Temperature and Pressure Controls

1 Constant Temperature Ensemble

One method is to use velocity scaling,

$$T_I = \frac{1}{3(N-1)} \sum_i m_i v_i^2 \quad (1)$$

$$\gamma = \sqrt{T/T_I} \quad (2)$$

$$\tilde{\mathbf{v}}_i = \gamma \mathbf{v}_i \quad (3)$$

The Nose-Hoover method for uses a dynamic "friction coefficient," ξ.

$$\mathbf{a_i} = \frac{1}{m_i}\mathbf{F}_i - \xi \mathbf{v}_i \quad (4)$$

$$\frac{d\xi}{dt} = \frac{1}{Q}(T_I - T) \quad (5)$$

2 Constant Pressure Ensemble

A constant pressure ensemble can be simulated by introducing tensor $\bar{L}$ for the box size. The physical position $\mathbf{r}$ of a particle is given by $r_\alpha = \sum_{\beta=1}^{3} L_{\alpha\beta} x_\beta$, where $\mathbf{a}$ is the dimensionless coordinate of the particle, with $0 \leq a_\alpha \leq 1$. The volume of the box is the determinant of $\bar{L}$, $\Omega = \det(\bar{L})$. For a pressure P, the equations of motion are

$$\frac{d^2\mathbf{r}}{dt^2} = \frac{1}{m_i}\mathbf{F}_i - (\bar{L}^T)^{-1} \frac{d\bar{L}^T}{dt} \frac{d\mathbf{r}}{dt} \quad (6)$$

$$\omega \frac{d^2\bar{L}}{dt^2} = (\bar{\pi} - p\bar{I})\Omega(\bar{L}^T)^{-1} \quad (7)$$

$$\bar{\pi} = \frac{1}{\Omega} \sum_i (m_i(\dot{\mathbf{r}}_i \dot{\mathbf{r}}_i) - \mathbf{r}_i \nabla_i V) \quad (8)$$

where $\bar{\pi}$ represents the internal shear.