Viscosity

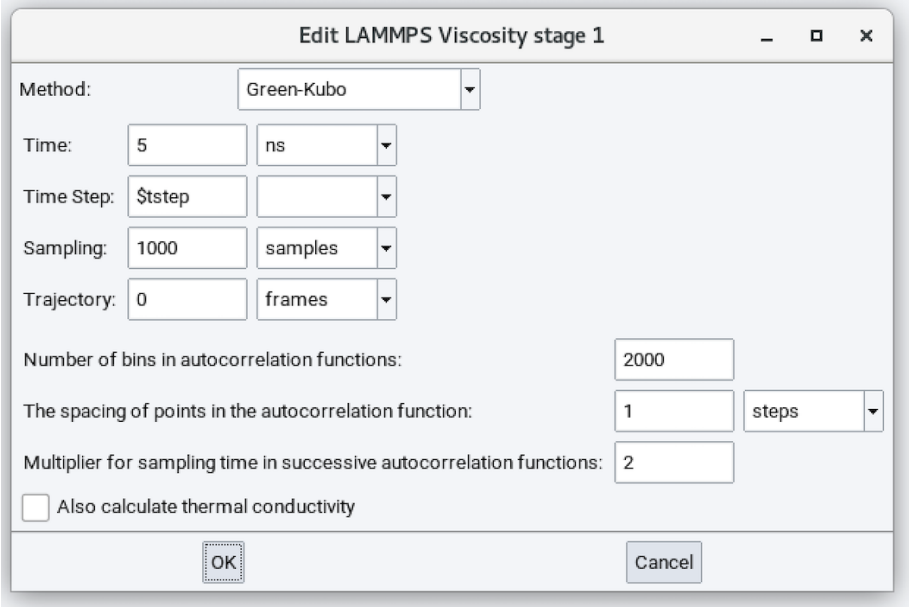
Contents

Key Benefits of *MedeA Viscosity*

- Automatic analysis including 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* Forcefield for advanced forcefield handling and assignment

1 Equilibrium Molecular Dynamics (EMD)

This is also known as the Green-Kubo Method, which calculates viscosity using the integral of the auto-correlation function of the shear (off-diagonal) components of the stress tensor. It is only applicable for homogeneous configurations, i.e., no defects, interfaces, multiple phases, etc. The required length of the simulation depends on the viscosity: higher viscosities require longer simulation times. Good approximations can be obtained for many organic systems, such as hydrocarbons, alcohols, ethers, esters, etc. A significant advantage is that it requires only moderate system sizes.



- *Method*: Green-Kubo
- *Time*: Duration of the simulation run (defaults to 5 ns).
- *Time Step*: Time step size employed in solving the equations of motion.

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- *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*: 2000
- *The spacing of points in the autocorrelation function*: 1 step
- *Multiplier for sampling time in successive autocorrelation functions*: 2
- ☐ *Also calculate thermal conductivity*: an option to also record the autocorrelation function of the heat flux and estimate thermal conductivity from the same dynamics trajectory.

Note: This option is only visible if you also have the *MedeA Thermal Conductivity* license.

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

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

```
Stage 6.4: Viscosity using Green-Kubo, NVE integration for 4 ns with a timestep of 1 fs
        The autocorrelation of the pressure tensor uses 2000 bins, starting with sampling every step,
        then every 2 steps, then every 4, etc.
              Property         Value   +/- Uncertainty    Units      After Steps   % Run
        ------------------  ----------     ----------- ------------- ------------ -------
                         t:  4000000.0                  fs
                         T:     295.61 +/- 0.58         K                       0     0.0%
                         P:       2925 +/- 11           atm                     0     0.0%
                         V:    25163.9 +/- 0            Ang^3                   0     0.0%
                       rho:     1.3497 +/- 0            g/mL                    0     0.0%
                    Etotal:    -324.54 +/- 0.031        kJ/mol                  0     0.0%
                      Epot:    -2208.5 +/- 3.7          kJ/mol                  0     0.0%
                      Ekin:     1883.9 +/- 3.7          kJ/mol                  0     0.0%
                      Evdw:    -2208.5 +/- 3.7          kJ/mol                  0     0.0%
                     Ecoul:           0 +/- 0            kJ/mol                  0     0.0%

     Property     Direct Integral       Fit        RMS        Units    Direct Time    %       Fit Time     %
--------------- -------------------- ---------- ---------- ---------- ---------- ---------- ---------- ---------
          eta x  0.18833 +/- 0.00064    0.17312    0.00062       mPa*s       4700       0.1%        593       0.0%
          eta y  0.16618 +/- 0.00029    0.16403    0.00077       mPa*s       1449       0.0%        498       0.0%
          eta z   0.1804 +/- 0.0065      0.1589       0.001      mPa*s      48512       1.2%        467       0.0%
    eta average   0.1796 +/- 0.0087      0.1635      0.0009      mPa*s      39200       1.0%        493       0.0%
```

Additionally, visualization of the autocorrelation function and the viscosity integral are available in the file {*stage_id*}*_SSt_decay_average.gif*. For example:

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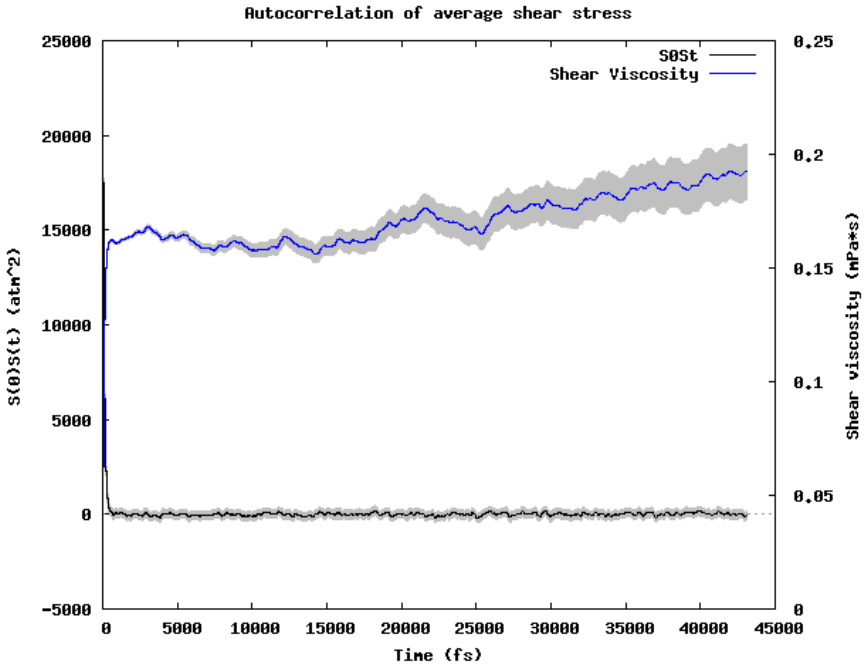

2 Reverse non-equilibrium molecular dynamics method (RNEMD)

This is also known as the Müller-Plathe [1] method, which induces a flow gradient (shear velocity or momentum flux) by performing momentum swaps between positive and negative shearing atoms, and monitoring the resulting velocity profile. Viscosity is then calculated using the slope of the induced shear velocity profile.

This method applies to all systems but requires elongated cells in the direction of flow. Higher viscosities, which arise from stronger interactions, require correspondingly longer cells. The effect of the cell cross-section should ideally be examined, and momentum transfer rate 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.

DOCUMENTATION

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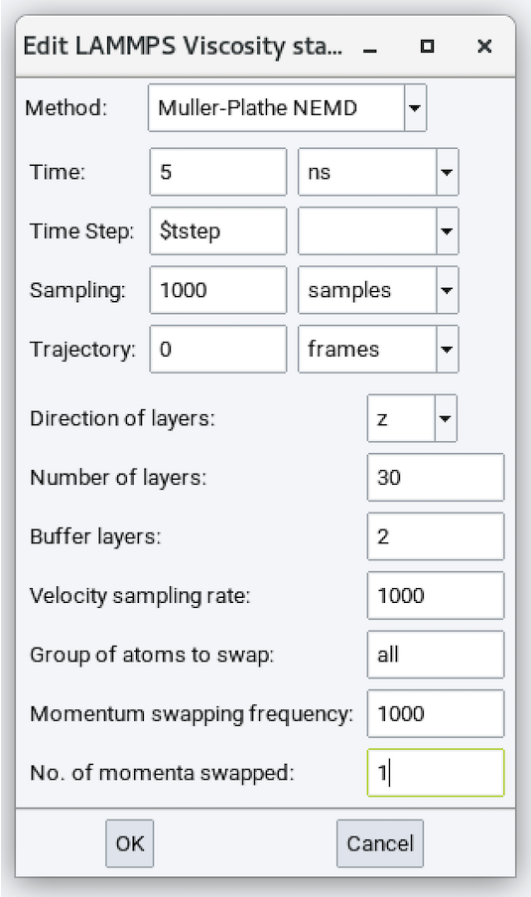

The required parameters are:

- *Method*: Muller-Plathe NEMD
- *Direction of layers*: Direction in which the shear velocity gradient should be established.
- *Number of layers*: Divides the above direction into this many layers to calculate the shear velocity profile.
- *Buffer layers*: Number of layers on and near the boundary that are not used in the final analysis.
- *Velocity scaling rate*: Sample shear velocity every this many steps. The default value of 1000 can usually be accepted.
- *Group of atoms to swap*: Defaults to all.
- *Momentum swapping frequency*: Defaults to 1000.
- *No. of momenta swapped*: Defaults to 1.

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

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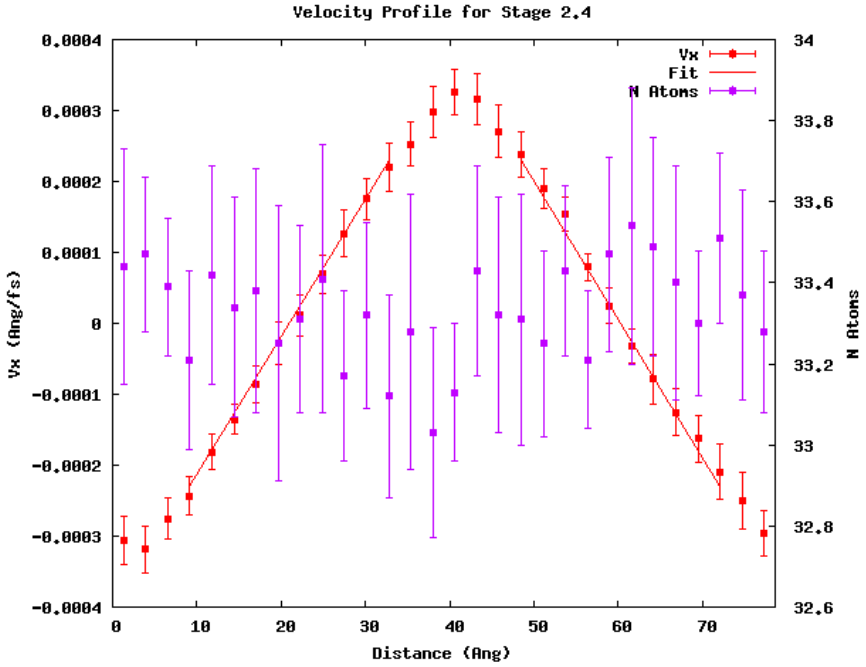
```
Stage 2.5: Thermal conductivity using Muller-Plathe NEMD, NVE integration for 1 ns with a timestep of 1 fs
           1 kinetic energies from group 'all' are interchanged every 1000 timesteps using 30 layers in z direction
             Property         Value   +/- Uncertainty    Units      After Steps   % Run
------------------------  -----------  ----------- ------------- ------------ -------
                      t:  1000000.0                 fs
                 deltaQ: 3807.2857676616081                kJ/mol
                   dQ/dt:     0.00382 +/- 2.5e-05     kJ/mol/fs               0     0.0%
                      t:  1000000.0                 fs
                      T:       99.67 +/- 0.16        K                       0     0.0%
                      P:        58.9 +/- 2.2         atm                     0     0.0%
                      V:     49140.9 +/- 0           Ang^3                   0     0.0%
                    rho:     1.34976 +/- 0           g/mL                    0     0.0%
                 Etotal:   -4192.679 +/- 0.046       kJ/mol                  0     0.0%
                   Epot:     -5434.5 +/- 1.9         kJ/mol                  0     0.0%
                   Ekin:      1241.8 +/- 2           kJ/mol                  0     0.0%
                   Evdw:     -5434.5 +/- 1.9         kJ/mol                  0     0.0%
                  Ecoul:           0 +/- 0           kJ/mol                  0     0.0%


             dT/dx(left):       0.434 +/- 0.073     K/Ang                   0     0.0%
                T0(left):        90.5 +/- 2         K                       0     0.0%
            dT/dx(right):        0.51 +/- 0.11      K/Ang                   0     0.0%
               T0(right):        88.8 +/- 1.9       K                       0     0.0%

                   dT/dx:       0.471 +/- 0.084     K/Ang                   0     0.0%
                      T0:        89.7 +/- 1.7       K                       0     0.0%
                  lambda:       0.108 +/- 0.019     W/(m*K)                 0     0.0%
```

Additionally, visualization of the shear velocity profiles is available as {*stage_id*}*_average_velocity_profile.png*. For example:



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