

The force.out output file

From GPUMD

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Brief Description

This file contains the per-atom forces of the atoms sampled at a given frequency.

The keyword which produces the current file

- `dump_force`

File format

```
fx_1(1) fy_1(1) fz_1(1)
fx_2(1) fy_2(1) fz_2(1)
...
fx_N(1) fy_N(1) fz_N(1)
fx_1(2) fy_1(2) fz_1(2)
vx_2(2) fy_2(2) fz_2(2)
...
fx_N(2) fy_N(2) fz_N(2)
...
```

Explanations

- There are three columns, corresponding to the x , y , and z components of the force.
- Each N consecutive lines correspond to one frame at a given time point.
- The number of lines equals the number of frames times N .
- $fx_m(n)$ is the x component of the m -th atom in the n -th frame.
- $fy_m(n)$ is the y component of the m -th atom in the n -th frame.
- $fz_m(n)$ is the z component of the m -th atom in the n -th frame.
- Force components are in units of eV/Å.

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