The dump velocity keyword

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Purpose

Dump the atom velocities to a text file named velocity.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 shoul have two parameters:

group grouping_method group_id

which means only dumping velocities of atoms in group <code>group_id</code> within the grouping method <code>grouping_method</code>. 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

velocity.out

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■ This page was last edited on 8 September 2020, at 20:59.