Project I

In this project you will solve the mystery of the water dimer, i.e. you will determine the minimum energy structure of two water molecules as modeled with the energy function described in class (remember to include the unit conversion factor for the electrostatic interactions that was added to the notes recently). The recommended programming language is Matlab. Matlab has a build in function calls to diagonalize matrices. If you program in a language different from Matlab you are not required to compute eigenvalues (see below). To compute the energy minimum of the dimer we will need the following

1. A function to compute the energy and the derivatives of the energy of $N$ water molecules, input data are the coordinate vector and the number of water molecules, output are the value of the energy and a vector of energy derivatives. You should have this function from the first homework. Remember to include the unit conversion factor for the electrostatic interactions.

2. A function to compute the second derivatives of the potential. Input data are the coordinates of the molecules and the number of water molecules, output is the matrix of second derivatives.

3. A function to determine if the current structure is likely to be a minimum (check the norm of the gradient (smaller than epsilon) and the second derivative matrix (all the eigenvalues must be non-negative). It accepts as input a structure, and the number of water molecules (in this case it will be two), and return true/false variable for convergence (true if gradient norm smaller than epsilon and all the second derivative eigenvalues are non negative).

4. A function to perform a single steepest descent minimization step. Input (and output) coordinate vectors, and step size. The function is checking internally that the step indeed reduces the value of the energy and if not it reduces the step size by a factor of 2 and re-try. If the energy is reduced in the first step, the step size is increased by 20 percent and returned as output, otherwise an unchanged step size is returned.

5. A function to perform a single Newton Raphson minimization. Input and output data are the coordinate set. Also input data are the number of water molecules

6. A function that generates an initial guess for the water dimer coordinate vector. Input: the number of water molecules, Output: vector of water coordinates.

7. A driver program that pick an initial guess and performs 100 steepest descent minimization steps followed up by 10 Newton Raphson minimization steps. It then checks the quality of the resulting structure (minimum or not?). If not, repeat again the cycle of 100 SDM and 10 NT steps. The energy, norm of potential gradient, and eigenvalues of the second derivative matrix should be reported.

After 1-7 are up and running it should not be a problem to determine the optimal dimer structure. In your report include the code and input/output samples. Also include a picture of the water dimer in which the atoms are drawn as spheres in a three-dimensional plot. The radii of the hydrogen should be drawn three times smaller than the radii of the oxygen atoms.