MSE 561 - Assignment 3
Molecular statics relaxation

(1) In this Assignment you will use the block and neighbor map you developed in the Assignment 2. You will employ the routines for calculation of the potential energy, forces, radial distribution function (RDF) and stresses that you developed also in the Assignment 2. All this is done using the L –J potential supplemented by a polynomial tail that provides for the cut-off at r_{cut} = 7.5Å, as explained in the description of the Lennard-Jones potential.

(2) Consider now the constructed block as a cluster with free surfaces. Use the steepest descent method to find a minimum energy configuration of this block. Investigate the effect of the choice of λ used in the relation $\Delta\mathbf{r}_i^{(m)} = \lambda\,\mathbf{F}_i^{(m)}$, upon the relaxation procedure. This means you try several values of λ and study the rate of convergence of the relaxation process. Do not forget that λ must never be too big, which means that any atomic displacement must be at least a factor of 20 smaller than the average separation of the nearest neighbors.

(4) Follow the relaxation process in two different ways **but concomitantly**. First, evaluate the energy and the maximum force in the block as a function of the number of iteration and plot this dependence. Secondly, evaluate the **total** stress tensor (i.e. components σ_{11}, σ_{22}, σ_{12}) during relaxation and follow its evolution during the relaxation process by plotting the stress components as a function of the number of iterations. This need not be done at every iteration step but always after a number, say 50, iterations. What is the final state of the stress? What is the final hydrostatic stress?

(5) Interpret the relaxed structure by:

(i) Displaying the structure such that circles represent atoms.

(ii) Determining the RDF for the relaxed structures. Compare this with the RDF of the unrelaxed structure that you made in the Assignment 2 from which you started the calculation.

(iii) Determine the atomic level hydrostatic stress and the shear stress σ_{12} at individual atoms.

Try to explain physically why the structure you obtained by relaxation is a minimum energy structure, what was formed during the relaxation and consider whether there might be other even lower energy structures. In particular, can you guess what might be the lowest energy structure i.e. the structure corresponding to the absolute lowest minimum of the energy.