1 Constant Temperature Ensemble

One method is to use velocity scaling,

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

\[ \gamma = \sqrt{T/T_I} \] (2)

\[ \dot{v}_i = \gamma v_i \] (3)

The Nose-Hoover method uses a dynamic “friction coefficient,” \( \xi \).

\[ a_i = \frac{1}{m_i} F_i - \xi v_i \] (4)

\[ \frac{d\xi}{dt} = \frac{1}{Q} (T_I - T) \] (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

\[ \frac{d^2 \mathbf{r}}{dt^2} = \frac{1}{m_i} F_i - (\bar{L}^T)^{-1} \frac{d\bar{L}^T}{dt} \frac{d\mathbf{r}}{dt} \] (6)

\[ \omega \frac{d^2 \bar{L}}{dt^2} = (\bar{\pi} - p\bar{l}) \Omega (\bar{L}^T)^{-1} \] (7)

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

where \( \bar{\pi} \) represents the internal shear.

\( \odot D. M. Ceperley 2000 \)