

The thermo.out output file

From GPUMD

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

Contents

- 1 Brief Description
- 2 The keyword which produces the current file
- 3 File format
- 4 Explanations

Brief Description

This file contains the global thermodynamic quantities sampled at a given frequency.

The keyword which produces the current file

- dump_thermo

File format

- If the simulation box is orthogonal, there are 9 columns in this output file, each containing the values of a quantity at increasing time points:

```
column  1 2 3 4  5  6  7  8  9
quantity T K U Px Py Pz Lx Ly Lz
```

- If the simulation box is triclinic, there are 15 columns in this output file, each containing the values of a quantity at increasing time points:

```
column  1 2 3 4  5  6  7  8  9 10 11 12 13 14 15
quantity T K U Px Py Pz ax ay az bx by bz cx cy cz
```

Explanations

- T is the temperature (in units of K)
- K is the kinetic energy (in units of eV) of the system
- U is the potential energy (in units of eV) of the system
- Px is the pressure (in units of GPa) in the x direction
- Py is the pressure (in units of GPa) in the y direction
- Pz is the pressure (in units of GPa) in the z direction
- Lx is the box length (in units of angstrom) in the x direction
- Ly is the box length (in units of angstrom) in the y direction
- Lz is the box length (in units of angstrom) in the z direction
- ax ay az bx by bz cx cy cz are the components (in units of angstrom) of the triclinic box matrix formed by the following vectors:

$$\mathbf{a} = a_x \mathbf{e}_x + a_y \mathbf{e}_y + a_z \mathbf{e}_z;$$

$$\begin{aligned}\mathbf{b} &= b_x \mathbf{e}_x + b_y \mathbf{e}_y + b_z \mathbf{e}_z; \\ \mathbf{c} &= c_x \mathbf{e}_x + c_y \mathbf{e}_y + c_z \mathbf{e}_z.\end{aligned}$$

Retrieved from "https://gpumd.zheyongfan.org/index.php?title=The_thermo.out_output_file&oldid=21352"

- This page was last edited on 23 August 2020, at 08:55.