Assignment 1 (assigned 1/3/06, due 1/12/06)

1. Apply the LJ potential to Ar3, and determine if the symmetrical linear or equilateral structure is lower in energy. Use realistic values of the LJ parameters for Argon. You can find these on the web.

Find the minima using the Newton-Raphson procedure as described in class.

Are both the linear and equilateral structures true minima, i.e., in the absence of any constraints? Note, that for the first part of the problem, you needed to consider only a single degree of freedom. To answer, the preceeding question, you need to allow for more than one degree of freedom.

In solving this problem, first set it up using internal coordinates. Then redo the problem using cartesian coordinates. Recall that the distance between two points in a plane is $R = \sqrt{(x2 - x1)^2 + (y2 - y1)^2}$.

2.Use the Newton-Raphson procedure to find the minimum of a Morse potential $V(x)=D[1 - e^{-ax}]^2$, in the case D and a =1. In writing a mathcad routine to accomplish this, try to write a program that detects if the calculations have converged sufficiently far, and, if so, exits. For a discussion of the Morse potential see http://en.wikipedia.org/wiki/Morse_potential