Spectrum: a short User's Guide

Spectrum is a utility to calculate the dynamical structure factor in liquids from the data of the particles trajectories. It was developed to process data obtained with LAMMPS package.

1. How to use it?
First, compile `spectrum.cpp` with g++:

```
g++ spectrum.cpp –o spectrum
```

You'll get the executable file `spectrum`. Now you can use it by typing

```
./spectrum spectrum.inp
```

where `spectrum.inp` is the file with input parameters of the calculation. Its structure is described below, an example file is distributed with the utility. After the processing, you'll get a set of output files.

2. Input/output files.
The program obtains input parameters from the file you type in the command line. It is constructed as follows:

```
Number of particles:

1000

Simulation box size:

11.183163

Number of simulation steps:

300000

Number of steps to skip:

0

Simulation timestep:

0.005

Dump step:

10

Min length of wavevector:

0

Max length of wavevector:
```

```
3

Omega Step:

0.005

Log file:

spectrum_log.txt

Vectors output file:

vectors.txt

Dump file:

dumpfile.dump

F(k, t) file:

Fkt.txt

S(k, omega) output file:

dynf.txt

###
```

We hope most of the lines are verbose enough. It should be explained that:
1. Simulation box is supposed to be cubic, its “size” is edge length.
2. Particles trajectories are presented as the consequence of dumps of all particles positions at different moments of time. These dumps are separated by constant time intervals

`tau = 'Simulation timestep'*'Dump step'` (dump is performed each `'Dump step'` simulation steps),

observation time is

`'Simulation timestep'*'Number of simulation steps'`.

If you use LAMMPS, just put as the parameters 3, 5, 6 in input file your values from commands `run`, `timestep` and `dump`, accordingly.

You may set the initial moment you want to consider using the fourth parameter in the input file. It is sometimes useful if the initial conditions are not equilibrium and you’d like to just skip several steps.

Two parameters (7^{th} and 8^{th}) sets the boundaries of k to calculate the dynamical structure factor S(k, omega). Minimal value of omega is zero, maximal one is determined using the value of dump time interval.

The following lines set names of output files and file of particles trajectories (dump file).

The structure of **dump file** is following:

Dump file consists of distinct dumps of coordinates of all the particles in the system. Their number equals `'Number of simulation steps''Dump step'`. First `'Number of steps to skip''Dump step'` dumps are dumps you don't intend to consider and they won't be used in calculation. Each dump consists of:

- 9 lines which mean nothing for the program, you can leave them blank or write a commentary.
- `'Number of particles'` lines each of those contains 3 float numbers – coordinates of particles at the moment of time.

After each dump there is no blank lines, next dump begins right after the previous one (in new line).

If you use LAMMPS, you can create such a dump file by command (example):

```
dump id all custom 20 dumpfile.dump x y z
```

Output files are:

Log.
The program writes a primitive log which contains time at that some key operations were performed. You may use it for test purposes to understand how fast the program runs and which parts of calculation are the most time-consuming.

Vectors output file.
Contains all the wavevectors used for calculation. At the top of the file there are also several lines with some checkout information on the work of vectors generating algorithm.

F(k,t) output file.
Contains values of intermediate scattering function. This file consists of four columns. The first one contains the lengths of wavevector, the second one – values of frequency, third and fourth ones – values of real and imaginary parts of the F(k,t), respectively. The results for each wavevector are followed by 3 blank lines.

S(k, omega) output file.
Contains values of the dynamical structure factor. The structure is the same as for F(k, t), but the second column is omega.

3. How does it work?
First, the program calculates the set of suitable wavevectors from the condition:

$k = \left(n_1\vec{i} + n_2\vec{j} + n_3\vec{k}\right)\cdot\frac{2\pi}{L}$, where L is linear size of simulation box (cubic edge length), $n_1, n_2, n_3 \in \square$.

In the present implementation, $n_1, n_2, n_3 \geq 0$. Minimum and maximum values of k are set in the input file; minimum one can't be smaller than $\frac{2\pi}{L}$ and maximum one can't be larger than $\frac{2\pi}{a}$, where a is an average interparticle distance.

Calculation of the dynamical structure factor is performed as following:
1) Calculation of "statical structure factor":

$$\rho_{\vec{k}}(t) = \sum_{j=1}^{N} \exp[i\vec{k}\vec{R}_j(t)].$$

2) Calculation of the intermediate scattering function:

$$F(\vec{k},t) = \frac{1}{N}\left\langle \rho^*_{\vec{k}} \rho_{\vec{k}}(t) \right\rangle.$$

If number of dumps the program considers (all the dumps excluding several first dumps we skip) is less than 2000 then maximum t here equals `'Simulation timestep'*'Number of dumps'`/2, else it equals 1000.

3) Calculation of the dynamical structure factor:

$$S(\vec{k},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} F(\vec{k},t)\exp(i\omega t)dt.$$