

The heatmode.out output file

From GPUMD

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Brief Description

This file contains the modal heat current generated by the Green-Kubo Modal Analysis (GKMA) method.

The keyword which produces the current file

- `compute_gkma` in `run.in`.

File format

This file reads:

$$\begin{array}{ccccc}
 J_{1,1}^{x,in} & J_{1,1}^{x,out} & J_{1,1}^{y,in} & J_{1,1}^{y,out} & J_{1,1}^z \\
 J_{1,2}^{x,in} & J_{1,2}^{x,out} & J_{1,2}^{y,in} & J_{1,2}^{y,out} & J_{1,2}^z \\
 : & : & : & : & : \\
 J_{1,n}^{x,in} & J_{1,n}^{x,out} & J_{1,n}^{y,in} & J_{1,n}^{y,out} & J_{1,n}^z \\
 J_{2,1}^{x,in} & J_{2,1}^{x,out} & J_{2,1}^{y,in} & J_{2,1}^{y,out} & J_{2,1}^z \\
 : & : & : & : & :
 \end{array}$$

- Each output is in units of $\text{eV}^{3/2}\text{amu}^{-1/2}$
- The indices denote the output number (left) and the bin (right).
- Each output will have n bins which are determined by the `compute_gkma` keyword inputs.

Tips

- The thermo (<https://github.com/AlexGabourie/thermo>) Python package contains code to process this output file.

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