ECE 559 Project #3

This project requires you to construct a real-valued EA to look for low energy configurations of small atomic clusters.

Atomic clusters are aggregates of atoms held together by the same forces that cause, for example, the formation of crystals. Cluster sizes vary from just a few atoms to hundreds of atoms. Among all of the possible atomic arrangements, the structure with the lowest total energy is the one of the most interest. (Not only is it the most stable configuration, but also the structure gives clues about what other atoms the cluster can react with.) The total energy of an atomic cluster with N atoms is

$$E = E(p_1, p_2, \ldots, p_N)$$

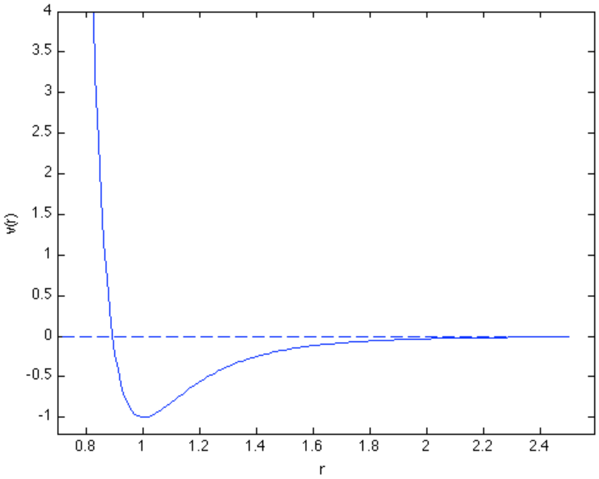
where p_k is the position of the k-th atom. ***Your objective in this project is to find the 3-D structure of an N=5 atom cluster with the lowest total energy.***

Summing up the potential energy between all pairs of atoms can approximate the total energy. That is,

$$E = \sum_{j=1}^{N-1} \sum_{k=j+1}^{N} v(r_{jk})$$

where r_{jk} is the Euclidean distance between atoms j and k and $v(r_{jk})$ is the pairwise potential energy. A commonly used pairwise potential energy function is the scaled Lennard-Jones potential energy function

$$v(r_{jk}) = \left(\frac{1}{r_{jk}}\right)^{12} - 2\left(\frac{1}{r_{jk}}\right)^{6}$$



Notice the minimum energy of $E = -1.0$ occurs at a Euclidean distance between atoms of $r_{jk} = 1.0$.

Each atom has *x*, *y*, *z* coordinates in 3-D space, which means the positions of an *N* atom cluster would take a total of $3N$ coordinates. But only $3N–6$ coordinates are needed if (*a*) the first atom is fixed at the origin, (*b*) the second atom lies only on the *x*-axis and (*c*) the third atom lies only in the *xy*-plane. All other atoms require 3 coordinates to specify their position. Hence, your genotype would only have to be a 9 component real vector.

Use a binary tournament to select parents and intermediate recombination as the primary variation operator. The mutation probability should be high (around 30%). Don't use strategy parameters in your mutation. Instead fix the standard deviation at $\sigma = 0.005$ for all object parameters. Use tournament selection to choose the survivors. All other EA parameters are your choice.

In your report you should plot the total energy per generation averaged over 10 runs. Also speculate on what you think is the lowest energy structure for the 5 atom cluster.