Due: June 10, 2019.

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

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

and $$U(r) = 0 \quad \text{for } r > r_c,$$

where

$$V(r) = \frac{A\sigma^{2}e^{-r/\sigma}}{r^2} + B e^{-2r/\sigma},$$

$$B/A = 0.5.$$ Fix $$r_c = L/2$$ in all cases. Consider $$N = 70$$ molecules in a cubic box of linear size $$L/\sigma$$ and fix $$L/\sigma$$ so that the density is $$\rho \sigma^3 = 0.7.$$ 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, $$p^* = \rho \sigma^3/A;$$ 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 $$\sum v^* = 0$$ and the kinetic energy per particle is equal to $$K^*/N = K/(AN) = 1.0.$$ 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 $$K^*/N = K/(AN) = 1.0$$ 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 total energy $$E(t) = U + K,$$ and the instantaneous temperature $$T(t) = 2K(t)/(3N).$$ Indicate with $$U^{(i)}(t)$$ 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 $$E^{(i)}(t) - E^{(1)}(t), \ i = 2, 3, \ldots,$$ 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.

e) [Errors and correlations.] Estimate average potential energy, pressure, and temperature, averaging the data for $$t > t^*_{eq}.$$ Estimate the autocorrelation times, expressed in physical units (not in time steps!), and the corresponding errors on the observables.