The kappamode.out output file

From GPUMD
Jump to navigationJump to search

Contents

Brief Description

This file contains the modal thermal conductivity generated by the Homogeneous Nonequilibrium Modal Analysis (HNEMA) method.

The keyword which produces the current file

- compute_hnema in run.in.

File format

This file reads:

$$
\begin{matrix}
\kappa_{1,1}^{x,in} & \kappa_{1,1}^{x,out} & \kappa_{1,1}^{y,in} & \kappa_{1,1}^{y,out} & \kappa_{1,1}^{z} \\
\kappa_{1,2}^{x,in} & \kappa_{1,2}^{x,out} & \kappa_{1,2}^{y,in} & \kappa_{1,2}^{y,out} & \kappa_{1,2}^{z} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\kappa_{1,n}^{x,in} & \kappa_{1,n}^{x,out} & \kappa_{1,n}^{y,in} & \kappa_{1,n}^{y,out} & \kappa_{1,n}^{z} \\
\kappa_{2,1}^{x,in} & \kappa_{2,1}^{x,out} & \kappa_{2,1}^{y,in} & \kappa_{2,1}^{y,out} & \kappa_{2,1}^{z} \\
\vdots & \vdots & \vdots & \vdots & \vdots
\end{matrix}
$$

- Each output is in units of $\mathrm{Wm^{-1}K^{-1/2}}$
- The indices denote the output number (left) and the bin (right).
- Each output will have n bins which are determined by the compute_hnema keyword inputs.

Tips

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

- This page was last edited on 11 August 2020, at 21:27.