The Chinese University of Hong Kong

PHYS4061 Computational Physics, 1st semester, 2019-2020

Project A Part I

Write a program to generate Sc, Bcc, Fcc, and Diamond crystalline structures.

Requirements:

- The simulation cell size should be adjustable in both periodicity and lattice constant,
- The shape of the cell should be cubic like (or tetragonal),
- Output in .xyz format, see reference and example below,
- The output can be plotted by using any graphic software such as VMD or VESTA. You are not required to send the picture to TA.
  - VMD: http://www.ks.uiuc.edu/Research/vmd/
  - VESTA: http://jp-minerals.org/vesta/en/

Since the structure you generated will be used in the following lab, storing the data inside the program and reuse them within the code is highly recommended.

Score will be deducted if the program has bad variable/function naming conventions or without adequate comments. Submit code and output to ylfchong@phy.cuhk.edu.hk

Due date: 24 Sep 2019

Score will be deducted if the submission is late.

Referenced file format

XYZ

https://en.wikipedia.org/wiki/XYZ_file_format

```
8
This line is comment, this cell is example of simple cubic
Si  0.000000000  0.000000000  0.000000000
Si  5.000000000  0.000000000  0.000000000
Si  0.000000000  5.000000000  0.000000000
Si  0.000000000  0.000000000  5.000000000
Si  5.000000000  5.000000000  0.000000000
Si  0.000000000  5.000000000  5.000000000
Si  5.000000000  0.000000000  5.000000000
Si  5.000000000  5.000000000  5.000000000
```

For animation, repeat the content from number of atoms to the end

```
8
Frame 1(This line is comment, not necessary to write frame number here)
Si  0.000000000  0.000000000  0.000000000
Si  5.000000000  0.000000000  0.000000000
Si  0.000000000  5.000000000  0.000000000
Si  0.000000000  0.000000000  5.000000000
Si  5.000000000  5.000000000  0.000000000
Si  0.000000000  5.000000000  5.000000000
Si  5.000000000  0.000000000  5.000000000
Si  5.000000000  5.000000000  5.000000000
8
Frame 2
Si  0.100000000  0.000000000  0.000000000
Si  5.100000000  0.000000000  0.000000000
Si  0.100000000  5.000000000  0.000000000
Si  0.100000000  0.000000000  5.000000000
Si  5.100000000  5.000000000  0.000000000
Si  0.100000000  5.000000000  5.000000000
Si  5.100000000  0.000000000  5.000000000
Si  5.100000000  5.000000000  5.000000000
8
Frame 3
```

Si	0.200000000	0.000000000	0.000000000
Si	5.200000000	0.000000000	0.000000000
Si	0.200000000	5.000000000	0.000000000
Si	0.200000000	0.000000000	5.000000000
Si	5.200000000	5.000000000	0.000000000
Si	0.200000000	5.000000000	5.000000000
Si	5.200000000	0.000000000	5.000000000
Si	5.200000000	5.000000000	5.000000000