Report for assign 7：

In this project, I developed four individual fortran 90 programs to realize the pair correlation function for simple cubic(sc), body centered cubic(bcc), face centered cubic(fcc) and hexagonal close packed(hcp) crystal. They are named sc.f90, bcc.f90, fcc.f90 and hcp.f90 respectively.

Pair correlation function g(r) is the probability to find a pair of distance r apart, which is essentially a density correlation function. In order to calculate g(r), we have four steps to go. Firstly, count the number of particles from r to r+dr. Secondly, divide the total count by the total number of particles in data. Thirdly, divide this number by the volume of the spherical shell 4*pi*r**2*dr. At last, divide the number by the particle number density, which ensure that g(r) = 1 for data without structure.

In all four fortran 90 programs, I used the same main structure. Primarily, I defined a function named distance to calculate the distance between the inputed point and the center point in the data. In the main program, I looped r from 0.1 to 10.1 with step width 0.1. The center point located at (10.0, 10.0, 10.0). The real variable “count” adds every point between r and r+dr. gr equals count/4/pi/r**2/N, which stands for the pair correlation function. Finally, I outputted r and gr into corresponding .dat file, and used gnuplot to plot 2D graph for each of them.

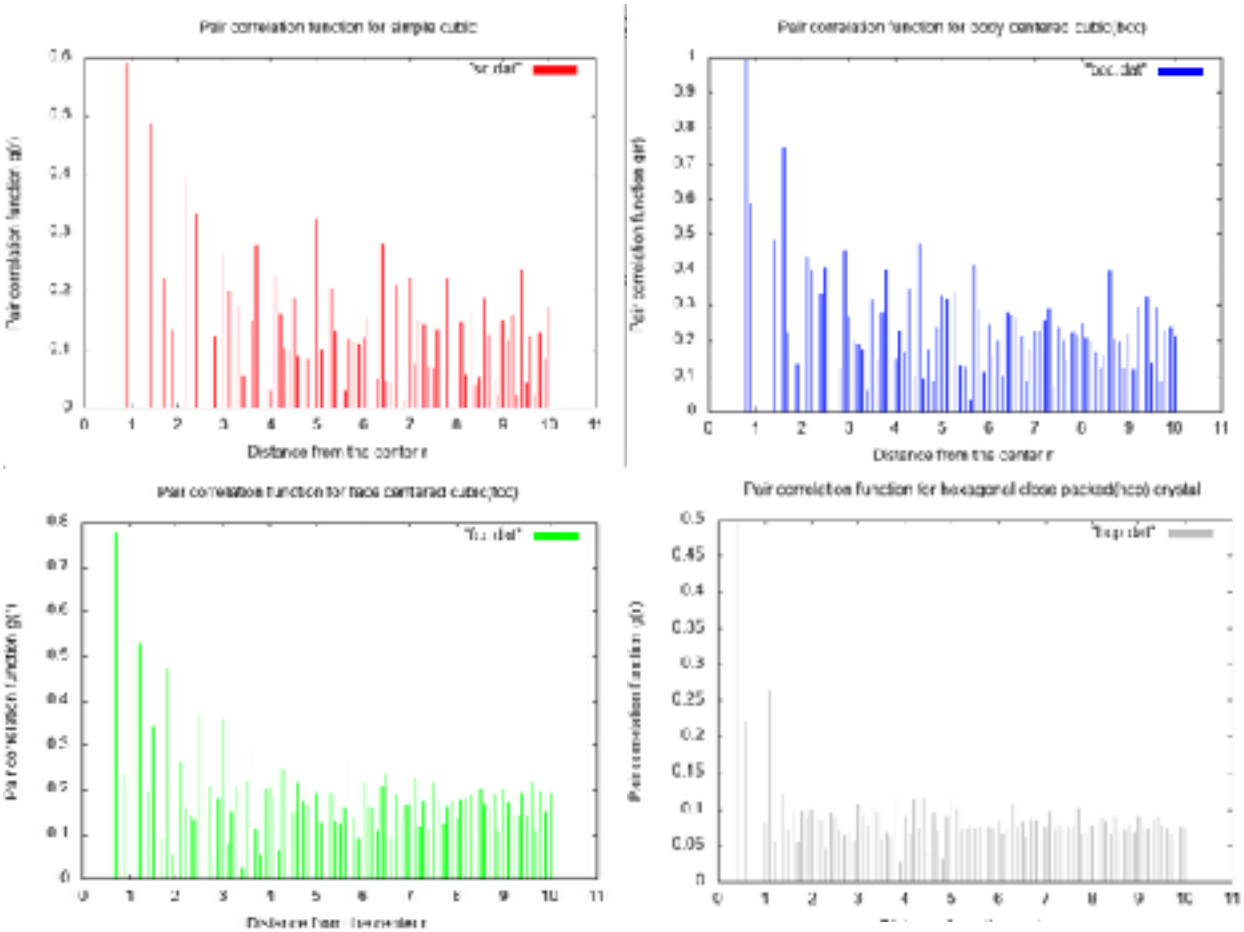
In sc.f90, I count the particles in simple cubic by looping i, j and k from 0.0 to 20.0 with step width 1.0.

In bcc.f90, I added more points that located at the body center of the lattice by looping i, j and k from 0.5 to 19.5 stepped 1.0.

In fcc.f90, I added more points on the face center of lattice based on sc.f90 like bcc.f90. The way I added these point is looping i from 0 to 20.0, j and k from 0.5 to 19.5. Whenever the program find a point at the range from r to r+dr, the variable “count” plus 3. The reason why I should plus 3 not 1 is that i, j and k are symmetric in this case, and I only counted the points at face center in j-k plane.

In hcp.f90, I set the step in z direction 1.0, in x direction sqrt(3) and y direction 3/2. I counted the particles in two different loop. The first loop starts at (0, 0, 0) and the second loop starts at (sqrt(3)/2, -1/2, 0). After these two loop, I counted all points in hcp crystal.

The graphs are stored in sc.png, bcc.png, fcc.png and hcp.png.



As the graph depicts, the minimum distance from the center point in sc, bcc and fcc are about 0.9, 0.8, 0.7. The reason why the minimum distance in simple cubic is not 1 is that I set the range as (r, r+dr]. This result that min(sc)>min(bcc)>min(fcc) is consistent with our expectation. Thus it confirms the accuracy of the data.

During the development of these program, I came across a situation that min(bcc) = 0.5 and min(fcc) = 0.9. I stuck at this point a little bit, but at a later time I noticed that I wrongly reset the value for j and k, from which I learnt that I should check whether I reset the value correctly or not after every loop.