

Winmostar tutorial

Gromacs

Viscosity · Dielectric constant

V8.007

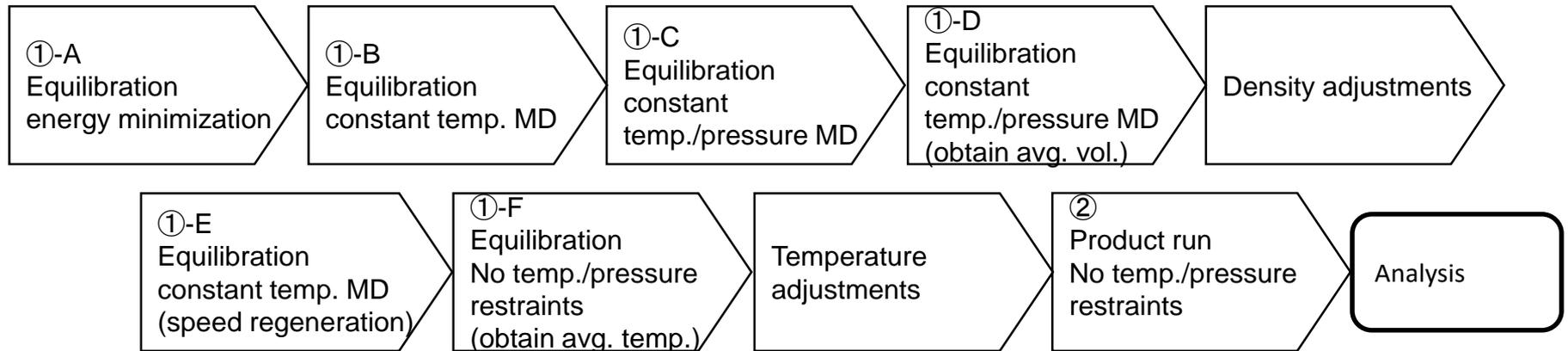
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Summary

In this tutorial, we will calculate viscosity and dielectric constant of liquid of water. Product run will be executed on a NVE ensemble (no restraints on temperature/pressure) to calculate physical properties sensitive to delicate movements of molecules. We will also show equilibration procedure for calculating NVE ensemble under target temperature/pressure.



Notes:

- The number of steps required for equilibration depends on the type of molecule and initial density varies and may be different from this example.
- To obtain accurate and reproducible results, the calculation requires long simulation times.
- The method for interaction calculations and/or the force field also affect the simulation results.

Configuration

You must set up Cygwin to use Gromacs on Winmostar.

- Obtain the installer for Cygwin, which contains the all programs needed by Winmostar, at https://winmostar.com/en/manual_en.html.

2. Installation Guides for Solvers

For Windows

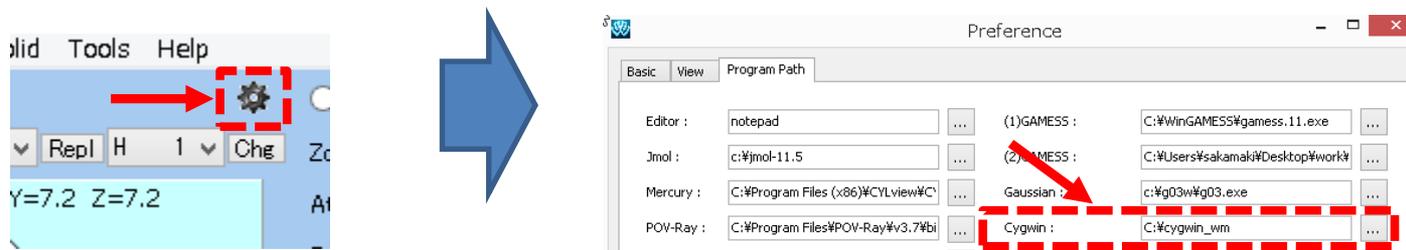
[cygwin_wm_v7_20160926.exe\(413MB\)](#) ※NWChem/Gromacs/Amber Window Build Package(Cygwin)

(For Experts)[NWChem/Gromacs/Amber Build with Cygwin](#) ※we recomend to use cygwin_wm_v7_20160926.exe

[GAMESS Installation Guide](#)

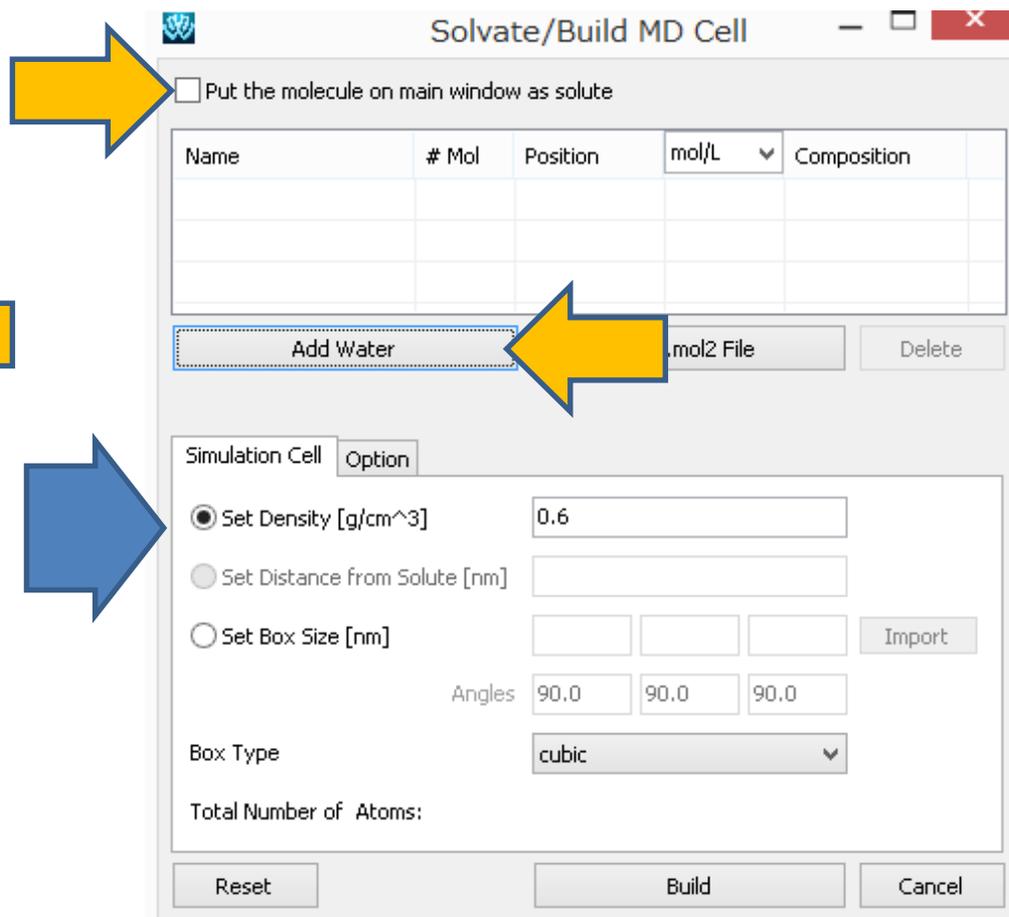
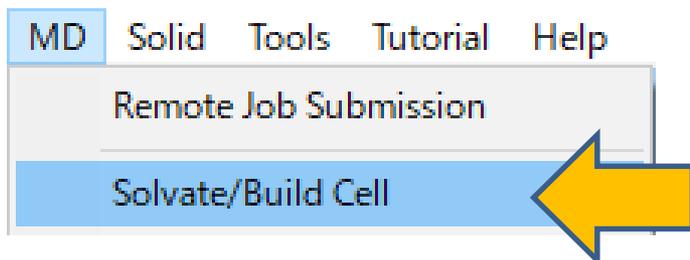
[LAMMPS Installation Guide](#)

- When you change the installation path for Cygwin from the default one, specify it on the preference panel.



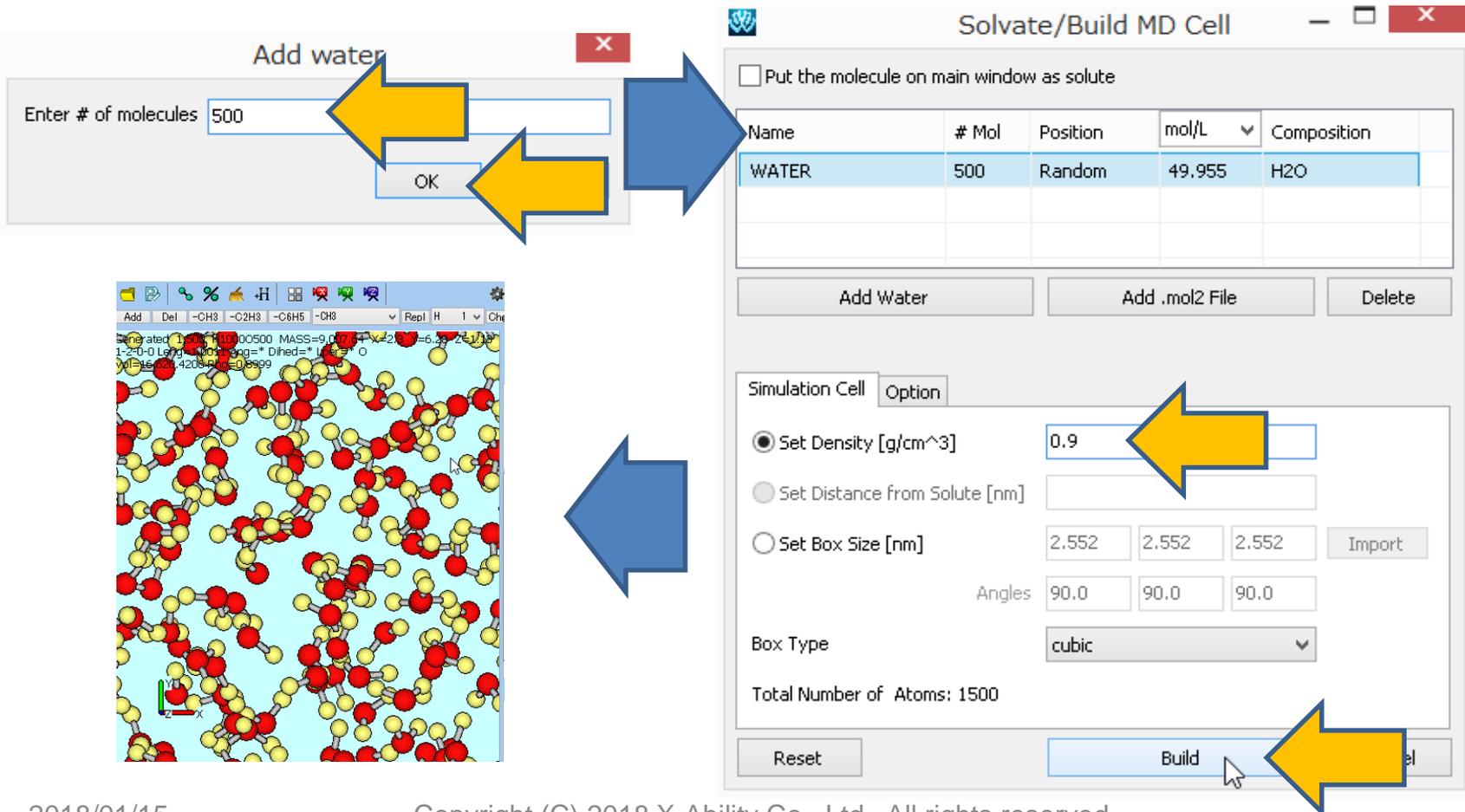
I. Build a simulation cell

1. Click **MD | Solvate/Build Cell**.
2. Uncheck **Put the molecule on main window as solute**.
3. Click **Add Water**.



I. Build a simulation cell

1. Set **Enter # of molecules** to **500**, then click **OK**.
2. Set **Set Density** to **0.9**, then click **Build**.



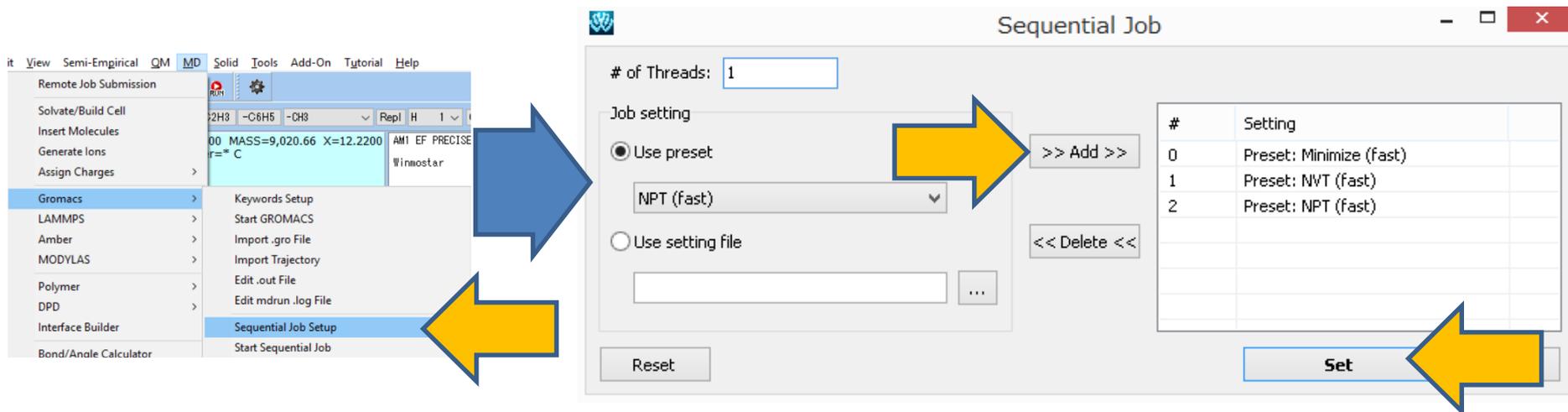
The screenshot shows the 'Solvate/Build MD Cell' window. In the top-left, an 'Add water' dialog box has 'Enter # of molecules' set to 500 and the 'OK' button highlighted. A yellow arrow points from this dialog to the main window. In the main window, the 'Simulation Cell' section has 'Set Density [g/cm³]' set to 0.9, with a yellow arrow pointing to the input field. Below this, the 'Build' button is highlighted with a yellow arrow. A blue arrow points from the 'Build' button to a 3D ball-and-stick model of a water simulation cell. The table in the main window is as follows:

Name	# Mol	Position	mol/L	Composition
WATER	500	Random	49.955	H2O

Other settings in the 'Simulation Cell' section include: 'Set Box Size [nm]' (2.552, 2.552, 2.552), 'Angles' (90.0, 90.0, 90.0), and 'Box Type' (cubic). The 'Total Number of Atoms' is 1500.

II. Equilibration (A - C)

1. Select **MD | Gromacs | Sequential Job Setup**.
2. Set Use preset to **Minimize (fast)** and click **>>> Add >>>**
3. Set Use preset to **NVT (fast)** and click **>>> Add >>>**
4. Set Use preset to **NPT (fast)** and click **>>> Add >>>**
5. After sequentially setting **Use presets**, click **Set**.
6. Next, select **MD | Gromacs | Start Sequential Job** and save files to begin job.



Sequential Job

of Threads: 1

Job setting

Use preset

NPT (fast)

Use setting file

>>> Add >>>

<<< Delete <<<

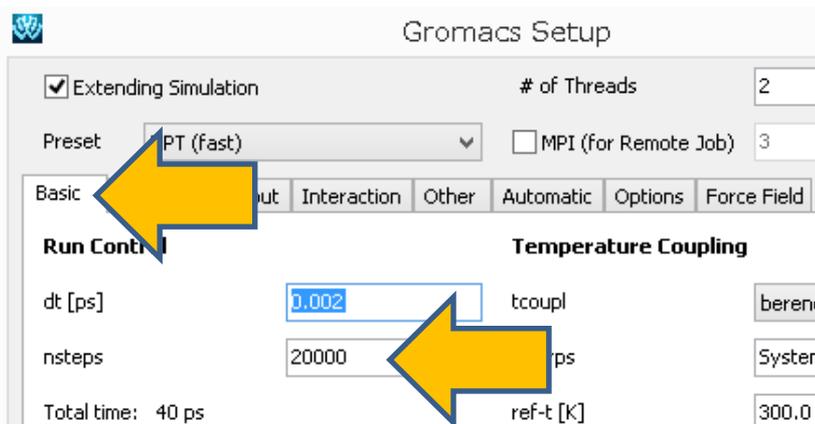
#	Setting
0	Preset: Minimize (fast)
1	Preset: NVT (fast)
2	Preset: NPT (fast)

Reset

Set

II. Equilibration (D) + Density Adjustment

1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. In the **Basic** tab, set **nsteps** to **25000**.
3. In the **Automatic** tab, check box for **Rescale box size...**
3. Click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.



Gromacs Setup

Extending Simulation # of Threads 2

Preset NPT (fast) MPI (for Remote Job) 3

Basic Output Interaction Other Automatic Options Force Field

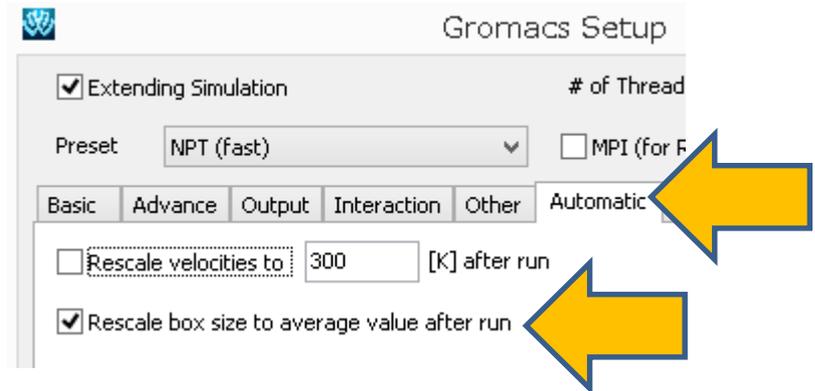
Run Control

dt [ps] 0.002 tcoupl berend

nsteps 20000 ps System

Total time: 40 ps ref-t [K] 300.0

Yellow arrows point to the 'Basic' tab, the 'nsteps' input field, and the 'dt' input field.



Gromacs Setup

Extending Simulation # of Thread

Preset NPT (fast) MPI (for F

Basic Advance Output Interaction Other Automatic

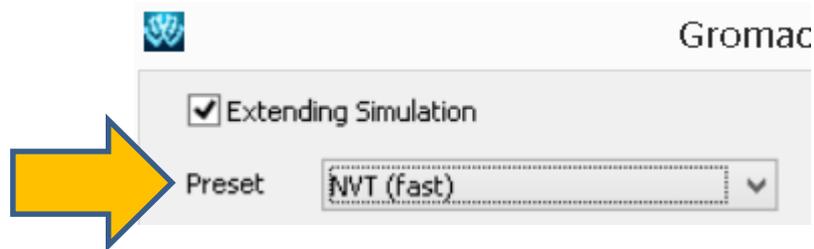
Rescale velocities to 300 [K] after run

Rescale box size to average value after run

Yellow arrows point to the 'Automatic' tab, the 'Rescale box size...' checkbox, and the 'Rescale velocities to' input field.

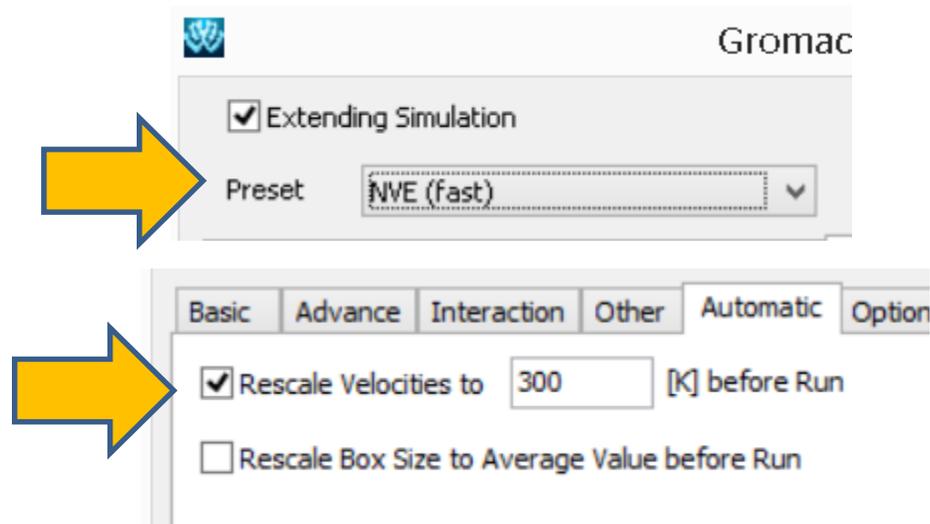
II. Equilibration (E)

1. After the calculation, Click **MD | Gromacs | Keywords Setup**.
2. Set **Preset** to **NVT (fast)**.
3. Click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.



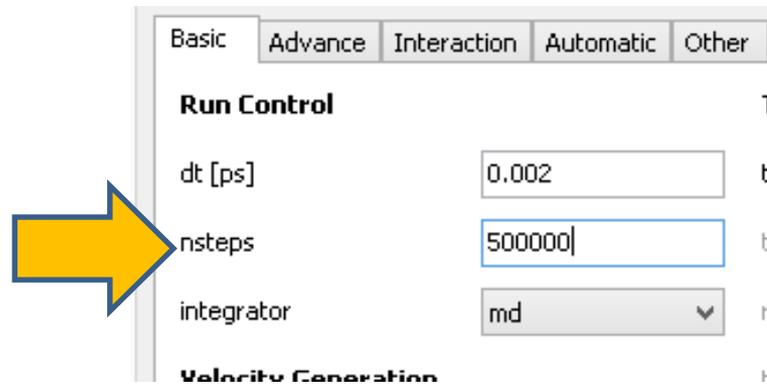
II. Equilibration (F)

1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Set **Preset** to **NVE (fast)**.
3. In the **Automatic** tab, check **Rescale Velocities to ...**.
4. Click **OK**.
5. Click **MD | Gromacs | Start Gromacs**.



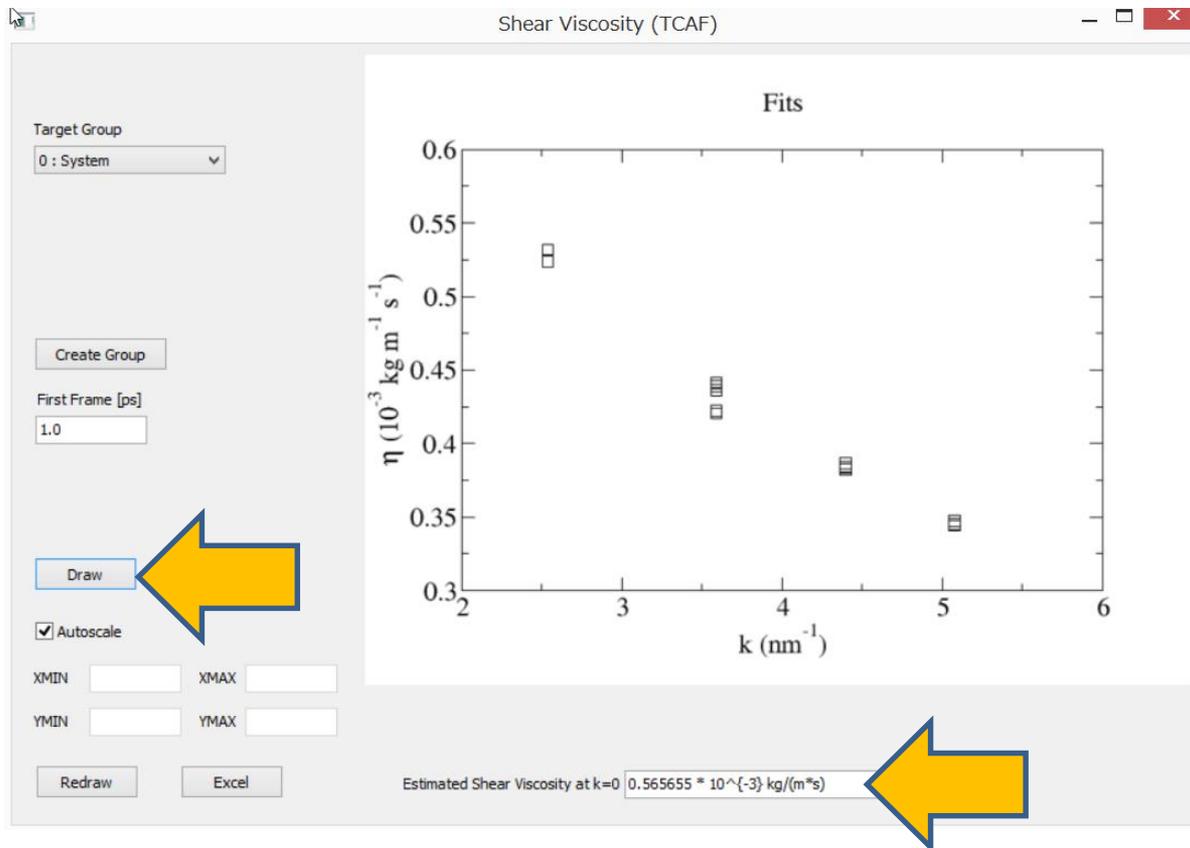
III. Product Run

1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. On **Basic** tab, set **nsteps** to **500000**.
3. Click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.



IV. Prediction of Viscosity

1. After the calculation, click **MD | Gromacs | Shear Viscosity**.
2. Open the default files; repeat 3 times.
3. Click **Draw** to draw the predicted value of Viscosity.



V. Prediction of Dielectric Constant

1. After the calculation, click **MD | Gromacs | Static Dielectric Constant**.
2. Open the default files; repeat 3 times.
3. Click **Draw** and set **Temperature [K]** to **300**, then click **OK**.
The predicted value of dielectric constant will be displayed.

