MSE 1022H, Homework #2: Molecular dynamics simulations

Due date: Wednesday, 29 Feb, 2012

A. INTERATOMIC POTENTIAL (15+20+5 = 40 points)

The generalized LJ potential energy function is defined as $V(r) = -\frac{A}{r^n} + \frac{B}{r^m}$, where the first term represents attraction while second term is for repulsion. The expression is equivalent to LJ potential for m=6, n=12, and therefore also known as 6-12 LJ potential.

a. Derive expressions for force, equilibrium atomic separation, r_0 (or bond-length), maximum binding energy, V_0 (=minimum potential energy at equilibrium separation).
b. Calculate r_0 and V_0 for the gold LJ potential that we used in HW1 (with parameters ε=0.458 eV and σ=2.569 Å). Also represent r_0 and V_0 in terms of parameters ε and σ for standard 6-12 LJ potential function. Draw the graphs of potential and force variation against atomic separation, and mark the above parameters on the graphs. Compare the values of r_0 and V_0 with EAM potential from HW1.
c. MgO and NaCl charge interactions can be represented by the following interatomic potential: $V(r) = -\frac{A(ze)^2}{r} + \frac{B}{r^9}$, where z =2 for MgO and z=1 for NaCl. Find the ratio of their equilibrium separations, assuming that *A* and *B* remain the same for both materials. How does that compare to experimental data?

B. MODIFYING A SIMPLE MD CODE (MATLAB) (10*6 = 60 points)

Using the MATLAB code for MD (files available on wiki), do the following. Attach only the subroutines/lines that you changed:

a. Subroutine for initializing velocities and temperature (300K) – using random numbers generated according to a Gaussian distribution. Now use this subroutine to initialize velocities rather than the given data file (*.rest) and compare plots (temp, ke, pe, total energy).
b. Subroutine for implementing Verlet scheme, compare results with Velocity Verlet scheme.
c. Subroutine for temperature control (300K) using velocity scaling thermostats. Plot curves.
d. Subroutine for CG minimization. Plot curves.
e. Fit a Buckingham potential to your LJ potential. Implement Buckingham potential for energy and force calculations and compare plots for two cases.
f. Finally, you should have a file that includes all of the above subroutines: (a) initialization of velocities and temperature, (b) velocity verlet scheme if run_style==dynamics, CG minimization if run_style==min, (c) temperature control: velocity scaling if temp_style==vel, Nose-Hoover if temp_style==nvt, (d) Buckingham potential if pot_style==buck, LJ if pot_style=lj. Now draw curves time (10000 steps) for following 2 cases:
   Case 1: Initial temperature = 200K, Velocity thermostat, Buckingham pot., run_style==dynamics
   Case 2: Initial temperature = 300K, Velocity scaling thermostat, LJ pot., run_style==dynamics.