimum state in energy but also various thermodynamic quantities as functions of temperature. In this talk, I will present some of the latest results of our protein folding simulations.