CE 530
Molecular Simulation

Assignment #1 Due: 09 February 2017

(1) For this problem you will collect data from the discontinuous molecular dynamics applet at http://www.etomica.org/app/modules/sites/swmd/swmd2d.html.

(a) Navigate to this applet, and run it for two state points (different temperatures and/or densities) for the ideal-gas model. Evaluate the group $Z = PA/NRT$, and report your value. Be sure to include error estimates. Also, remember to reset the averages whenever you change the state parameters.

(b) Then change to the hard-sphere model. Evaluate Z for a range of densities, and plot your results, showing confidence limits on the values. Run one of the densities at two different temperatures, and include both points on your graph. Also include on the plot the empirical equation of state given by Wood:

$$\frac{PA}{NRT} = 1 + 1.81380\,\hat{\rho}\,\frac{1 - 0.356780\hat{\rho} + 0.021447\hat{\rho}^2}{1 - 1.775171\hat{\rho} + 0.787808\hat{\rho}^2}$$

where $\hat{\rho} = \rho / \rho_0$, with ρ the number density N/A, and $\rho_0 = \frac{2}{d^2\sqrt{3}}$ is the close-packed density (d is the disk diameter).

(2) Derive the expression for the impulse given in Slide 9 of Lecture 2, using the momentum- and energy-conservation formulas that precede it.

(3) Derive an expression for the (vector) impulse applied to two square-well atoms as they approach each other from outside their wells. Let the diameter of the wells be λ and the depth of the wells be ε.

(4) Surface tension has the units of dynes/cm. Develop a dimensionless surface tension variable using molecular constants for a Lennard-Jones fluid.

(5) A Lennard-Jones simulation was performed at $T^* = 1.4$ and $\rho^* = 0.8$. The simulation produced a dimensionless pressure of 2.856 and a dimensionless internal energy of -5.612. To what physical conditions (in K and moles/L) do these state conditions correspond, and what are the corresponding values of the pressure and energy (in MPa and kJ/mol). Use parameter values for Argon (σ = 3.465 Angstroms, ε/k = 113.5 K).