

The dump force keyword

From GPUMD

[Jump to navigation](#)[Jump to search](#)

Contents

- 1 Purpose
- 2 Grammar
- 3 Examples
 - 3.1 Example 1
 - 3.2 Example 2
- 4 Output file

Purpose

Dump the atom forces to a text file named force.out.

Grammar

```
dump_force interval <options>
```

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

```
group grouping_method group_id
```

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

Examples

Example 1

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

```
dump_force 10
```

before the run keyword.

Example 2

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

```
dump_force 10 group 2 1
```

Output file

- force.out

Retrieved from "https://gpumd.zheyongfan.org/index.php?title=The_dump_force_keyword&oldid=21597"

-
- This page was last edited on 8 September 2020, at 21:00.