Homework 3 (CSM3)

Due: June 4, 2020.

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

$$U(r) = V(r) - V(r_c) + \frac{r}{r_c}(r_c - r)V'(r_c) \qquad \text{for } r < r_c$$

and $U(r) = 0$ for $r > r_c$, where

$$V(r) = \epsilon \left[\frac{\sigma^2 e^{-r/\sigma}}{r^2} + \alpha e^{-2r/\sigma} \right],$$

with $\alpha = 0.3$. Fix $r_c = L/2$ in all cases. Consider $N = 60$ molecules in a cubic box of linear size L/σ, use periodic boundary conditions (i.e. the minimum-image convention to compute distances) and fix L/σ so that the density is $\rho\sigma^3 = 0.7$. Use reduced units. Length, $r^* = r/\sigma$; energy, $E^* = E/\epsilon$; time, $t^* = t/\sigma\sqrt{\epsilon/m}$; velocities, $v^* = v\sqrt{m/\epsilon}$; pressure, $p^* = p\sigma^3/\epsilon$; temperature $T^* = k_B T/\epsilon$. In the following, $E, v, p, t \ldots$ will always refer to the different quantities in reduced units.

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 $K/N = 1.0$. Perform a MD run using the velocity Verlet updating scheme with time step $\Delta t = 0.002$, stopping at $t = 1$. At the end rescale the velocities so that $K/N = 1.0$ and save this final 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 analyses (points b,c,d,e,f) only for the stable runs.

b) [**Trajectory divergence.**] Plot $E^{(k)}(t) - E^{(1)}(t)$, $k = 2, 3, 4, 5$, 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 $E^{(k)}(t)$, $k = 1, \ldots$ verify that the energy is approximately constant.

d) [**Thermalization.**] Plot $P^{(k)}(t)$ and $T^{(k)}(t)$ versus time and estimate the time t_{eq} at which equilibrium is reached. Do this calculation for each k. Note that the starting procedure already thermalizes the system, so we are looking here at the effect of the second velocity rescaling: if the rescaling is small, the system may be in equilibrium already for $t = 0$.

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.

For questions: Meet meeting `https://meet.google.com/fgx-evds-mgc` Friday 05/22, Tuesday 05/26, Friday 05/29, Monday 06/01. Always at 6:00pm.