I. BASIC MOLECULAR DYNAMICS

Text Reference: Frenkel&Smit, Section 4.1 - 4.3, 6.1.1

Code Reference: ./ExampleCode/tps_integrator.f90

i) **[Getting an integrator!]**

1. Consider a one-dimensional harmonic oscillator (HO),

$$H = \frac{p^2}{2m} + V(q), \quad V(q) = \frac{1}{2} m\omega^2 q^2 \tag{1}$$

with $m = 1$, $\omega = 1$. Implement Euler, Verlet, velocity-Verlet integrator and propagate a trajectory $q(t)$, $v = \dot{q}(t)$ starting from a non-trivial initial condition, i.e. $p(0) \neq 0$ or $q(0) \neq 0$. Use $\Delta t = 0.001$ for the integration step. Compare numerical result with the analytical one.

2. Plot kinetic, potential and total energy along the trajectories. Check energy conservation along the trajectory by defining

$$\bar{E} = \int dt\, E(t) \Big/ \int dt \tag{2}$$

and

$$\sigma_E^2 = \int dt\ |E(t) - \langle E\rangle|^2 \Big/ \int dt \tag{3}$$

Compare energy mean and variance from different integrators and time steps.

3. Repeat the calculations for an asymmetrical Morse oscillator (MO)

$$V(q) = D_e \left(1 - e^{-aq}\right)^2 . \tag{4}$$

with $a = 1$. Choose proper D_e s.t. HO in *i*)-1 is the second-order expansion of MO here. Quantitatively describe the difference between trajectories from two oscillators.

ii) **[From NVE to NVT ensemble]**

1. (Static quantity) Simulate second moment of position

$$\langle q^2\rangle = \int dpdq\, e^{-\beta H} \times q^2 \tag{5}$$

of the HO in *i*)-1 with Andersen thermostat at $\beta = 1$. Experimenting the frequency of stochastic collisions in the thermostat to ensure a proper sampling. Compare numerical result with the analytical one.

2. (Static quantity) Sample the distribution . Plot the histogram.

3. (Dynamical quantity)