第 11 回計算分子科学コロキウム

Enhancing classical and quantum molecular simulations with colored noise

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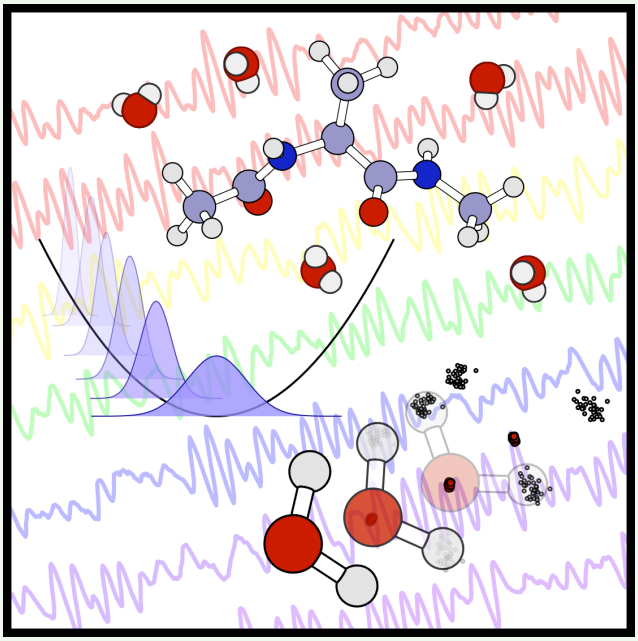
場所　　自然科学 5 号館　6 講



概 要

Langevin dynamics model the coupling of a Hamiltonian system to a bath by introducing a viscous friction term and a noisy force, which is modelled as white noise (not correlated in time). Introducing a history dependence in the friction and noise terms is not only crucial to model a physically realistic bath, but also opens up endless possibilities of fine-tune the sampling properties of molecular dynamics with unprecedented control. I will introduce the Generalized Langevin Equation formalism, and discuss how colored (correlated) noise can be used to manipulate atomistic simulations by increasing sampling efficiency, stabilizing multiple time step integrators, and controlling the extent of disturbance to the intrinsic dynamics. I will also briefly discuss how the same formalism can be used to obtain out-of-equilibrium simulations, which can be tuned to reproduce accurately the quantum mechanical behavior of atomic nuclei at a fraction of the cost of a conventional path integral molecular dynamics simulation.

問合せ先　数物科学類　計算科学コース
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