The compute gkma keyword

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Purpose

The `compute_gkma` keyword is used to calculate the modal heat current using the Green-Kubo Modal Analysis (GKMA) method [Lv 2016].

Grammar

```
compute_gkma sample_interval 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.
- `first_mode` is the first mode in the eigenvector.in 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_gkma 10 1 27216 f_bin_size 1.0
```

This means that (1) you want to calculate the modal heat current with the GKMA method; (2) the modal heat flux will be sampled every 10 steps; (3) the range of modes you want to include of calculations are from 1 to 27216; (4) you want to bin the modes by frequency with a bin size of 1 THz.

Example 2

```
compute_gkma 10 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_gkma 10 1 27216 bin_size 10
```

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

Output file

- heatmode.out

Caveats

- This computation can be very memory intensive. The memory requirements are comparable to the size of the eigenvector.in file.
- Depending number of steps run, sampling interval, and number of bins, the heatmode.out output file can become very large as well (i.e. many GBs)
- This keyword cannot be used in the same run as the compute_hnema keyword. The keyword appeared last will be used in the run.

References

- [Lv 2016] Wei Lv and Asegun Henry, *Direct calculation of modal contributions to thermal conductivity via Green-Kubo modal analysis* (https://doi.org/10.1088/1367-2630/18/1/013028), New J. Phys. **18**, 013028 (2016).