

CS 428: Homework I ([*] =15 points bonus)
Due Thursday Sept 14 at 2:30PM.

1. Write a Matlab function that computes the interaction energy of N water molecules and the forces that they exert on each other. It is useful to separate the calculation to different functions, one function that computes the internal energy of the water molecules, and one function that computes the Lennard Jones and electrostatic interactions. The input should be the coordinate vector and the number of water molecules and the output the potential value and the gradient of the potential. Check the analytical gradient by a finite difference formula.
2. Construct five trial configurations for a water dimer (your choice of a minimum energy configuration) and evaluate their energies. Did you hit a minimum?
3. Write steepest descent algorithm to minimize the energy of the water dimer and minimize it. Report a plot of the relative conformation of the molecules. Prepare a Matlab movie that follows the minimization path.
4. (*) Write a code that computes the second derivative of the energy of the water dimer.
5. (*) Refine the optimal structure obtained from the steepest descent minimization using Newton Raphson minimization. Report the changes in structure/energy

In your submission include code, input, and output and a brief explanation. Both electronic and hard copies are required (send your electronic copy to ron@cs.cornell.edu)