The compute hnemd keyword

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Purpose

This keyword is used to calculate the thermal conductivity using the HNEMD method [Fan 2019].

Grammar

```
compute_hnemd output_interval Fe_x Fe_y Fe_z
```

- The first parameter is the output interval.
- The next three parameters are the x, y, and z components of the external driving force $\vec{F}_{\rm e}$ in units of Å^{-1}.
- Usually, there should be only one nonzero component of $\vec{F}_{\rm e}$. According to Eq. (8) of [Fan 2019]:
  - Using a nonzero x component of $\vec{F}_{\rm e}$, one can obtain the xx, yx and zx components of the thermal conductivity tensor.
  - Using a nonzero y component of $\vec{F}_{\rm e}$, one can obtain the xy, yy and zy components of the thermal conductivity tensor.
  - Using a nonzero z component of $\vec{F}_{\rm e}$, one can obtain the xz, yz and zz components of the thermal conductivity tensor.

Examples

Example 1

- An example of the keyword is:

```
compute_hnemd 1000 0.00001 0 0
```

- This means that
  - you want to calculate the thermal conductivity using the HNEMD method;

    - the thermal conductivity will be averaged and output every 1000 steps (the heat current is sampled for every step);
    - the external driving force is along the x direction and has a magnitude of 10^{-5} Å^{-1}.
- Note that one should control the temperature when using this keyword. Otherwise, the system will be heated up by the external driving force. **For this purpose, the Nose-Hoover chain thermostat is recommended. The Langevin thermostat cannot be used for this purpose because it will affect the dynamics of the system.**

Example 2

```
compute_hnemd 1000 0 0.00001 0
```

- This is similar to the above example, but the external driving force is applied along the y direction.

Output file

- kappa.out

Related tutorial

- Tutorial: Thermal transport from NEMD and HNEMD

References

- [Fan 2019] Zheyong Fan, Haikuan Dong, Ari Harju, and Tapio Ala-Nissila, *Homogeneous nonequilibrium molecular dynamics method for heat transport and spectral decomposition with many-body potentials* (https://doi.org/10.1103/PhysRevB.99.064308), Phys. Rev. B **99**, 064308 (2019).