Heinrich–Heine–Universität Düsseldorf
Institut für Theoretische Physik II
Computational Physics
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Problem 7.1: **Nosé-Hoover thermostat**

The equations of motion for a two-dimensional system of N particles coupled to a Nosé-Hoover thermostat can be written as follows

$$\dot{\vec{r}}_i = \frac{1}{m}\vec{p}_i \tag{1}$$

$$\dot{\vec{p}}_i = \vec{F}_i - \frac{1}{Q}p_\eta \vec{p}_i \tag{2}$$

$$\dot{\eta} = \frac{1}{Q}p_\eta \tag{3}$$

$$\dot{p}_\eta = \sum_{i=1}^{N} \frac{1}{m}\vec{p}_i^{\,2} - 2Nk_BT \tag{4}$$

with $i = 1, \ldots, N$ the particle index, m the mass of a particle, η the extra degree of freedom for the heat bath, p_η the momentum corresponding to η, Q a coupling parameter, T the temperature of the heat bath, $\vec{r}_i$ and $\vec{p}_i$ respectively the position and momentum of particle i, $\vec{F}_i$ the force on particle i, and k_B the Boltzmann constant.

a) Implement the Nosé-Hoover thermostat in the MD programme for the WCA system of exercise 6.1, using the algorithm, as derived in the lecture from the Liouville operator splitting.

b) Consider a system of 144 particles (initial configuration from problem 6.1) in a square box with linear dimension $L = 14\sigma$. Start a simulation at $T = 1.5$ and change the temperature of the thermostat to $T = 1.0$ after $t = 5\tau$ ($\tau = \sqrt{m\sigma^2/\varepsilon}$). Determine the time series of the system's temperature up to $t_{max} = 10\tau$ for the following cases:

   - $Q' = 100$ (weak coupling)
   - $Q' = 1$
   - $Q' = 0.01$ (strong coupling)

   with $Q' = Q/2Nk_B$. Plot and discuss the results.

Problem 7.2: **Fluctuations**

In the microcanonical (NVE) ensemble, the heat capacity at constant volume, C_V, can be obtained in a d-dimensional system from

$$\frac{C_V}{Nk_B} = \frac{d}{2}\left(1 - \frac{2}{dN}\frac{\langle \Delta K^2 \rangle}{N\,(k_BT)^2}\right)^{-1} \tag{5}$$

where $\langle \Delta K^2 \rangle = \langle K^2 \rangle - \langle K \rangle^2$ quantifies the fluctuations of the kinetic energy K. In the canonical (NVT) ensemble, C_V is given by

$$\frac{C_V}{Nk_B} = \frac{\langle \Delta E^2 \rangle}{N\,(k_BT)^2} \tag{6}$$

where $\langle \Delta E^2 \rangle = \langle E^2 \rangle - \langle E \rangle^2$ describes the fluctuations of the total energy E.

a) Determine C_V for the two-dimensional WCA system of exercise 7.1 using a canonical MD simulation with Nosé-Hoover thermostat at $T = 1.0$.

b) Now determine C_V from a microcanonical MD simulation.

Hint: To compute averages, use only the data after the system is equilibrated.