**ChEn 513**

**Homework #7**

**Problem #1**

Do problem #4 from Section 9.9.1.

**Problem #2**

Do problem #5 from Section 9.9.1.

**Problem #3**

Use the Transport Simulator Workbook to determine the diffusion coefficient for Ar at 300 K and 10 MPa. Find values using the MSD and the autocorrelation function methods.

**Problem #4**

Set up a 3-D MD simulation of LJ molecules in a cubic cell that is periodic in the x and y directions but has a solid surface at the top and bottom of the cell in the z direction as shown in the figure at the right. The dimensionless LJ potential model should be used for the interactions between the molecules, but the interactions between the molecules and the wall should be modeled with

where *b* is the molecule-wall energy well depth divided by the molecule-molecule energy well depth and *z*+ is the perpendicular distance of the molecule from a point 0.5 dimensionless units beyond the wall. Note that by centering the LJ interaction site for the wall at *z*+ = -0.5 and *z*+ = *L* + 0.5, this will allow the molecules to touch the wall’s surface. You should run your simulation for the case of *T+* = 1.0, **0.6 and *b* = 3. Prepare a histogram of average number of molecules versus the dimensionless *z* coordinate and explain any observed nonuniformity in density in the *z* direction. Hint: You will likely need to make a change in subroutine grider so that the initial centers of the molecules are not close to the either *z* boundary or the wall-molecule potential will be very high due to overlap of the molecule with the wall.