The compute hnema keyword

From GPUMD
Jump to navigationJump to search

Contents

- 1 Purpose
- 2 Grammar
- 3 Examples
  - 3.1 Example 1
  - 3.2 Example 2
  - 3.3 Example 3
- 4 Output file
- 5 Caveats
- 6 References

Purpose

The `compute_hnema` keyword is used to calculate the modal thermal conductivity using the Homogeneous Nonequilibrium Modal Analysis (HNEMA) method [Gabourie 2020].

Grammar

```
compute_hnema sample_interval output_interval Fe_x Fe_y Fe_z first_mode last_mode bin_option size
```

- `sample_interval` is the sampling interval (in number of steps) used to compute the heat modal heat current. Must be a divisor of `output_interval`.
- `output_interval` is the interval to output the modal thermal conductivity. Each modal thermal conductivity output is averaged over all samples per output interval.
- `Fe_x` is the x direction component of the external driving force $\mathbf{F_e}$ in units of Å^{-1}.
- `Fe_y` is the y direction component of the external driving force $\mathbf{F_e}$ in units of Å^{-1}.
- `Fe_z` is the z direction component of the external driving force $\mathbf{F_e}$ in units of Å^{-1}.
- `first_mode` is the first mode in the eigenvector.in file file to include in the calculation.
- `last_mode` is the last mode in the eigenvector.in file to include in the calculation.
- `bin_option` determines which binning technique to use: `bin_size` or `f_bin_size`.
- `size` defines how the modes are added to each bin. If `bin_option` = `bin_size`, then this is an integer describing how many modes are included per bin. If `bin_option` = `f_bin_size`, then binning is by frequency and this is a float describing the bin size in THz.

Examples

Example 1

```
compute_hnema 10 1000 0.000008 0 0 1 27216 f_bin_size 1.0
```

This means that (1) you want to calculate the modal thermal conductivity with the HNEMA method; (2) the modal thermal conductivity will be sampled every 10 steps; (3) the average of all sampled modal thermal conductivities will be output every 1000 time steps; (4) the external driving force is along the x direction and has a magnitude of 0.8×10^{-5} Å^{-1} (5) the range of modes you want to include of calculations are from 1 to 27216; (6) you want to bin the modes by frequency with a bin size of 1 THz.

Example 2

```
compute_hnema 10 1000 0.000008 0 0 1 27216 bin_size 1
```

This example is identical to Example 1, except the modes are binned by count. Here, each bin only has one mode (i.e. all modes are output).

Example 3

```
compute_hnema 10 1000 0.000008 0 0 1 27216 bin_size 10
```

This example is identical to Example 2, except each bin has 10 modes.

Output file

- kappamode.out

Caveats

- This computation can be very memory intensive. The memory requirements are comparable to the size of the eigenvector.in file.
- This keyword cannot be used in the same run as the compute_gkma keyword. The keyword used last will be used in the run.

References

- [Gabourie 2020] Alexander J. Gabourie, Zheyong Fan, and Eric Pop, in preparation.