LAMMPS Brownian Dynamics

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1 Derivation

The motion of equation for Langevin Dynamics(LD) is the following

$$m\ddot{x} = f(x) - m\gamma\dot{x} + R(t)$$

where $\langle R(0)R(t)\rangle = 2kTm\gamma\delta(t)$. $\gamma = \zeta/m$ where ζ is the drag coefficient. If $\gamma = \zeta/m \to \infty$, the bath becomes infinitely dissipative. We can neglect acceleration part of the equation then

$$\dot{x} = \frac{1}{\gamma m}f(x) + \frac{1}{\gamma m}R(t) = \frac{1}{\gamma m}f(x) + R'(t)$$

where $\langle R'(0)R'(t)\rangle = (2kT/m\gamma)\delta(t)$.

The Euler integration for this equation is

$$x(t+\Delta t) - x(t) = \frac{\Delta t}{m\gamma}f(x) + \sqrt{\frac{2kT\Delta t}{m\gamma}}\omega(t) = \frac{\Delta t}{m\gamma}[f(x) + \sqrt{\frac{2kTm\gamma}{\Delta t}}\omega(t)]$$

This is the equation we implemented in *fix_langevin_overdamp.cpp* and *fix_nve_overdamp.cpp*.