PHYS4061 Project A Part IV

Yip Hoi Tung 1155092406
1155092406@link.cuhk.edu.hk 7th Dec, 2018

**Remarks:**

My program "Project_A_Part_IV" is written in Python 2.7. It imports automatically another two python scripts which are modified versions of Project A Part I. Parameters were hard-coded into them such that they produce .xyz files of Fcc Xenon (for Lennard-Jones (LJ) potential) and Diamond Silicon (for Tersoff potential) lattices for Part IV's use.

If you want to modify the lattices' details, you can find the files under \Project_A_Part_I. You can alter the structure, lattice constant, periodicities and element label in the function get_inputs() (line 7). Correspondingly, you might need to adjust the distance cut-off (LJ: line 550 and/or Tersoff: line 627).

There are four parts in the script you can uncomment to use. They are steepest descent (SD) for LJ potential (line 566), conjugate gradient (CG) for LJ potential (line 587), SD for Tersoff potential (line 644) and CG for Tersoff potential (line 665).

For each part, 1) .xyz file for the atoms, 2) neighbor list and 3) .xyz file for the frames of energy minimization (ready for VMD) are outputted under the same directory of the python script.

**Methods:**

The program calculates gradient numerically for both potentials. The method is to alter each coordinate of each atom one at a time and calculate the change in total energy each time to get the corresponding slope. So, there will be 3N components in the gradient for N atoms. The step for the numerical differentiation was chosen to be 1.0% of the lattice constant (adjustable).

Line minimization for computing how long to travel along the gradient, the secant method was used. The step for computing the slope of the gradient was taken to be 1.0% of each gradient component (adjustable).

Perturbation was done to the atoms by moving each coordinate of each atom by a random distance within the interval [-x, x) where x = 20.0% of lattice constant.

Iteration in the SD/CG is set to stop when the discrepancy between minimum total energy and the total energy in the current step is smaller than 1.0%.

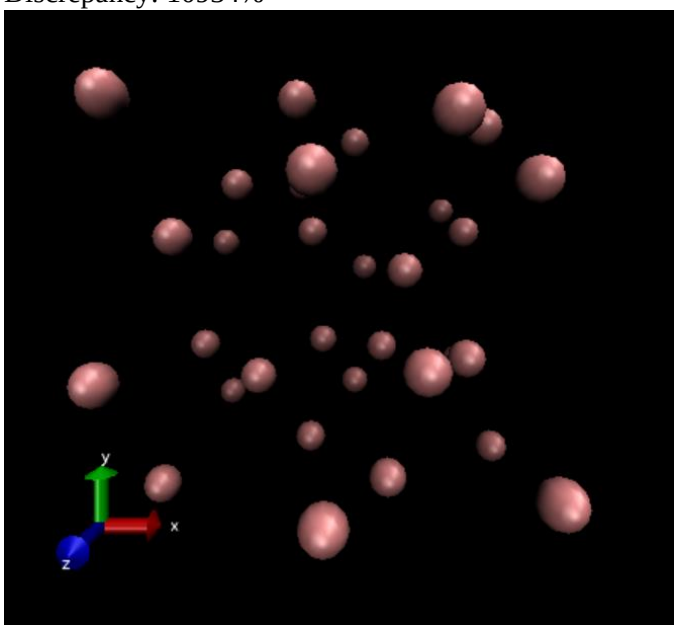
Parameters used in the LJ/Tersoff potentials follow from Part III which were shown to be correct.

**Results:**

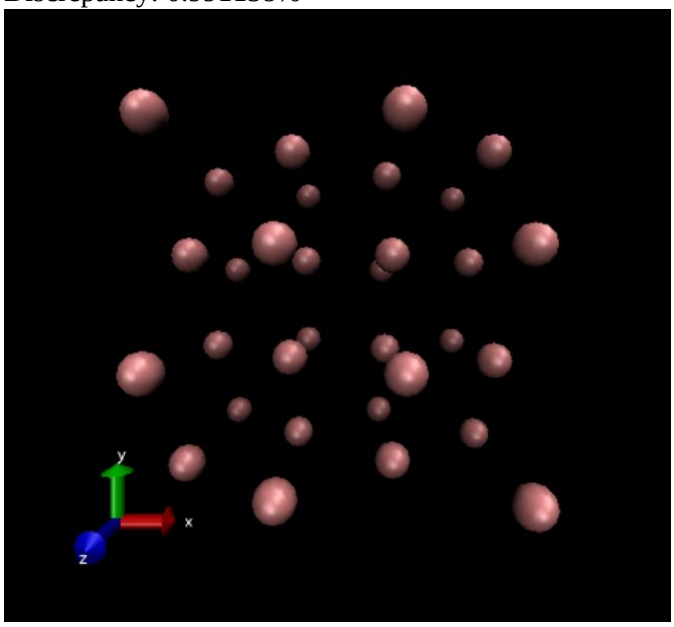
*SD for LJ potential:*

1. Xenon; Fcc; 2*2*2; lattice constant 6.13Å; distance cut-off 6.129Å;
   Minimum total energy: -5.90179e-12erg;
   Total energy at start (perturbed): 6.39401e-10erg

   **Start:**
   Frame: 0;
   Total energy now: 6.39401e-10erg;
   Discrepancy: 10934%

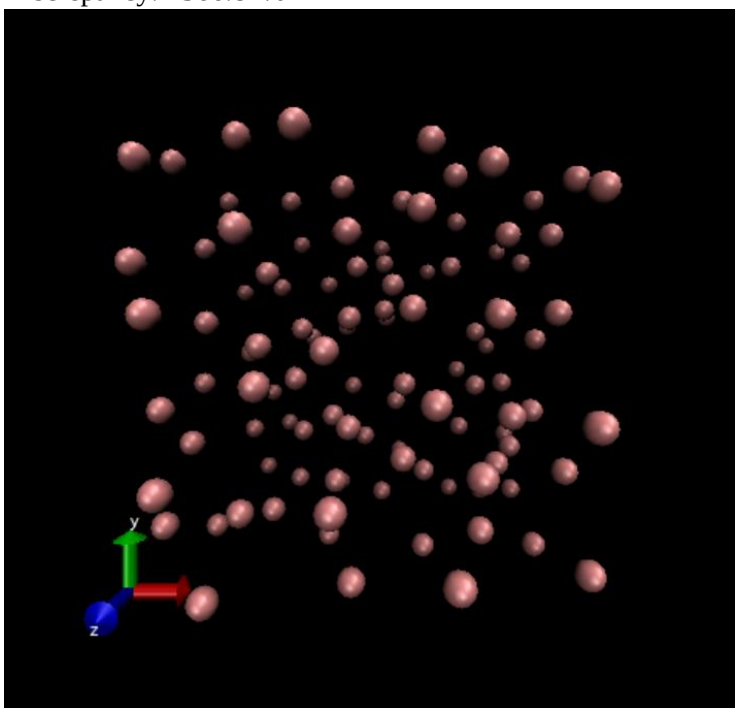



   **End:**
   Frame: 134;
   Total energy now: -5.8433e-12erg;
   Discrepancy: 0.991158%

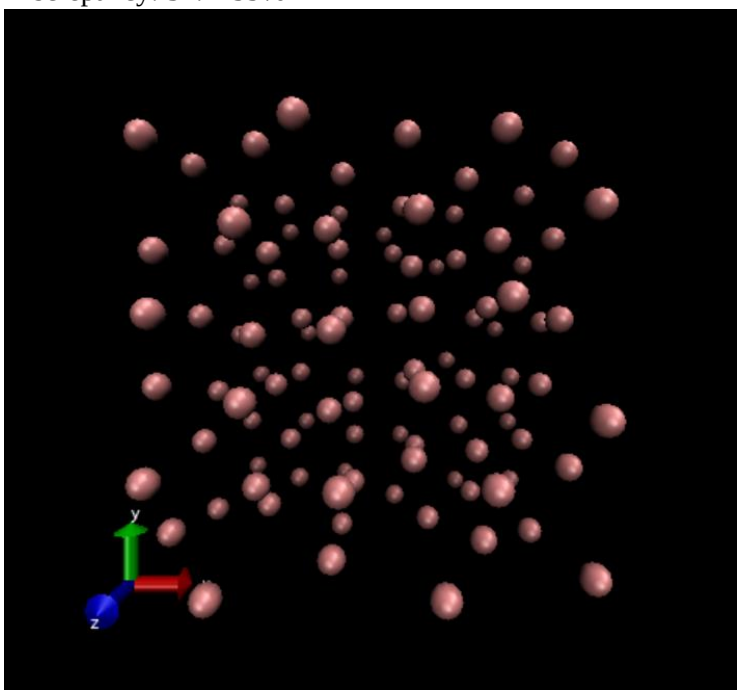


2. Xenon; Fcc; 3*3*3; lattice constant 6.13Å; distance cut-off 9.194Å;
   Minimum total energy: -2.71621e-11erg;
   Total energy at start (perturbed): 1.15897e-09erg

   **Start:**
   Frame: 0;
   Total energy now: 1.15897e-09erg;
   Discrepancy: 4366.87%



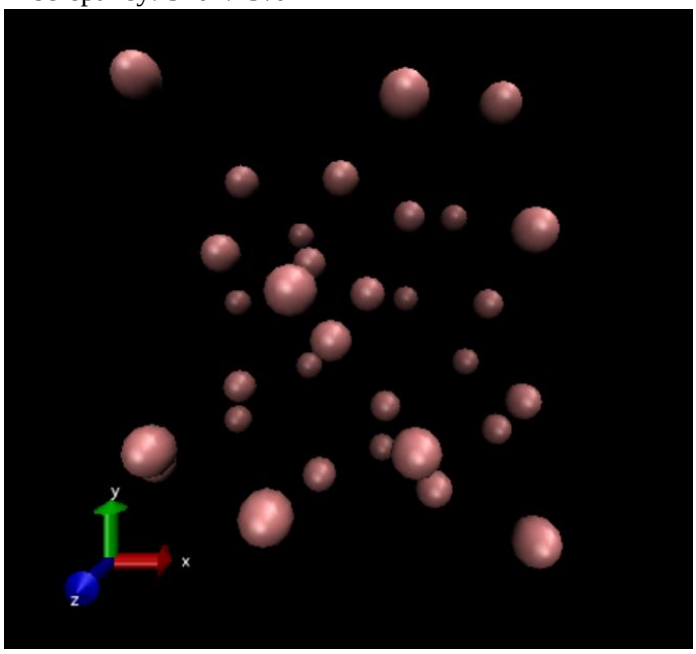

   **End:**
   Frame: 29;
   Total energy now: -1.82665e-11erg;
   Discrepancy: 32.7499%



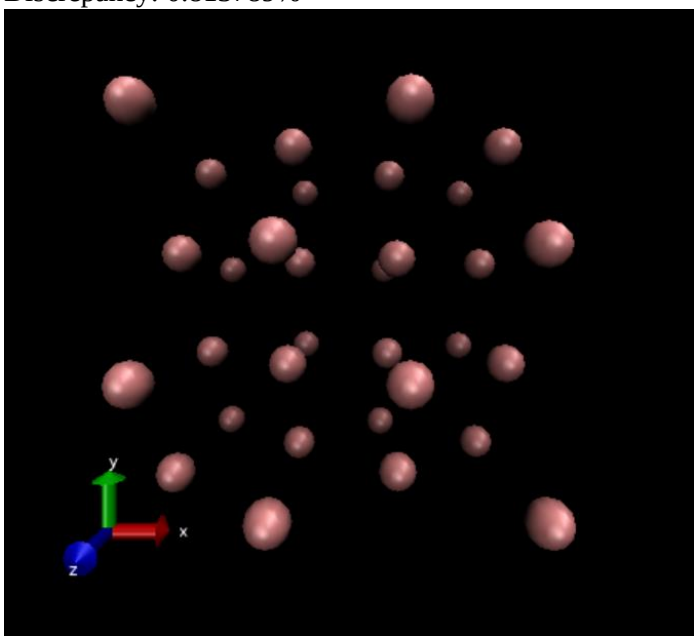
*CG for LJ potential:*

1. Xenon; Fcc; 2*2*2; lattice constant 6.13Å; distance cut-off 6.129Å;
   Minimum total energy: -5.90179e-12erg;
   Total energy at start (perturbed): 1.95038e-10erg

   **Start:**
   Frame: 0;
   Total energy now: 1.95038e-10erg;
   Discrepancy: 3404.73%

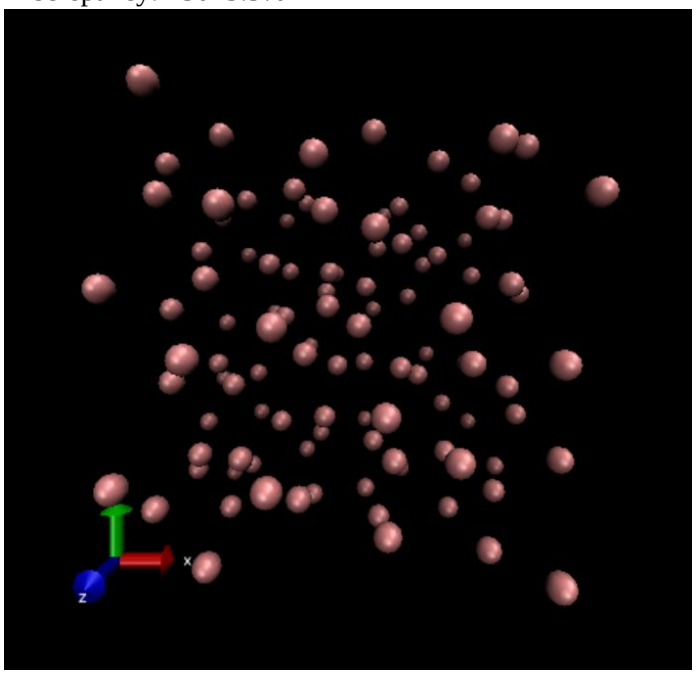



   **End:**
   Frame: 54;
   Total energy now: -5.85377e-12erg;
   Discrepancy: 0.813789%

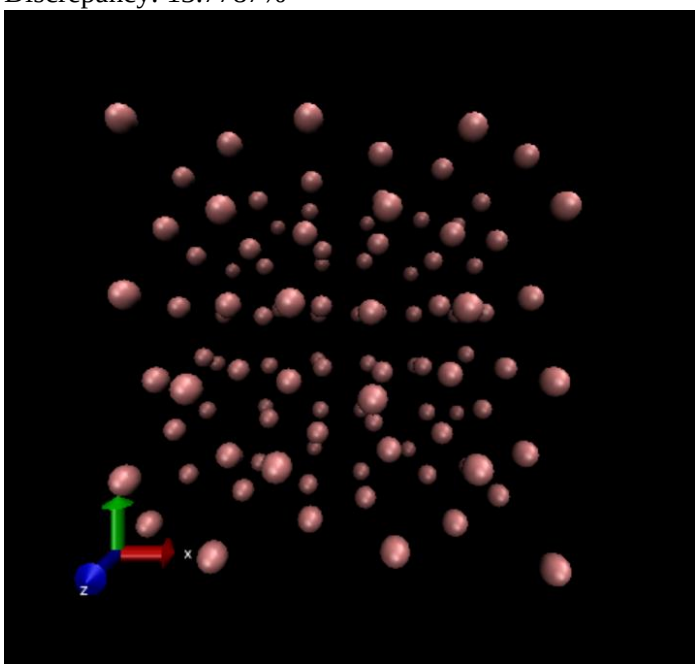


2. *(1st run)* Xenon; Fcc; 3*3*3; lattice constant 6.13Å; distance cut-off 9.194Å;
   Minimum total energy: -2.71621e-11erg;
   Total energy at start (perturbed): 3.5103e-09erg

   **Start:**
   Frame: 0;
   Total energy now: 3.5103e-09erg;
   Discrepancy: 13023.5%

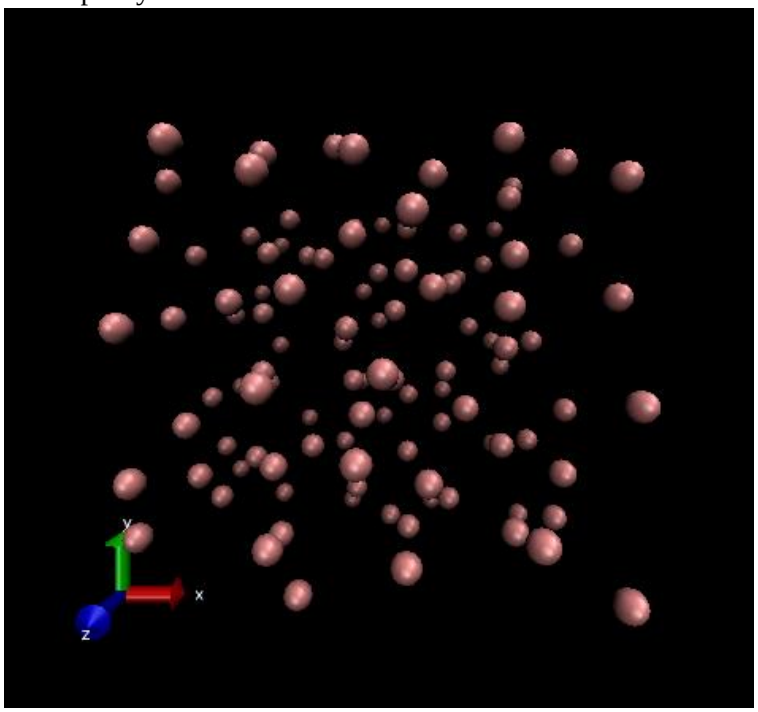



   **End:**
   Frame: 30;
   Total energy now: -2.34195e-11erg;
   Discrepancy: 13.7787%

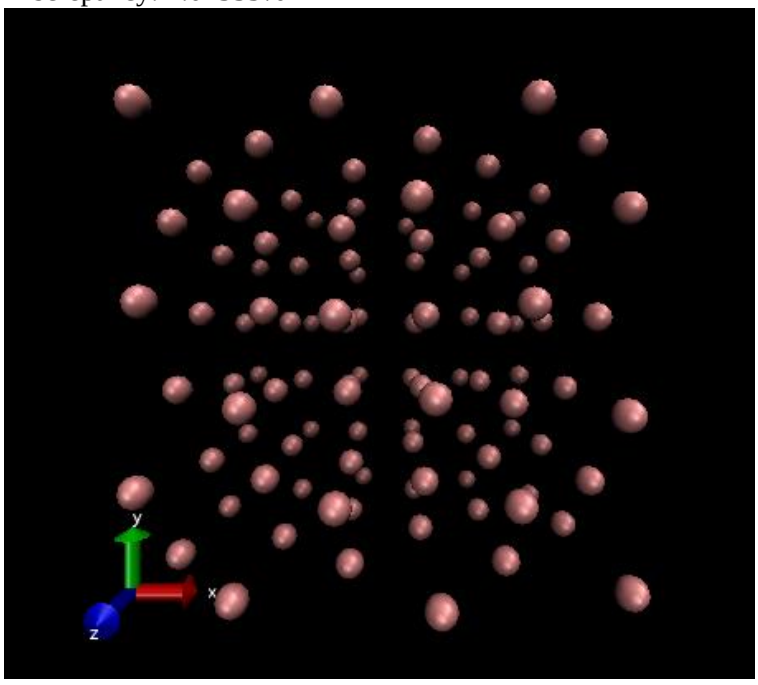


3. *(2nd run)* Xenon; Fcc; 3*3*3; lattice constant 6.13Å; distance cut-off 9.194Å;
   Minimum total energy: -2.71621e-11erg;
   Total energy at start (perturbed): 5.99944e-09erg

   **Start:**
   Frame: 0;
   Total energy now: 5.99944e-09erg;
   Discrepancy: 22187.5%



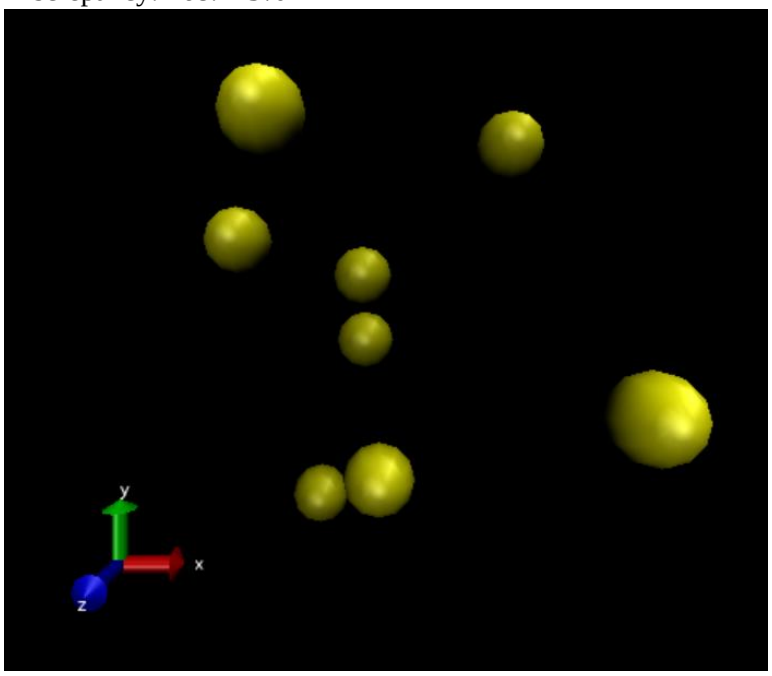

   **End:**
   Frame: 83;
   Total energy now: -2.52565e-11erg;
   Discrepancy: 7.01553%



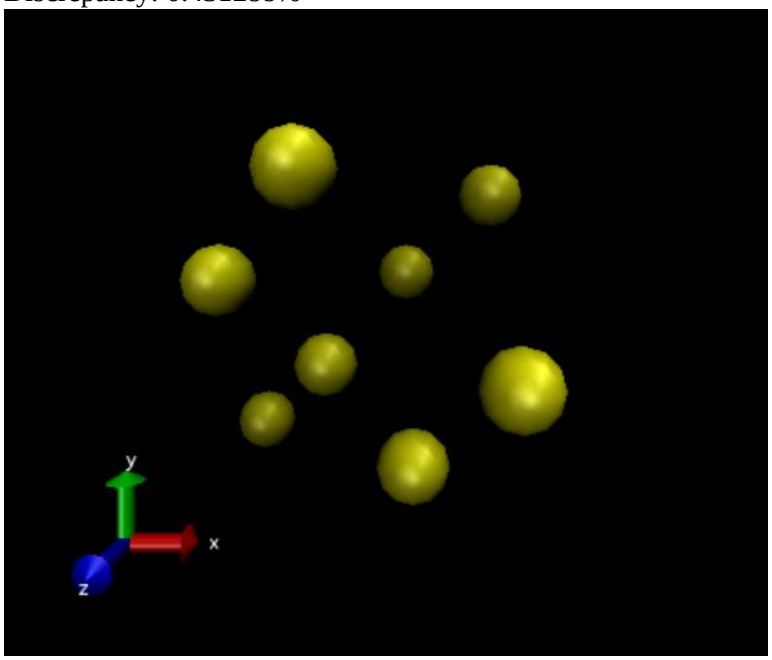
*SD for Tersoff potential:*

1. Silicon; Diamond; 1*1*1; lattice constant 5.43Å; distance cut-off 2.714Å**;**
   Minimum total energy: -37.0377erg;
   Total energy at start (perturbed): 25.3424erg

   **Start:**
   Frame: 0;
   Total energy now: 25.3424erg;
   Discrepancy: 168.423%



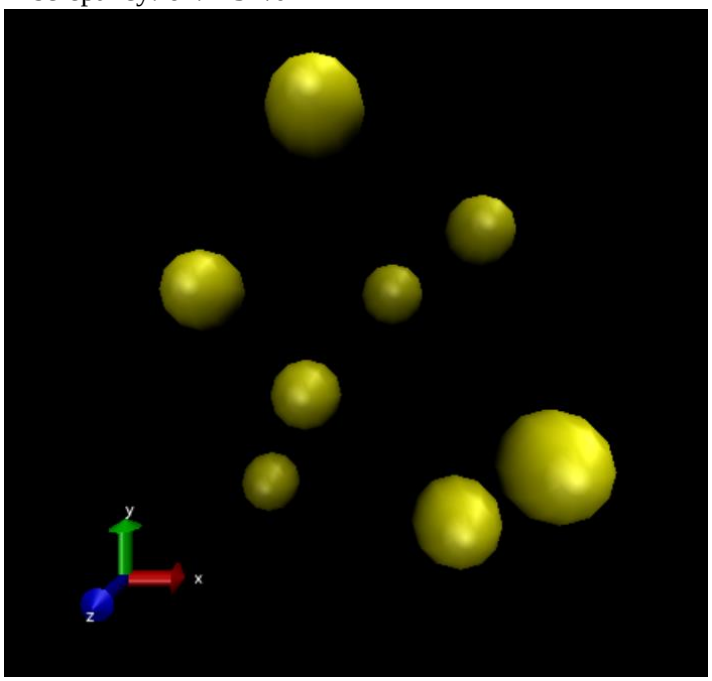

   **End:**
   Frame: 36;
   Total energy now: -36.878erg;
   Discrepancy: 0.431288%



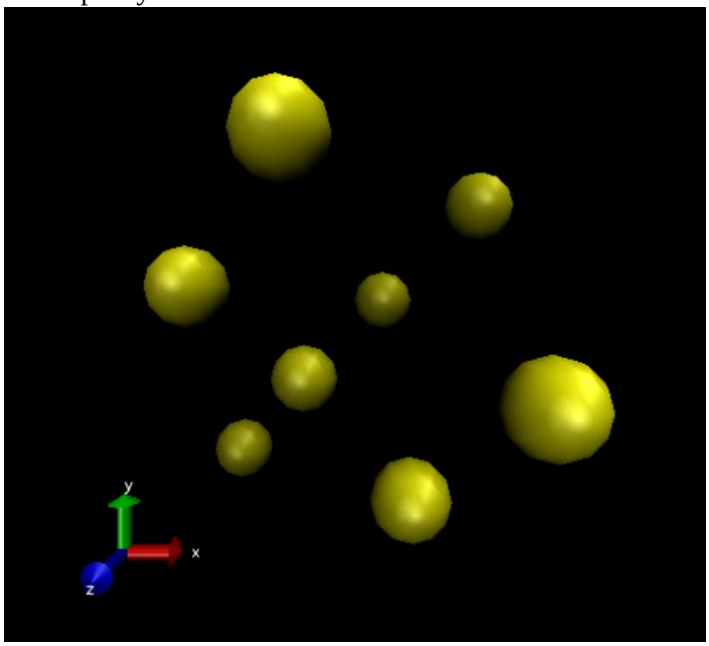
*CG for Tersoff potential:*

1. Silicon; Diamond; 1*1*1; lattice constant 5.43Å; distance cut-off 2.714Å**;**
   Minimum total energy: -37.0377erg;
   Total energy at start (perturbed): -13.288erg

   **Start:**
   Frame: 0;
   Total energy now: -13.288erg;
   Discrepancy: 64.1231%




   **End:**
   Frame: 7;
   Total energy now: -36.6713erg;
   Discrepancy: 0.989469%



All the associated files and screenshots of the above results are also put under \Sample Output Files for your information. Thank you.