

## Homework 3 (CSM3)

Due: June 16, 2017.

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

$$U(r) = \frac{A\sigma^2 e^{-r/\sigma}}{r^2} \quad \text{for } r < r_c,$$

$U(r) = 0$  for  $r > r_c$ . Fix  $r_c = L/2$  in all cases. Consider  $N = 60$  molecules in a cubic box of linear size  $L/\sigma$  and fix  $L/\sigma$  so that the density is  $\rho\sigma^3 = 0.6$ . 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  $K^*/N = K/(AN) = 1.0$ . 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.

- Identify the runs that give *stable* results. Do the following analysis only for the stable runs.
- [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.
- [Energy conservation.]** From the plots of  $E^{(k)}(t)$ ,  $k = 1, \dots$  verify that the energy is approximately constant.
- [Thermalization.]** Plot  $P^{(k)}(t)$  and  $T^{(k)}$  versus time and estimate the time  $t_{\text{eq}}^*$  at which equilibrium is reached.
- [Errors and correlations.]** Estimate average potential energy, pressure, and temperature, averaging the data for  $t > t_{\text{eq}}^*$ . Estimate the autocorrelation times and the corresponding errors on the observables. Always apply the tail correction.