# Problem set 2

Due: January 24

1. What scaling behavior does an MD scheme have with respect to the total number of particles N, without applying techniques such as neighbor lists or bins, and why? Provide an example for this scaling behavior with some pseudocode.

   Discuss strategies that may provide better scaling. Are such strategies applicable for Columbic interactions?

2. Assuming the LJ potential with nearest neighbor interactions, what is the energy difference between these two atomic configurations (left=string, right=bent structure):
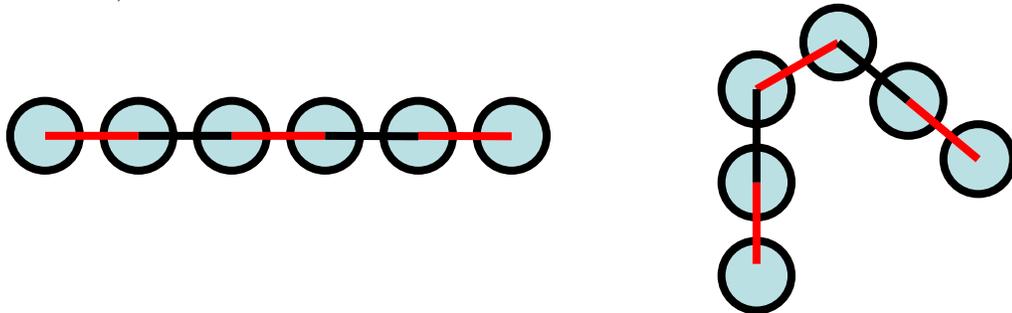
   The red and black lines indicate an equal distance between atoms corresponding to the equilibrium separation. Discuss what implications this may have for modeling such a one-dimensional string of atoms.

3. The JAVA applet (http://polymer.bu.edu/java/java/LJ/index.html) provides a simple MD simulation code for particles interacting according to a LJ pair potential.

   Set up the simulation so you have periodic boundary conditions. Leave the potential parameters identical but change the temperature to 0.01 and the density to 1.19. Perform a constant temperature *NVT* simulation.

   a. Plot snapshots of the system configuration after the simulation has approached steady state (you can confirm this using the "Potential Energy vs. Time" plot). Describe the atomic mechanisms and structures you observe.

   b. Change the density to 0.85, 0.75 and 0.5 while leaving the temperature at 0.01. How does the structure of the system change for each choice of the density?

   c. For a density of 0.85, determine the critical temperature at which the system starts to melt, *i.e.* the initial crystalline order disappears. Describe the procedure you used to determine the critical melting temperature.

Hint: Use the "trajectory" visualization scheme. ("Color Particles - Trajectories").

d. By playing with the interaction parameters for G-B and between B-B, study under what condition you can generate a decomposition of the structure into islands of either blue or green atoms. You may do this for a density of 0.85 and temperature below the melting temperature.

Note: The density in the applet relates to the size of each atom; which is related to the parameter s in the LJ potential.

4. Calculation of elastic coefficients from energy density function.

   For this problem please read section "2.3 An Energy Approach to Elasticity" in the write-up for the first lecture (Basic Continuum Mechanics).
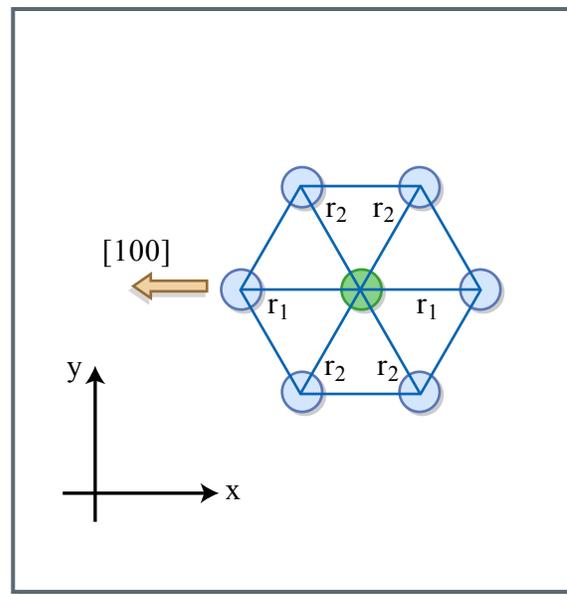

Figure by MIT OCW.

It can be shown that the energy density for a 2D triangular lattice is

$$\Phi(\varepsilon_{ij}) = \frac{\sqrt{3}}{8}\phi''\left(3\varepsilon_{xx}^2 + 2\varepsilon_{xx}\varepsilon_{yy} + 3\varepsilon_{yy}^2 + (\varepsilon_{yx} + \varepsilon_{xy})^2\right), \tag{1}$$

where ϕ'' is the second derivative of the interatomic potential evaluated at the equilibrium distance r_0.

From this expressions, calculate Young's modulus E for a 12:6 LJ potential, expressed as a function of the LJ parameters σ and ε, where Young's modulus gives a direct relation between the tensile strain and the tensile stress.

Does Young's modulus depend on the pulling direction x vs. y, *i.e.* is the material anisotropic?

Hint: To obtain this value, calculate the elasticity tensor coefficients, write the stress-strain relations, and adapt the strain in the direction orthogonal to the pulling direction to the uniaxial stress state (*i.e.* stress orthogonal to pulling direction is zero).