

The velocity.out output file

From GPUMD

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Brief Description

This file contains the velocities of the atoms sampled at a given frequency.

The keyword which produces the current file

- `dump_velocity`

File format

```
vx_1(1) vy_1(1) vz_1(1)
vx_2(1) vy_2(1) vz_2(1)
...
vx_N(1) vy_N(1) vz_N(1)
vx_1(2) vy_1(2) vz_1(2)
vx_2(2) vy_2(2) vz_2(2)
...
vx_N(2) vy_N(2) vz_N(2)
...
```

Explanations

- There are three columns, corresponding to the x , y , and z components of the velocity.
- Each N consecutive lines correspond to one frame at a given time point.
- The number of lines equals the number the number of frames times N .
- $vx_m(n)$ is the x component of the m -th atom in the n -th frame.
- $vy_m(n)$ is the y component of the m -th atom in the n -th frame.
- $vz_m(n)$ is the z component of the m -th atom in the n -th frame.
- Velocity components are in units of \AA ps^{-1} .

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