

Winmostar tutorial  
Gromacs  
Viscosity · Dielectric constant  
V7.025

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2017/8/8

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# Configure

**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](https://winmostar.com/en/manual_en.html).

2. Installation Guides for Solvers

For Windows

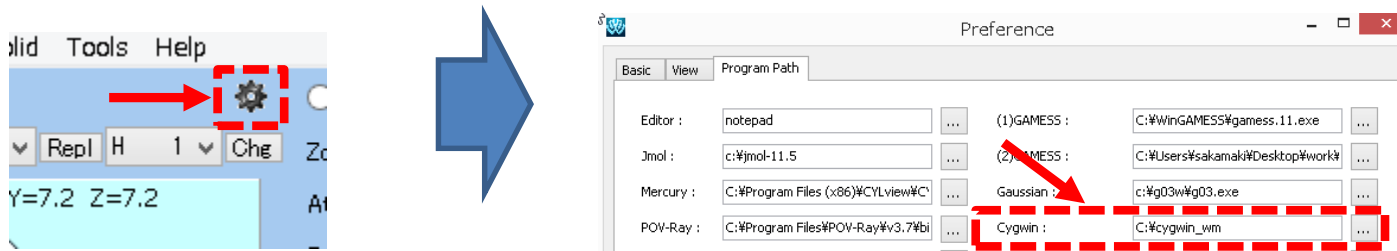
[cygwin\\_wm\\_v7\\_20160926.exe\(413MB\)](#) ※NWChem/Gromacs/Amber Window Build Package(Cygwin)

(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.



# Note

- The simulation steps required are dependent on molecular species and initial density.
- To obtain accurate and reproducible results, you have to set long simulation time.
- The method for interaction calculations and/or the force field also affect the simulation results.

# 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**.

The screenshot shows the 'Solvate/Build MD Cell' dialog box in the X-Ability software. The 'MD' menu is highlighted, and the 'Solvate/Build Cell' option is selected. The dialog box has the checkbox 'Put the molecule on main window as solute' unchecked. The 'Add Water' button is highlighted. The 'Simulation Cell' tab is active, showing 'Set Density [g/cm<sup>3</sup>]' selected with a value of 0.6, and 'Box Type' set to 'cubic'.

Name	# Mol	Position	mol/L	Composition

Simulation Cell Option

Set Density [g/cm<sup>3</sup>] 0.6

Set Distance from Solute [nm]

Set Box Size [nm] Import

Angles 90.0 90.0 90.0

Box Type cubic

Total Number of Atoms:

Reset Build Cancel

# 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/cm<sup>3</sup>]' selected and set to 0.9, with a yellow arrow pointing to the input field. Below this, the 'Box Type' is set to 'cubic' and 'Total Number of Atoms' is 1500. A yellow arrow points to the 'Build' button at the bottom right. A table in the center shows the composition of the cell:

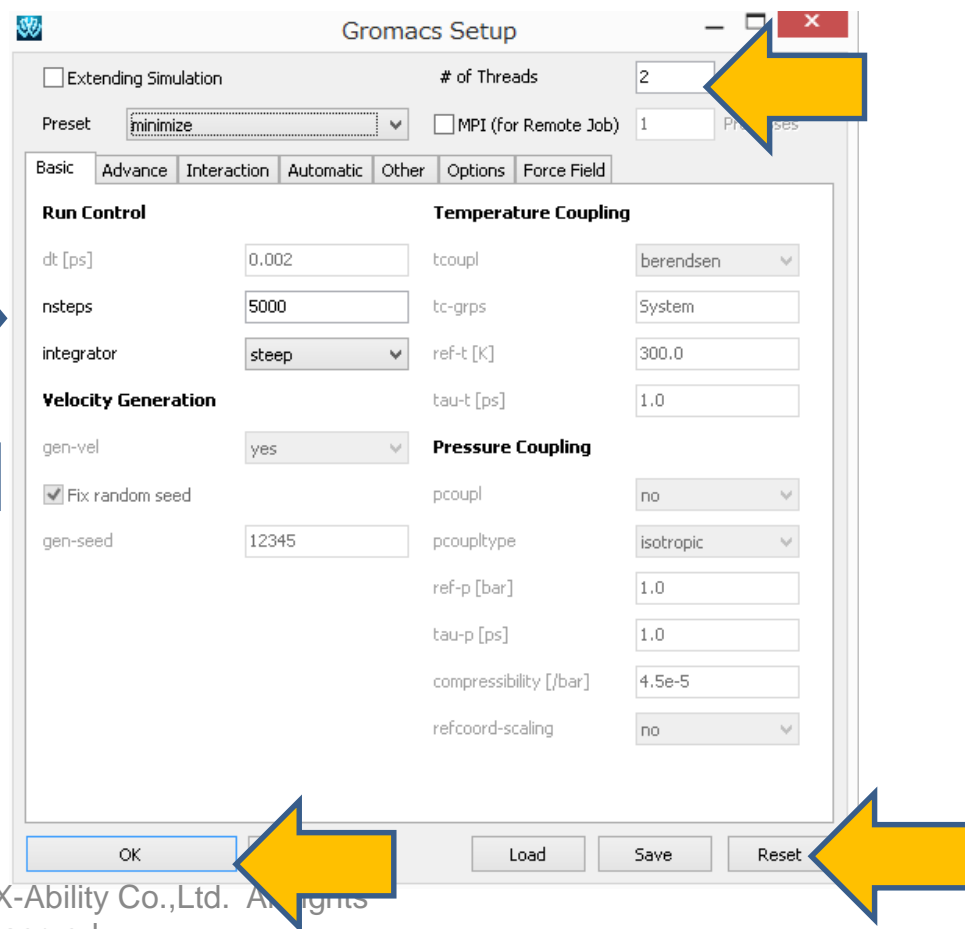
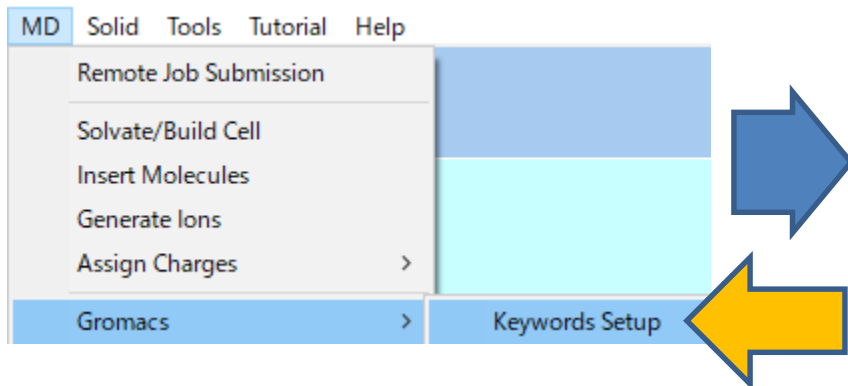
Name	# Mol	Position	mol/L	Composition
WATER	500	Random	49.955	H2O

At the bottom left, a 3D ball-and-stick model of the simulation cell is shown, containing numerous water molecules (red and white spheres) and a few yellow spheres representing the solute. A blue arrow points from the 'Build' button to this model.

## II. Execute simulations

### 1. Equilibration (Energy minimization)

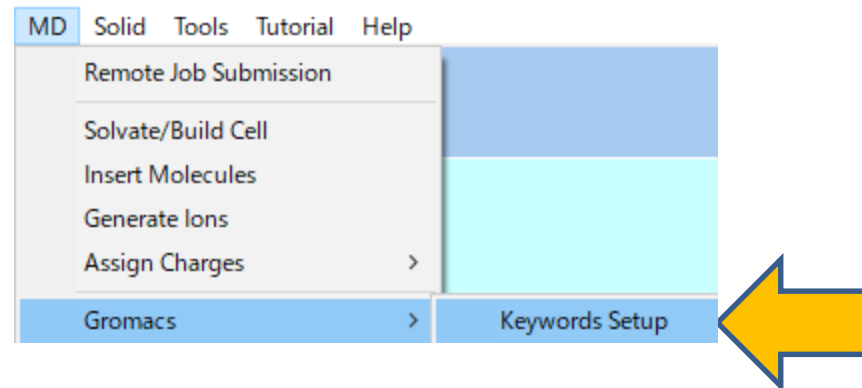
1. Click **MD | Gromacs | Keywords Setup**.
2. Click **Reset**.
3. Set **# of Threads** to a parallel number, then click **OK**.



## II. Execute simulations

### 1. Equilibration (Energy minimization)

1. Click **MD | Gromacs | Start Gromacs**.
2. Save the coordination file as **water.gro**, topology file as **water.top**.  
Then Cygwin will be launched and Gromacs process will begin.

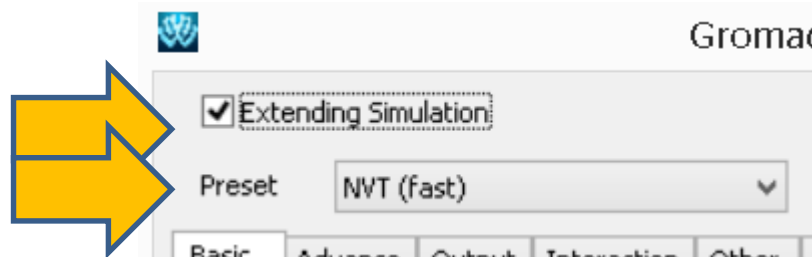




## II. Execute simulations

### 1. Equilibration (*NVT*)

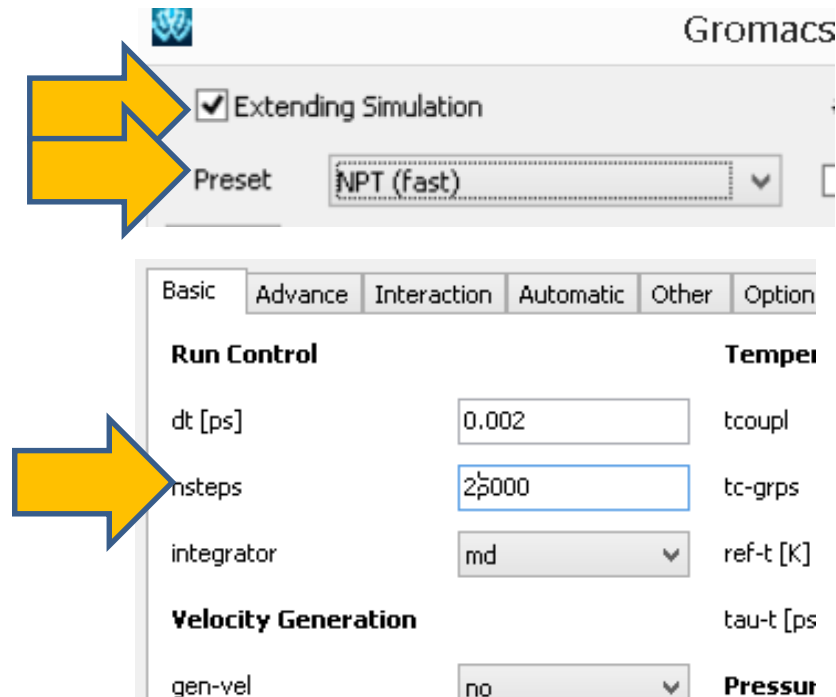
1. After the calculation, Click **MD | Gromacs | Keywords Setup**.
2. Check **Extending Simulation**, set **Preset** to **NVT (fast)**.
3. Click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.



## II. Execute simulations

### 1. Equilibration (*NPT*)

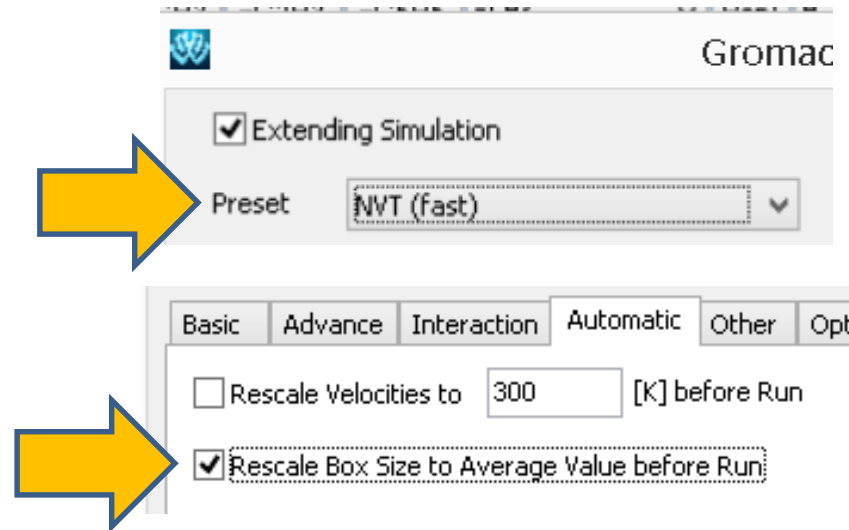
1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Set **Preset** to **NPT (fast)**, **nsteps** to **25000**.  
(when **nsteps** is modified, **Preset** will be automatically set to (**custom**).)
3. Click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.



## II. Execute simulations

### 1. Equilibration (*NVT* 2)

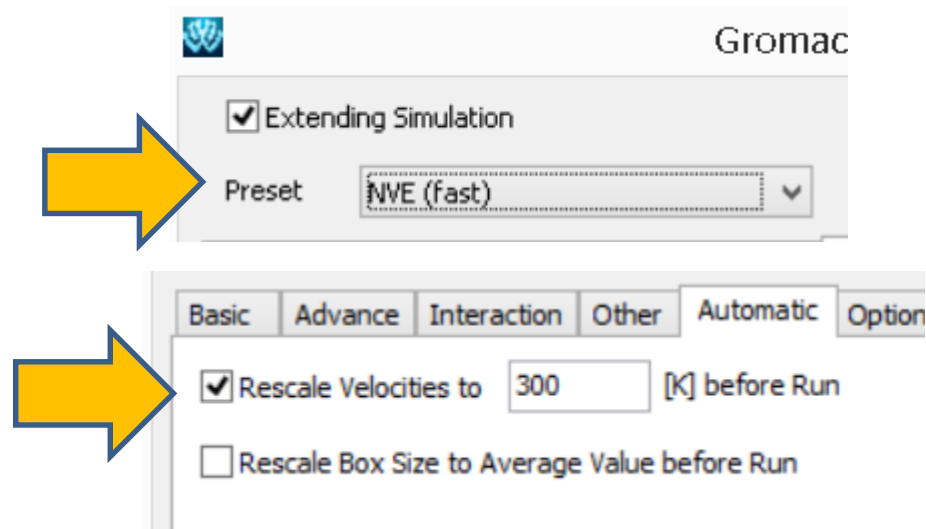
1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Set **Preset** to **NVT (fast)**.
3. On **Automatic** tab, check **Rescale Box Size to Average Value before Run**.
4. Click OK.
5. Click **MD | Gromacs | Start Gromacs**.



## II. Execute simulations

### 1. Equilibration (No Temperature and Pressure control)

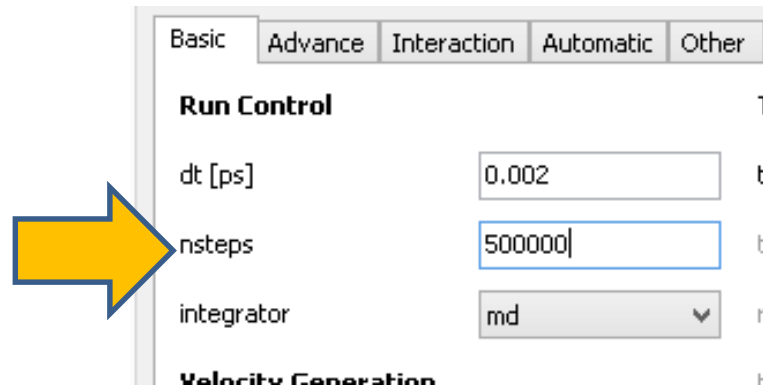
1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. Set **Preset** to **NVE (fast)**.
3. On **Automatic** tab, check **Rescale Velocities to ...**.
4. Click **OK**.
5. Click **MD | Gromacs | Start Gromacs**.



## II. Execute simulations

### 2. Product run

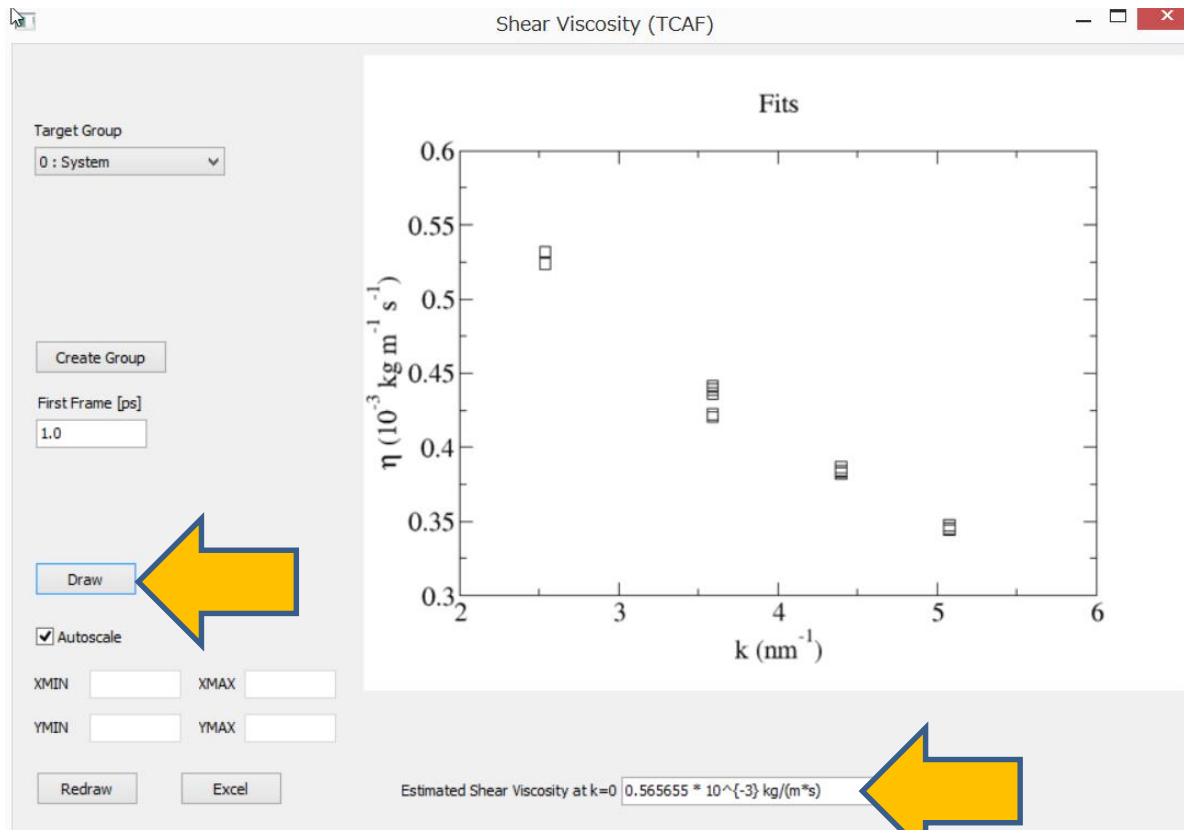
1. After the calculation, click **MD | Gromacs | Keywords Setup**.
2. On **Basic** tab, set **nsteps** to **500000**.
3. Click **OK**.
4. Click **MD | Gromacs | Start Gromacs**.



## III. Analyze

### 1. 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.



## III. Analyze

### 2. 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.

