Velocity Rescaling Method for Temperature Control in MD Simulations

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1 Algorithm

The velocity rescaling method algorithm is as follows:

1. **Initialize:** Assign initial velocities to particles based on the Maxwell-Boltzmann distribution for a given temperature T_{initial}.

2. **Calculate Kinetic Energy:** At each time step t, compute the current kinetic energy of the system:

$$E_{\text{kinetic}}(t) = \frac{1}{2} \sum_{i=1}^{N} m_i v_i^2(t)$$

   where m_i is the mass and $v_i(t)$ is the velocity of particle i, and N is the total number of particles.

3. **Compute Target Kinetic Energy:** Based on the desired temperature T_{target}, the target kinetic energy is:

$$E_{\text{kinetic, target}} = \frac{3}{2} N k_B T_{\text{target}}$$

   where k_B is Boltzmann's constant.

4. **Determine Scaling Factor:** The scaling factor λ is calculated as:

$$\lambda = \sqrt{\frac{E_{\text{kinetic, target}}}{E_{\text{kinetic}}(t)}}$$

5. **Rescale Velocities:** Rescale the velocities of all particles:

$$v_i(t+1) = \lambda \cdot v_i(t)$$

6. **Iterate:** Repeat steps 2-5 at each subsequent time step.