Generalized-ensemble algorithms for classical and quantum simulations

Yuko Okamoto

High Performance Computing Division, Information Technology Center
and
Global Engagement Center, International Affairs
Nagoya University, Nagoya, Aichi 464-8601, Japan

Conventional Monte Carlo and molecular dynamics simulations are greatly hampered by the multiple-minima problem, where the simulations tend to get trapped in some of astronomically large number of local-minimum energy states. In order to overcome this difficulty, we have been advocating the uses of generalized-ensemble algorithms which are based on non-Boltzmann weight factors (for reviews, see, e.g., Refs. [1-6] and for our recent algorithm developments and their applications, see, e.g., Refs. [7-17]). With these algorithms we can explore a wide range of the conformational space. The advantage of generalized-ensemble algorithms such as multicanonical algorithm and replica-exchange method (or, parallel tempering) lies in the fact that from only one simulation run, one can obtain various thermodynamic quantities as functions of temperature and other physical parameters such as pressure, etc. by the reweighting techniques. In this talk, I will present the latest results of our applications of generalized-ensemble simulations to complex systems.

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