

The D.out output file

From GPUMD

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Purpose

- This file contains the dynamical matrices $D(\vec{k})$ at different k points.

File format

- It has $3 * N_{\text{basis}} * N_{\text{kpoints}}$ rows and $6 * N_{\text{basis}}$ columns, where N_{basis} is the number of basis atoms in the unit cell defined in the basis.in file and N_{kpoints} is the number of k points in the kpoints.in file.
- Each consecutive $3 * N_{\text{basis}}$ rows correspond to one k point. For each k point, the first $3 * N_{\text{basis}}$ columns correspond to the real part and the second $3 * N_{\text{basis}}$ columns correspond to the imaginary part. Schematically, the file is organized as:

```
D_real(k_0) D_imag(k_0)
D_real(k_1) D_imag(k_1)
...
```

- The matrix elements are in units of $\text{eV \AA}^{-2} \text{amu}^{-1}$.

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