MedeA Thermal Conductivity: Reliable Heat Transport Properties from Classical Simulations

Contents

Key Benefits of *MedeA Thermal Conductivity*

- Automatic analysis including the fitting of results
- Quick and easy validation based on graphs, reported fitting errors, and access to all intermediate results through the convenient web interface
- Integrated with *MedeA Forcefields* for advanced forcefield handling and assignment

Note: Generally, there are two contributions to the thermal conductivity of any material:

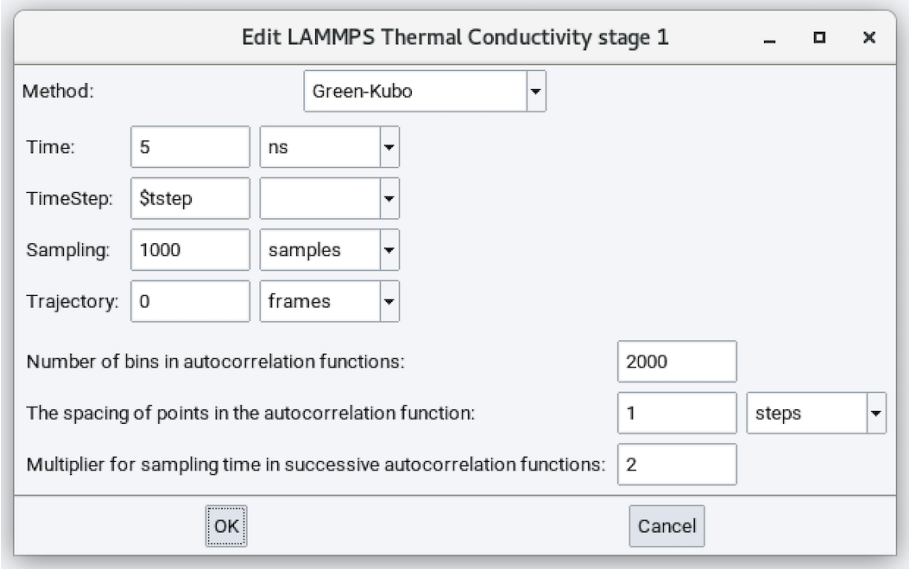
- Electronic contribution: depends on the electronic band structure, electron scattering, and electron-phonon interaction.
- Lattice contribution: depends mainly on the phonons (atom vibrations) and phonon scattering.

MedeA Thermal Conductivity calculates the lattice contribution to the thermal conductivity using forcefield methods. When necessary, you may also use *MedeA VASP* and *MedeA Electronics* to calculate the electronic contribution.

1 Equilibrium Molecular Dynamics (EMD)

The equilibrium molecular dynamics (EMD) method for computing the thermal conductivity, also known as the Green–Kubo method, uses the integral of the autocorrelation function of the heat flux. This method is only applicable for homogeneous configurations, i.e., no defects, interfaces, multiple phases, etc. The required length of the simulation depends on the thermal conductivity, with higher conductivities requiring longer simulation times. The EMD method provides reasonable approximations for systems with small atomic charges, such as hydrocarbons, many semiconductor alloys, etc. A significant advantage is that only moderate system sizes are required.

DOCUMENTATION



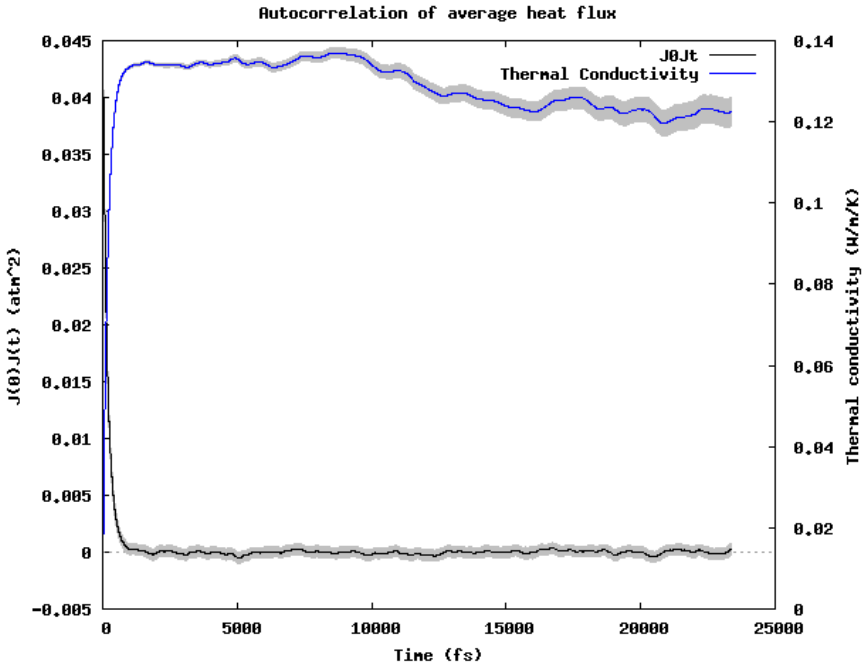
- *Method*: Green–Kubo.
- *Time*: Duration of the simulation run.
- *Time Step*: Time step size employed in solving the equations of motion.
- *Sampling:* Number of samples employed in performing averaging. This parameter does not affect dynamics.
- *Trajectory:* Number of trajectory frames saved during the molecular dynamics calculation. This parameter does not affect dynamics.
- *Number of bins in autocorrelation function*: The default is `2000`.
- *The spacing of points in the autocorrelation function*: The default is `1` steps.
- *Multiplier for sampling time in successive autocorrelation functions*: The default is `2`.

After completing a simulation, results are written to *Job.out*. For example:

```
Stage 4.4: Thermal conductivity using Green-Kubo, NVE integration for 5 ns with a timestep of 1 fs
        The autocorrelation of the heat flux uses 2000 bins, starting with sampling every step,
        then every 2 steps, then every 4, etc.
              Property         Value   +/- Uncertainty    Units      After Steps   % Run
        -----------------  ----------     ----------- ------------ ------------ -------
                        t:  5000000.0                  fs
                        T:     296.43 +/- 0.47         K                       0     0.0%
                        P:     2911.9 +/- 7.6          atm                     0     0.0%
                        V:    24036.6 +/- 0            Ang^3                   0     0.0%
                      rho:    1.41286 +/- 0            g/mL                    0     0.0%
                   Etotal:   -289.408 +/- 0.03         kJ/mol                  0     0.0%
                     Epot:    -2178.6 +/- 3            kJ/mol                  0     0.0%
                     Ekin:     1889.2 +/- 3            kJ/mol                  0     0.0%
                     Evdw:    -2178.6 +/- 3            kJ/mol                  0     0.0%
                    Ecoul:           0 +/- 0            kJ/mol                  0     0.0%


     Property     Direct Integral       Fit        RMS        Units   Direct Time    %       Fit Time     %
--------------- ------------------- ---------- ---------- ---------- ---------- ---------- ---------- ---------
       lambda x  0.12289 +/- 0.00056    0.13654    0.00026      W/m/K       7220       0.1%        934       0.0%
       lambda y  0.13786 +/- 0.00035    0.14067    0.00094      W/m/K       4520       0.1%       3472       0.1%
       lambda z   0.1307 +/- 0.0012      0.1355     0.0002      W/m/K      14240       0.3%       2638       0.1%
 lambda average   0.1234 +/- 0.0026      0.1343     0.0002      W/m/K      21216       0.4%       1162       0.0%
```

Additionally, visualization of the autocorrelation function and its integral, the thermal conductivity, are available as {*stage_id*}*_JJt_decay_average.gif*. For example:



Hint: If you are modeling fluid systems and would also like to calculate viscosity from the autocorrelation function of the stress tensor using the Green–Kubo algorithm, and you have a license for *MedeA Viscosity*, you can use a checkbox in the **Viscosity** stage to calculate both the thermal conductivity and the viscosity:

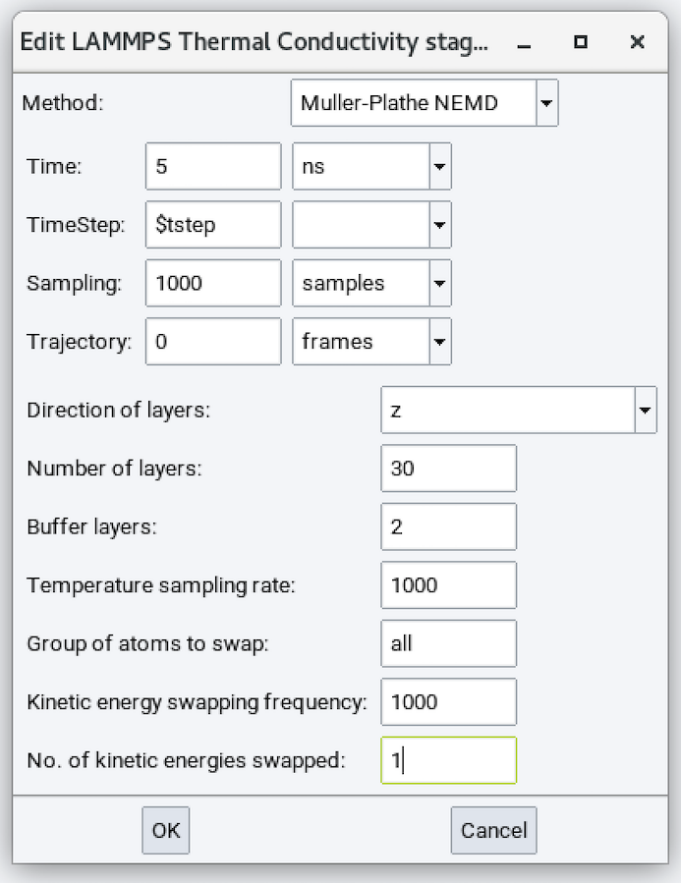
☐ *Also calculate thermal conductivity*

This option reduces computational expense when you would like to calculate both the viscosity and the thermal conductivity in a single stage!

2 Reverse Non-Equilibrium Molecular Dynamics Method (RNEMD)

The reverse non-equilibrium molecular dynamics method, also known as the Müller-Plathe [1] method, induces a temperature gradient (heat flux) by performing kinetic energy swaps between atoms in hot and cold regions, and monitors the resulting temperature profile. The thermal conductivity is calculated as the ratio of the heat flux to the slope of the temperature profile. The method applies to all systems but requires elongated cells in the direction of heat transfer. Higher conductivities, which arise from longer phonon mean free path lengths, require correspondingly longer cells. The effect of the cell cross-sectiontional area and length should ideally be examined, and the heat transfer rate (flux) may need to be optimized, requiring some user intervention.

[1] Florian Müller-Plathe and Dirk Reith, "Cause and Effect Reversed in Non-Equilibrium Molecular Dynamics: an Easy Route to Transport Coefficients", *Computational and Theoretical Polymer Science* 9, no. 3 (1999): 203-209.



The different parameters are:

- *Method*: Muller-Plathe NEMD
- *Direction of layers*: Direction in which the temperature gradient should be established.
- *Number of layers*: Divides the above direction into this many layers to calculate the temperature profile.
- *Buffer layers*: Number of layers on and near the boundary that are not used in the final analysis.
- *Temperature sampling rate*: Sample temperature profile every this many steps. The default value of `1000` is usually acceptable.
- *Group of atoms to swap*: Defaults to all.
- *Kinetic energy swapping frequency*: Defaults to `1000`.
- *No. of kinetic energies swapped*: Defaults to `1`.

After completing a simulation, results are written to *Job.out*. For example:

```
Stage 4.4: Thermal conductivity using Muller-Plathe NEMD, NVE integration for 5 ns with a timestep of 1 fs
           1 kinetic energies from group 'all' are interchanged every 1000 timesteps using 30 layers in z direction
             Property         Value   +/- Uncertainty     Units       After Steps   % Run
------------------  -----------      ------------ -------------- ------------ -------
                 t:  5000000.0                    fs
                 T:     302.24 +/- 0.42           K                           0     0.0%
                 P:     1003.5 +/- 5.8            atm                         0     0.0%
                 V:    32748.5 +/- 0              Ang^3                       0     0.0%
               rho:     1.0127 +/- 0              g/mL                        0     0.0%
            Etotal:    162.819 +/- 0.04           kJ/mol                      0     0.0%
              Epot:    -1718.1 +/- 2.6            kJ/mol                      0     0.0%
              Ekin:     1880.9 +/- 2.6            kJ/mol                      0     0.0%
              Evdw:    -1718.1 +/- 2.6            kJ/mol                      0     0.0%
             Ecoul:          0 +/- 0              kJ/mol                      0     0.0%
                 t:  5000000.0                    fs
            deltaQ: 44739.100364551974                kJ/mol
               dQ/dt:   0.008882 +/- 2.7e-05      kJ/mol/fs                 500    10.0%


        dT/dx(left):       2.59 +/- 0.17         K/Ang                       0     0.0%
           T0(left):      244.8 +/- 3.2          K                           0     0.0%
       dT/dx(right):       2.74 +/- 0.18         K/Ang                       0     0.0%
          T0(right):      242.7 +/- 4.9          K                           0     0.0%

             dT/dx:       2.67 +/- 0.16         K/Ang                       0     0.0%
                T0:      243.7 +/- 3.1          K                           0     0.0%
            lambda:     0.0697 +/- 0.0041       W/(m*K)                   500    10.0%
```

Additionally, visualization of the temperature profiles is available as {*stage_id*}*_average_temperature_profile.png*. For example: