

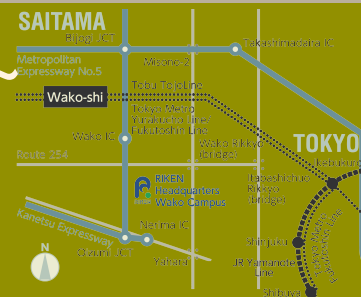


Enhanced sampling
techniques for spin and
biomolecular simulations

Prof. Yuko Okamoto
(Nagoya University)



September 16th (Tue.) 14:00 ~
Suzuki Umetaro Hall
RIKEN Wako campus



Conventional Monte Carlo (MC) and molecular dynamics (MD) simulations of complex systems are greatly hampered by the multiple-minima problem, where the simulations tend to get trapped in some of a huge 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. With these algorithms we can explore a wide range of the configurational space. The advantage of generalized-ensemble algorithms such as multicanonical algorithm (MUCA), simulated tempering (ST), and replica-exchange method (REM) lies in the fact that from only one simulation run, one can obtain various thermodynamic quantities as functions of temperature and other parameters of the system. Recently, we have given a general formulation for multidimensional MUCA, ST, and REM. In this talk, I will present the recent results of various applications of generalized-ensemble algorithms to complex systems.

The colloquium comprises
three short talks by the iTHES
members in addition to
Prof. Okamoto's lecture:

14:00- N. Yamanaka (iTHES-phys)

14:15- T. Shirakawa (iTHES-cond)

14:30- K. Maeda (iTHES-bio)

14:45- 15:00 break

15:00- Y. Okamoto (Nagoya)

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