

The velocity keyword

From GPUMD

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Purpose

- This keyword is used to initialize the velocities of the atoms in the system according to a given temperature.

Grammar

- This keyword only has one parameter, which is the initial temperature of the system:

```
velocity initial_temperature
```

- The temperature is in units of kelvin (K).

Examples

Example 1

- For example, the command

```
velocity 10
```

means that one wants to set the initial temperature to 10 K.

Caveats

- The initial velocities generated do not follow the Maxwell distribution, but this is not a problem at all. During the MD simulation, Maxwell distribution will be automatically developed within a short time.
- The total linear and angular momenta are zeroed.
- If there are already velocity data in the `xyz.in` file, the initial temperature will not be used and the velocities will be initialized as those in the `xyz.in` file.

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