Homework 3 (CSM3)

Due: May 29, 2015.

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

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

$U(r) = 0$ for $r > r_c$. Fix $r_c = L/2$ in all cases. Consider $N = 75$ molecules in a cubic box of linear size L/σ and fix L/σ so that the density is $\rho\sigma^3 = 0.5$. Use reduced units. Length, $r^* = r/\sigma$; energy, $E^* = E/A$; time, $t^* = t/\sigma\sqrt{A/m}$; velocities, $v^* = r^*/t^*$; 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.

Time-step dependence. Perform four MD runs using the velocity Verlet updating scheme. Start all runs from the **same** starting configuration (the one computed in the previous step). Use $\Delta t^* = 0.003$ (run 1), 0.009 (run 2), 0.027 (run 3), 0.081 (run 4), 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) [**Trajectory divergence.**] Plot $E^{(2)}(t) - E^{(1)}(t)$, $E^{(3)}(t) - E^{(1)}(t)$, and $E^{(4)}(t) - E^{(1)}(t)$ 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.

b) [**Energy conservation.**] From the plots of $E^{(k)}(t)$, $k = 1, 2, 3, 4$ verify that the energy is approximately constant. Compute its standard deviation for the four runs.

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

d) [**Errors and correlations.**] Estimate average potential energy, pressure, and temperature in the three cases, averaging the data for $t > t^*_{\text{eq}}$. Estimate carefully the errors on the results.

Dependence on the starting configuration. Generate a new starting configuration and perform a new run with $\Delta t^* = 0.009$. Compute t^*_{eq}, average potential energy, pressure, and temperature.