

The dump thermo keyword

From GPUMD

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Purpose

Dump some global thermodynamic quantities.

Grammar

- This keyword only requires a single parameter, which is the output interval (number of steps) of the global thermodynamic quantities:

```
dump_thermo interval
```

- This keyword will produce the output file thermo.out.

Examples

To dump the global thermodynamic quantities every 1000 steps for a run, one can add

```
dump_thermo 1000
```

before the run keyword.

Caveats

- This keyword is not propagating. That is, its effect will not be passed from one run to the next.

Output file

- thermo.out

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- This page was last edited on 22 August 2020, at 17:18.

