

The dump velocity keyword

From GPUMD

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Purpose

Dump the atom velocities to a text file named v.out.

Grammar

```
dump_velocity interval <options>
```

- The interval parameter is the output interval (number of steps) of the atom velocities.
- The <options> can only be group now.
- The option group should have two parameters:

```
group grouping_method group_id
```

which means only dumping velocities of atoms in group `group_id` within the grouping method `grouping_method`. If this option is not used, velocities will be dumped for all the atoms.

Examples

Example 1

To dump all the velocities every 10 steps for a run, one can add

```
dump_velocity 10
```

before the run keyword.

Example 2

Similar to the above example, but only for atoms in group 1 within grouping method 2

```
dump_velocity 10 group 2 1
```

Output file

- v.out

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