Project

You need to model a cluster of N spherical particles of diameter $\sigma = 3.4$ Å . Assume that each pair of particles interact with each other via the Lennard-Jones potential of the form

$$V = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

where $\varepsilon = 0.238$ kcal/mol and r is the distance between the interacting pair of particles.

The total potential energy of the system can be evaluated by considering summation over all interacting pairs in the above equation.

Step 1 : You need to generate an initial configuration of the system such that no two particles are separated by a distance (*i.e.*, center to center distance) either less than the diameter of the particle or greater than 2.5σ.

Step 2 : Generate 10 different initial configurations and determine the total potential energy of the system for each of these configurations.

Step 3 : Design an algorithm (or use the steepest descent algorithm) to determine the least-energy configuration of the system.

Step 4 : How do the number of energy minima and number of maxima/saddle points vary with N? You need to vary N from 2 to 20 (19 such clusters).

Step 5 : For N=8, find the minimum energy path connecting any two minimum energy structures of this cluster. A minimum energy path is the least-energy path that the system would take to evolve from one structure to the other. You may use the nudged-elastic band method/algorithm to determine the minimum energy path.