The kappa.out output file

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Brief Description

This file contains the running thermal conductivity (RTC) from the HNEMD method.

The keyword which produces the current file

- compute_hnemd in run.in

File format

- This file reads:
    - column 1: $\kappa_x^{\text{in}}(t)$ (in units of W/mK)
    - column 2: $\kappa_x^{\text{out}}(t)$ (in units of W/mK)
    - column 3: $\kappa_y^{\text{in}}(t)$ (in units of W/mK)
    - column 4: $\kappa_y^{\text{out}}(t)$ (in units of W/mK)
    - column 5: $\kappa_z^{\text{tot}}(t)$ (in units of W/mK)

- The RTC have been decomposed as described in this paper (https://doi.org/10.1103/PhysRevB.99.06430 8). This decomposition is useful for 2D materials but is not necessary for 3D materials. For 3D materials, one can sum up some columns to get the conventional data. That is:

$$\kappa_x^{\text{tot}}(t) = \kappa_x^{\text{in}}(t) + \kappa_x^{\text{out}}(t);$$

$$\kappa_y^{\text{tot}}(t) = \kappa_y^{\text{in}}(t) + \kappa_y^{\text{out}}(t).$$

Tips

- Only the potential part of the heat current has been considered. To simulation systems in which the convective heat current is important, one needs to modify the code.

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- This page was last edited on 3 June 2019, at 17:01.