

## Input format description

The input format for atomic coordinates for the software is in a text .xyz format. The first line contains the number of atoms. The second line contains lower and upper limits of computation cell in x, y and z separated with spaces as

$x_{min} x_{max} y_{min} y_{max} z_{min} z_{max}$

All the other lines contain  $x$ ,  $y$  and  $z$  coordinates of each atom separated with spaces as

$x y z$

Examples of input files can be found in the input\_examples folder.

## Description of xrdmp.in and xrdmp.list input files

The file "xrdmp.in" contains input parameters and flags used in the calculations. The list of the parameters and their description in the order they appear in the file is listed below.

- NB – Number of bins used to calculate the absolute values of  $Q$ . The bin size for  $Q$  is calculated using this parameter as  $\Delta Q = (Q_{max} - Q_{min})/NB$  where  $Q_{max}$  and  $Q_{min}$  are maximum and minimum values of  $Q$ . Keep it low in order to improve  $Q$  resolution.  
Value Type: Positive Integer
- Nbins – Number of bins used to calculate the absolute values of  $r_k$ . The bin size for  $r_k$  is calculated using this parameter as  $\Delta r_k = R_{cut}/(Nbins - 1/2)$ . Keep it below characteristic distance in your system.  
Value Type: Positive Integer.
- NRCFLAG – Flag which defines if periodic boundary conditions (PBC) are applied. If equals 0 than no PBC applied, if = 1 than PBC applied in all three directions (x, y and z). If = 2 than PBC are applied only in x and y directions. Value Type: Positive Integer.
- WFLAG – Flag which defines if window function is applied. If = 0 than window function is not used, if = 1 than window function is used as described in the paper. Value Type: Positive Integer.
- dtheta – Angular step to calculate  $\vec{e}_Q$ . Units: degrees. Value type: Positive real.
- Qmax – maximum value of  $Q$  in reciprocal space. Units:  $\text{\AA}^{-1}$ . Value type: Positive real.
- Rcut – cut-off distance for interatomic distances used when calculating the histogram and the window function. Units:  $\text{\AA}$ . Value type: Positive real.
- MULT\_FLAG – Flag which defines whether normalization is used (=1) or not (=0) as described in the paper. Value type: Positive integer.

The file "xrdmp.list" contains file names which are used for reading the atomic positions and writing output data. The first line (UNIT 14) contains the name of parameter file "xrdmp.in" and should be left intact. The second line (UNIT 15) contains the name of .xyz file described in the

previous section. The third line (UNIT 17) contains the name of the file used for output of two-dimensional diffraction profile. The fourth line (UNIT 18) contains the name of the file which is used for the output of one-dimensional diffraction profile obtained through the angular averaging of the two-dimensional diffraction profile.

The output (UNIT 17 and UNIT 18) is organized as follows. The file with 2-d diffraction profile (UNIT 17) contains  $Q_x$  in the first column,  $Q_y$  in the second column and the magnitude of the structure factor  $S(Q_x, Q_y)$  in the third column. The file with 1-d diffraction profile (UNIT 18) contains the absolute value of  $Q$  in the first column and  $S(Q)$  in the second column. The  $Q$  units used in the output are inverse of distance units used in the input file (.xyz) with atomic coordinates. For instance, if atomic positions are set in angstroms than the  $Q$  units in the output (UNIT 17 and UNIT 18) will be in inverse angstroms.

### **Compiling and running**

The code was written following Fortran90 standard and tested using IntelMPI. Other MPI implementations were not tested with this code and correct work is not guaranteed.

### **Description of input examples**

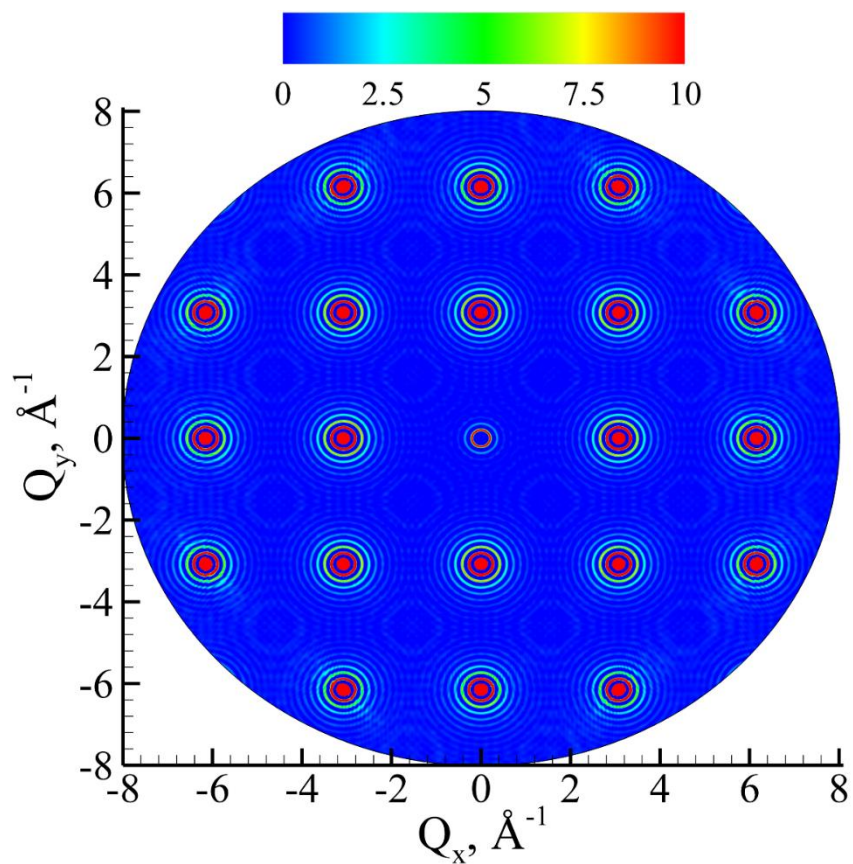
There are four test systems which are provided together with the code in input\_examples subfolder. Their brief description is given below.

- FCC\_32.xyz: A FCC gold system which contains 32,000 atoms thermalized for 350 picoseconds at 300 K and zero pressure in NPT ensemble with periodic boundary conditions applied in all three directions.
- Liq\_32.xyz: A liquid gold system which contains 32,000 atoms thermalized for 140 ps after melting at 1300 K and zero pressure in NPT ensemble with periodic boundary conditions applied in all three directions.
- FCC\_256.xyz: A FCC gold system which contains 256,000 atoms thermalized for 350 picoseconds at 300 K and zero pressure in NPT ensemble with periodic boundary conditions applied in all three directions.
- Liq\_256.xyz: A liquid gold system which contains 256,000 atoms thermalized for 140 ps after melting at 1300 and zero pressure in NPT ensemble with periodic boundary conditions applied in all three directions.

### **Results of Input Examples**

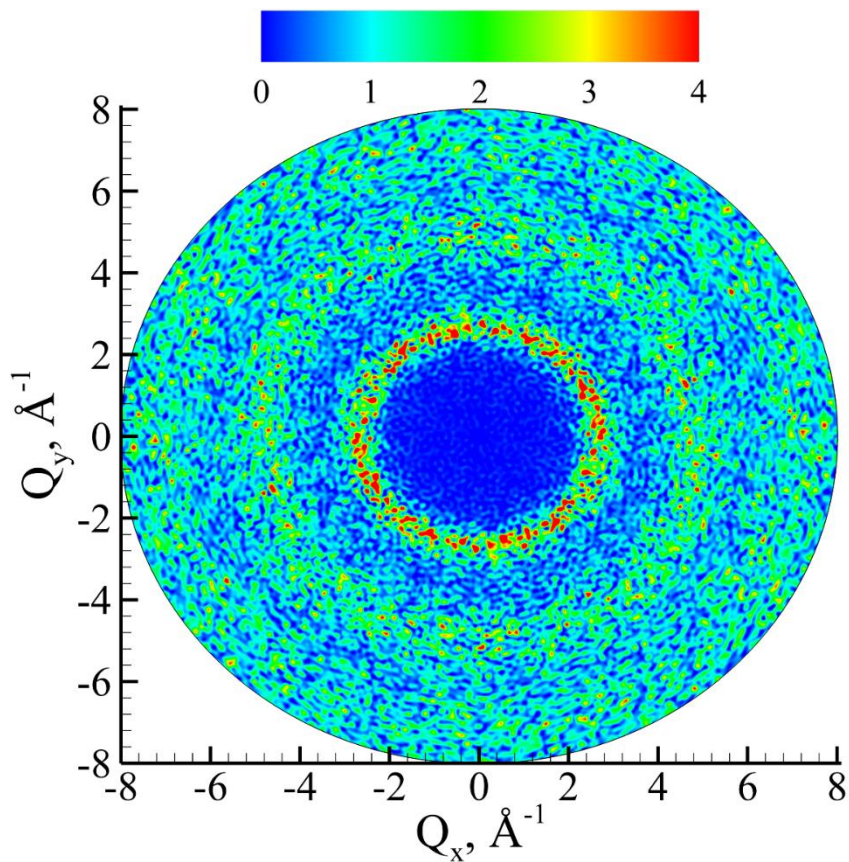
Below are two-dimensional diffraction profiles calculated for the input examples and list of parameter values used by the software to obtain them.

**FCC\_32.xyz**



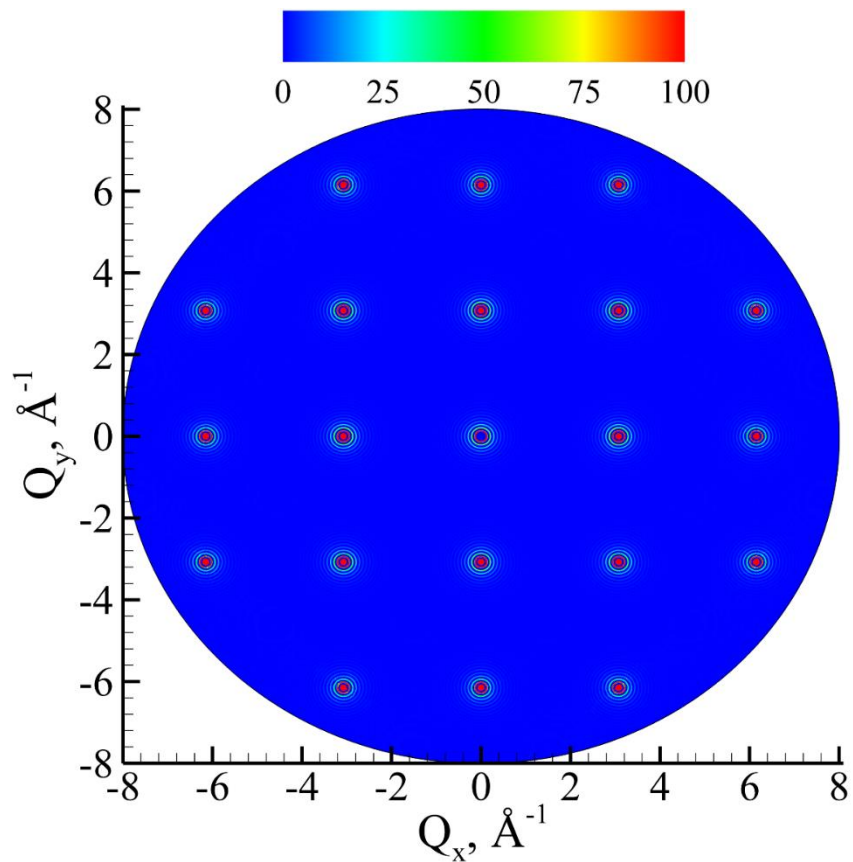
**Parameters:** NB = 300, Nbins = 2000, NRCFLAG = 2, WFLAG = 1, dtheta = 0.5, Qmax = 8.0, Rcut = 30.0, MULT\_FLAG = 1

**Liq\_32.xyz**



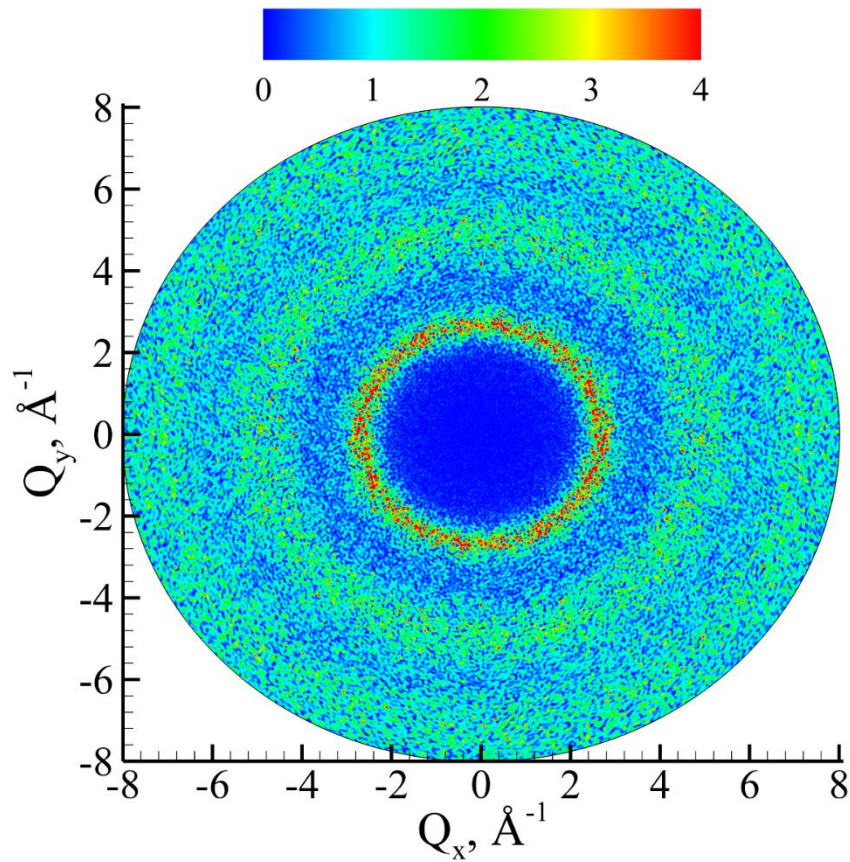
**Parameters:** NB = 300, Nbins = 2000, NRCFLAG = 1, WFLAG = 0, dtheta = 1.0, Qmax = 8.0, Rcut = 30.0, MULT\_FLAG = 1

**FCC\_256.xyz**



**Parameters:** NB = 600, Nbins = 2000, NRCFLAG = 1, WFLAG = 1, dtheta = 0.25, Qmax = 8.0, Rcut = 80.0, MULT\_FLAG = 0

**Liq\_256.xyz**



**Parameters:** NB = 300, Nbins = 2000, NRCFLAG = 1, WFLAG = 0, dtheta = 0.5, Qmax = 8.0, Rcut = 80.0, MULT\_FLAG = 1