

The kpoints.in input file

From GPUMD

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Purpose

This file is used to specify the k points needed for `src/phonon`.

File format

- The format of this file must be as follows:

```
N_kpoints
kx(0) ky(0) kz(0)
kx(1) ky(1) kz(1)
...
kx(N_kpoints-1) ky(N_kpoints-1) kz(N_kpoints-1)
```

- Here,
 - `N_kpoints` is the number of k points you want to consider.
 - The remaining lines give the k vectors (in units of $1/A$) you want to consider.

Tips

- The user has to make sure that the k vectors are defined in the reciprocal space with respect to the unit cell chosen in the `basis.in` file.

Related pages

- See the tutorial on phonon dispersion for an explicit example.

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