

## Homework 3 (CSM3)

Due: June 4, 2021.

The purpose of this exercise is that of performing a simple Molecular Dynamics (MD) simulation.

**Model.** Consider a system of monoatomic molecules interacting via a potential

$$U(r) = \frac{A\sigma^2 e^{-r/\sigma}}{r^2}.$$

Perform simulations with the truncated and shifted potential  $V_{\text{sh}}(r) = V(r) - V(r_c)$  for  $r \leq r_c$  and  $V_{\text{sh}}(r) = 0$  for  $r > r_c$ , fixing  $r_c = L/2$  in all cases. Use periodic boundary conditions, so that distances are always computed using the minimum-image convention. Consider  $N = 80$  molecules in a cubic box of linear size  $L/\sigma$  and fix  $L/\sigma$  so that the density is  $\rho\sigma^3 = 0.75$ . Use reduced units. Length,  $r^* = r/\sigma$ ; energy,  $E^* = E/A$ ; time,  $t^* = t/\sigma\sqrt{A/m}$ ; velocities,  $v^* = v\sqrt{m/A}$ ; pressure,  $p^* = p\sigma^3/A$ ; temperature  $T^* = k_B T/A$ .

**Starting configuration.** Generate a starting configuration such that: a) the molecules are randomly distributed in the box; b) the velocities are random, such that  $\sum \mathbf{v}^* = 0$  and the kinetic energy per particle is equal to  $\frac{2}{3}K^*/N = \frac{2}{3}K/(AN) = 1.0$ . Save the generated configuration on disk.

Perform MD runs using the velocity Verlet updating scheme. Start all runs from the **same** starting configuration (the one computed in the previous step). Use  $\Delta t^* = 0.002$  (run 1), 0.006 (run 2), 0.018 (run 3), 0.054 (run 4), 0.162 (run 5), stopping the simulation at  $t^* = 30$  in all cases. After each updating step measure the potential energy  $U(t)$ , the instantaneous pressure  $P(t)$ , the total energy  $E(t) = U + K$ , and the instantaneous temperature  $T(t) = 2K(t)/(3N)$ . Indicate with  $U^{(1)}(t)$  the potential energy computed in run 1 at time  $t$ , with  $U^{(2)}(t)$  that computed in run 2, and so on. Use the same notation for all observables.

a) Identify the runs that give *stable* results. Do the following analysis only for the stable runs.

b) [**Trajectory divergence.**] Plot  $E^{(i)}(t) - E^{(1)}(t)$ ,  $i = 2, 3, \dots$ , as a function of time (be careful to select the same time for the different runs). Do the same plots for the pressure and the instantaneous temperature.

c) [**Energy conservation.**] From the plots of  $E^{(k)}(t)$ ,  $k = 1, \dots$  verify that the energy is approximately constant.

d) [**Thermalization.**] Plot  $P^{(k)}(t)$  and  $T^{(k)}$  versus time and estimate the time  $t_{\text{eq}}^*$  at which equilibrium is reached.

e) [**Errors and correlations.**] Compute the autocorrelation function in equilibrium  $C(t)$  for the potential energy, the virial, and the kinetic energy. Report in a single plot the autocorrelation functions for the energy as computed in the runs with different time step, as a function of the physical time  $t$  (not as a function of the number of time steps). Do the same for the virial and for the kinetic energy. Estimate the corresponding autocorrelation times, expressed in physical units (not in time steps!).

f) [**Averages**] Estimate average potential energy, pressure, and temperature, averaging the data for  $t > t_{\text{eq}}$ . Use the results of point e) for the autocorrelation times to estimate the correct error.