13.2: Brownian Dynamics

The Langevin equation for the motion of a Brownian particle can be modified to account for an additional external force, in addition to the drag force and random force. From Newton's Second Law:

$$m\ddot{x} = f_d + f_r(t) + f_{ext}(t)$$

where the added force is obtained from the gradient of the potential it experiences:

$$f_{ext} = -\frac{\partial U}{\partial x} \tag{13.2.1}$$

With the fluctuation-dissipation relation $\langle f_r(t) f_r(t')\rangle = 2\zeta k_B T \delta(t-t')$, the Langevin equation becomes

$$m\ddot{x} + (\partial U/\partial x) + \zeta\dot{x} - \sqrt{2\zeta k_B T}R(t) = 0 \tag{13.2.2}$$

Here $R(t)$ refers to a Gaussian distributed sequence of random numbers with $\langle R(t)\rangle = 0$ and $\langle R(t)R(t')\rangle = \delta(t-t')$.

Brownian dynamics simulations are performed using this equation of motion in the diffusion-dominated, or strong friction limit $|m\ddot{x}| \ll |\zeta\dot{x}|$. Then, we can neglect inertial motion, and set the acceleration of the particle to zero to obtain an expression for the velocity of the particle

$$\dot{x}(t) = \frac{\frac{\partial U}{\partial x}}{\zeta} - \sqrt{2k_B T/\zeta}R(t)$$

We then integrate this equation of motion in the presence of random perturbations to determine the dynamics $x(t)$.

Readings

1. R. Zwanzig, Nonequilibrium Statistical Mechanics. (Oxford University Press, New York, 2001).
2. B. J. Berne and R. Pecora, Dynamic Light Scattering: With Applications to Chemistry, Biology, and Physics. (Wiley, New York, 1976).