The dump force keyword

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Purpose

Dump the atom forces to a text file named f.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 shoul 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

• f.out

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