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Winmostar tutorial

Gromacs

Vapor Pressure・Surface Tension

V8.007

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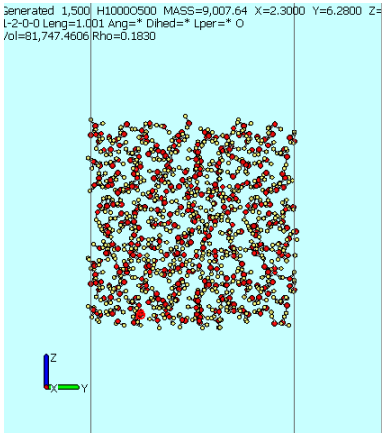
Summary

In this tutorial, we will calculate vapor pressure and surface tension with a vapor-liquid equilibration.



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 longer simulation time. Convergence of calculation of interfacial tension is especially slow.
- The method for interaction calculations and/or the force field also affect the simulation results.
- If necessary, execute equilibrium calculation in the liquid phase before vacuum layer insertion.

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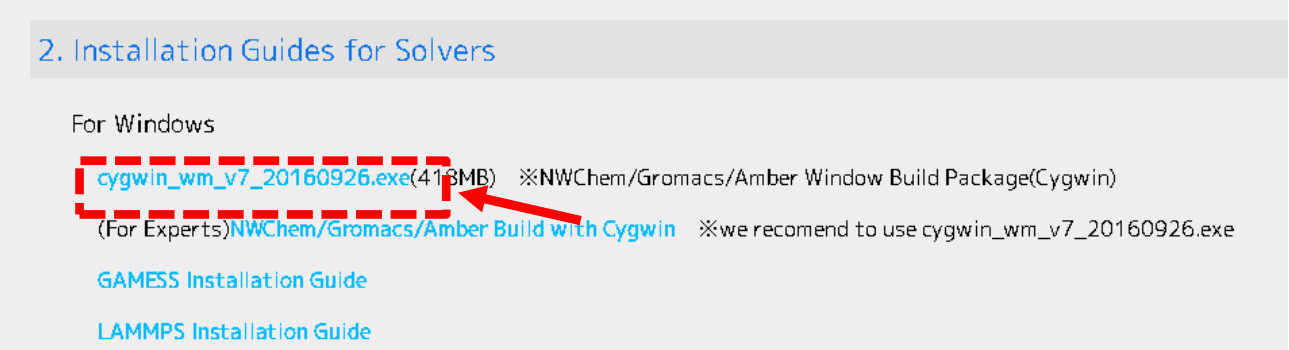
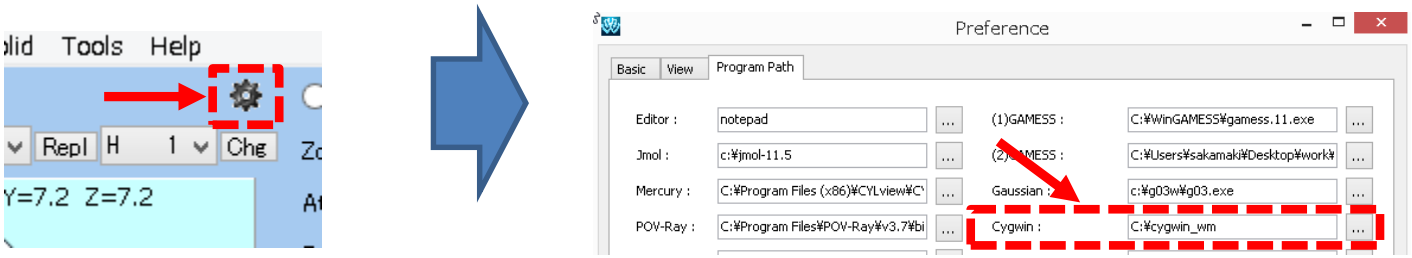
Configuration

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.



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



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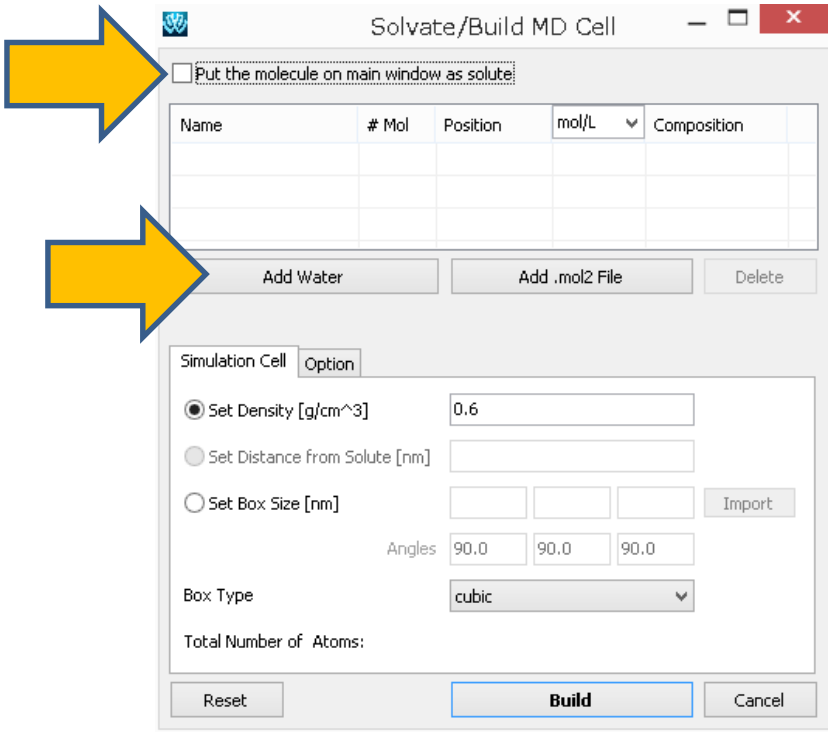
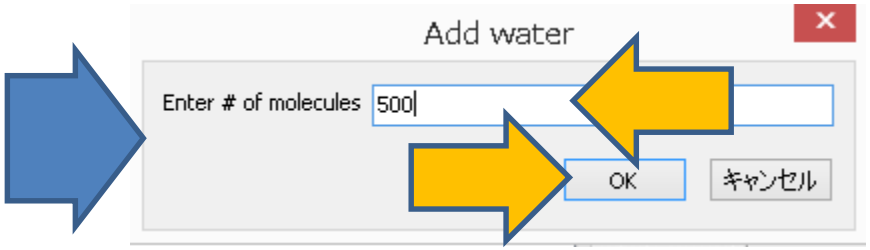
I. Build a simulation cell

1. Click **MD** | **Solvate/Build Cell**.
2. Uncheck **Put the molecule on main window as solute**.
3. Click **Add water**. Set **Enter # of molecules** to **500**.
4. Click **OK**.





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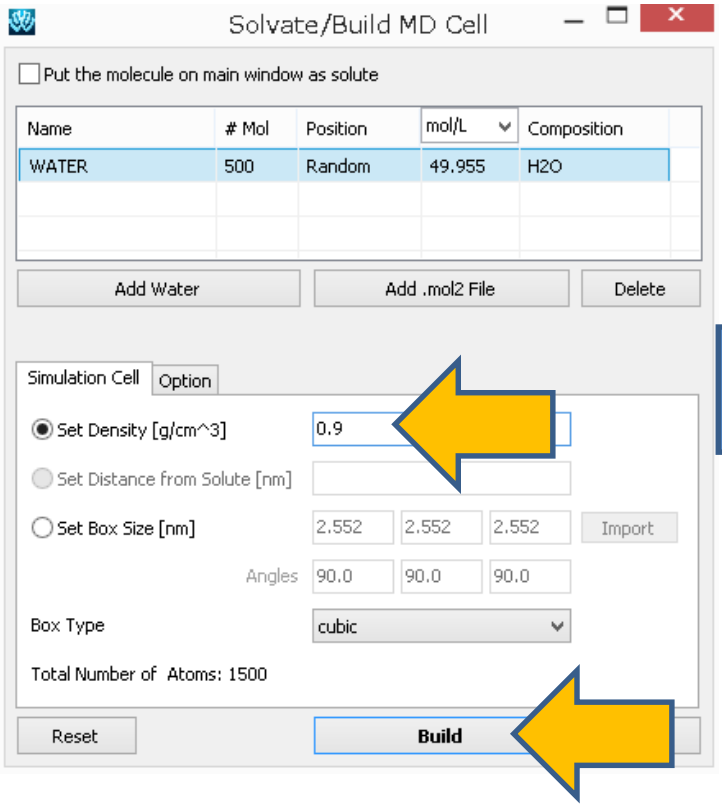
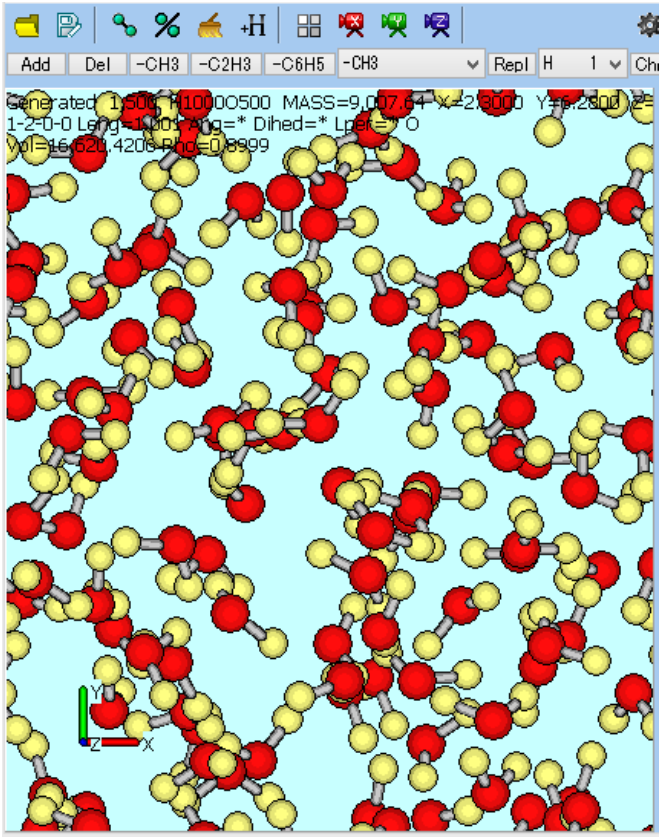
I. Build a simulation cell

1. Set **Set Density** to **0.9**.
2. Click **Build**.





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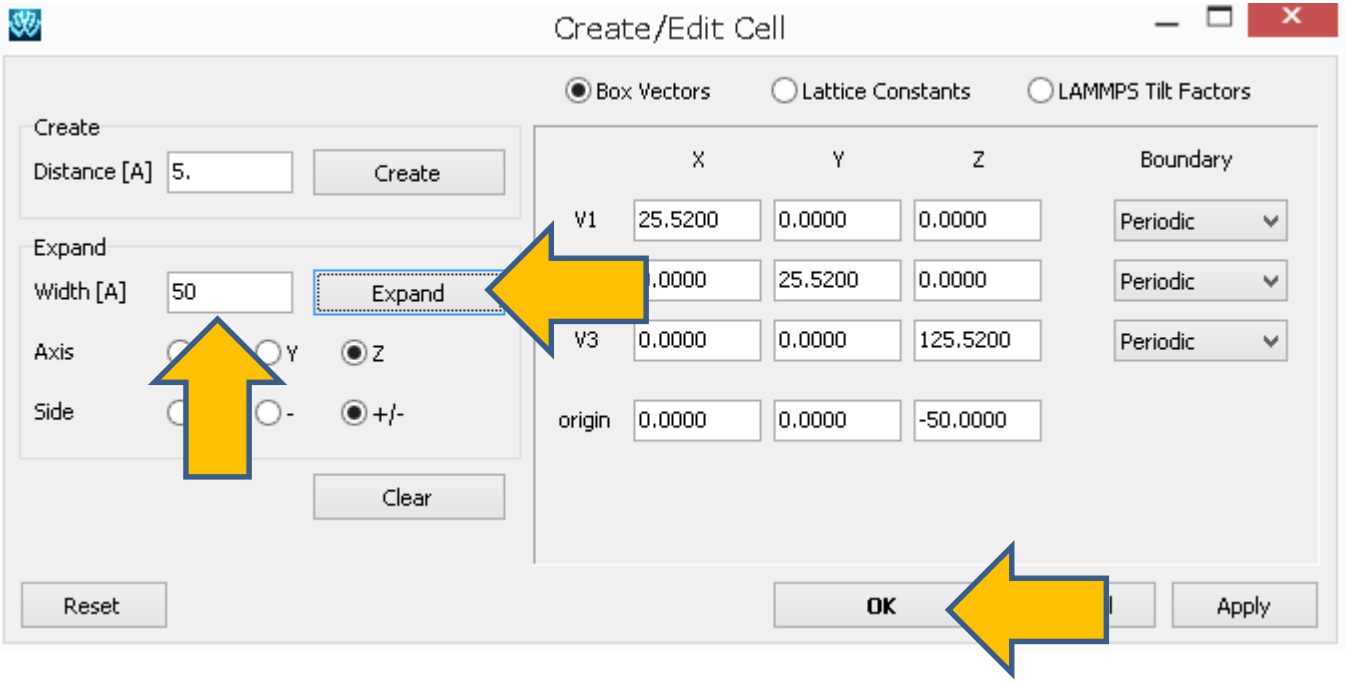
I. Build a simulation cell

1. Click **Edit** | **Solvate/Build Cell**.
2. On **Expand**, set **Width** to **50**, then click **Expand**.
3. Click **OK**.



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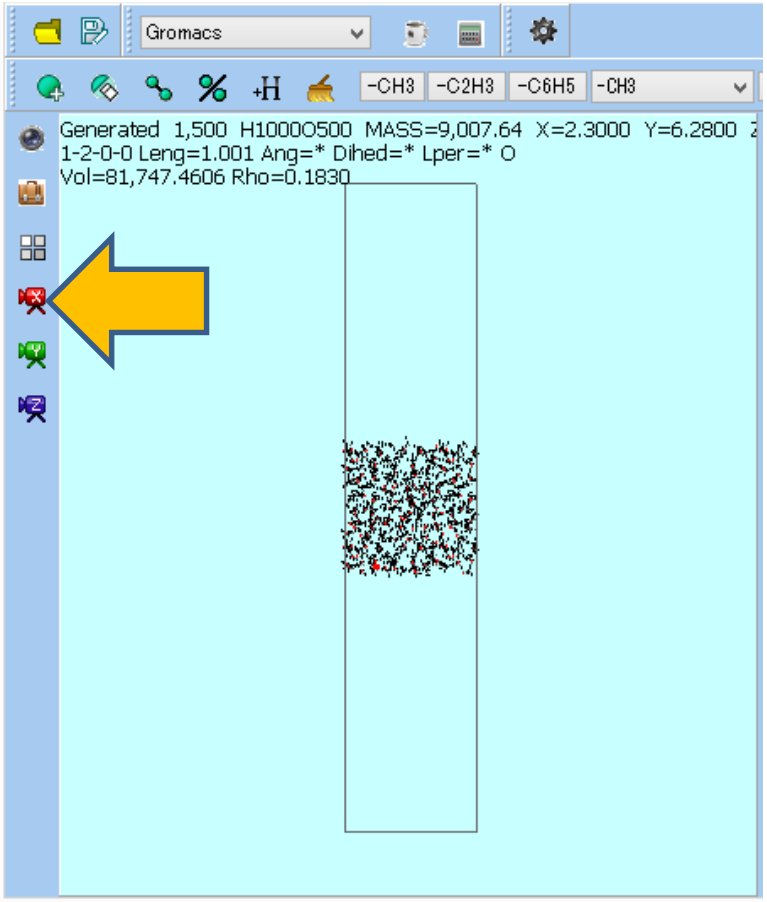
I. Build a simulation cell

Click the red X camera icon to the left of the main window,
then zoom out the camera. Vapor - liquid equilibration system has been built.



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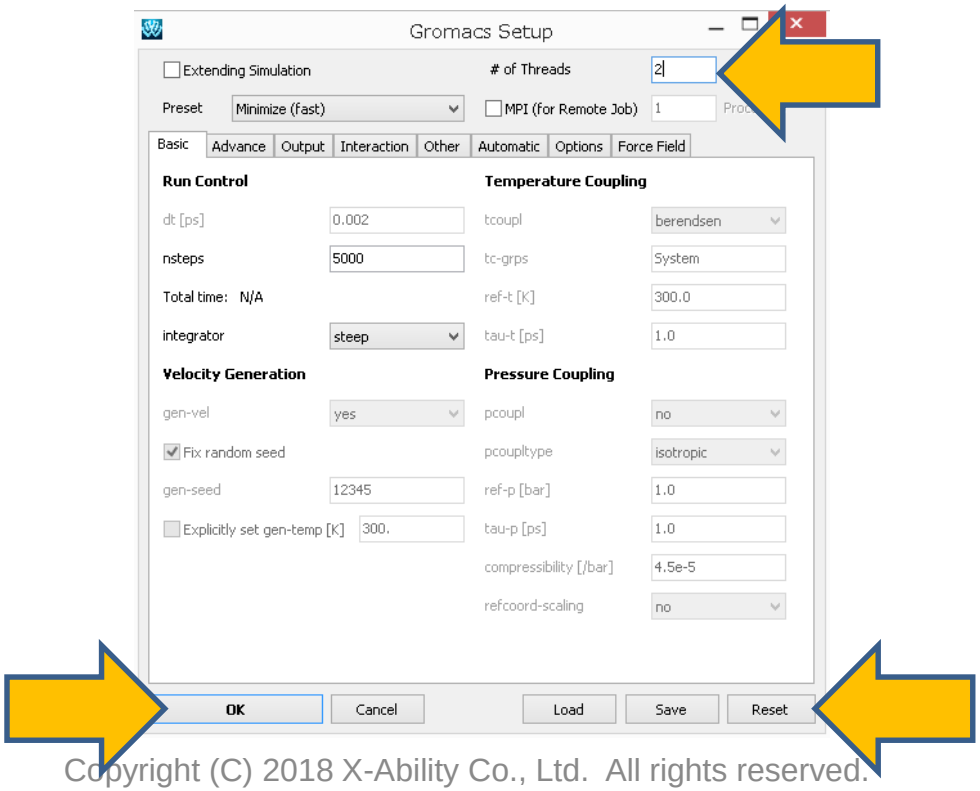
II. Equilibration

1. Click **MD** | **Gromacs** | **Keywords Setup**.
2. Click **Reset**.
3. Click **# of Threads** and set to a parallel number, then click **OK**.
4. Click **MD** | **Gromacs** | **Start Gromacs**.
5. Save the coordinate file as **spce500k.gro**, the topology file as **spce500k.top**.



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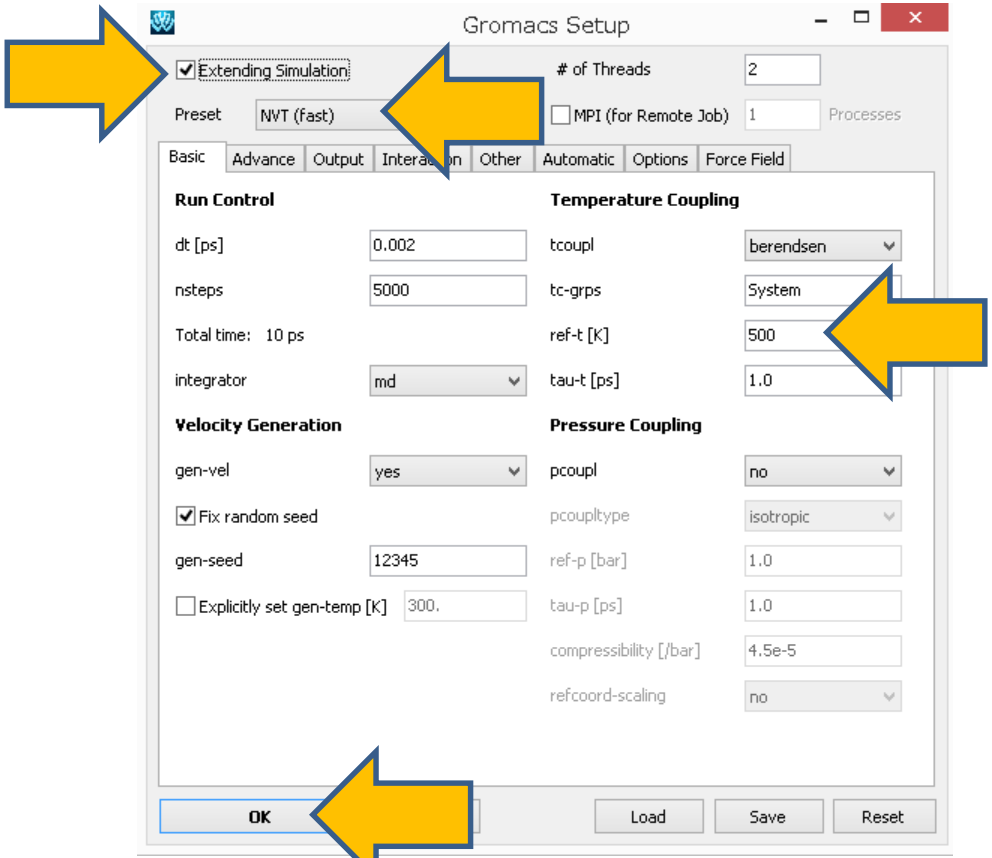
II. Equilibration

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Check the box for **Extending Simulation**.
3. Set **Preset** to **NVT (fast)**, **ref-t [K]** to **500**, then click **OK**.
4. Click **MD** | **Gromacs** | **Start Gromacs**.



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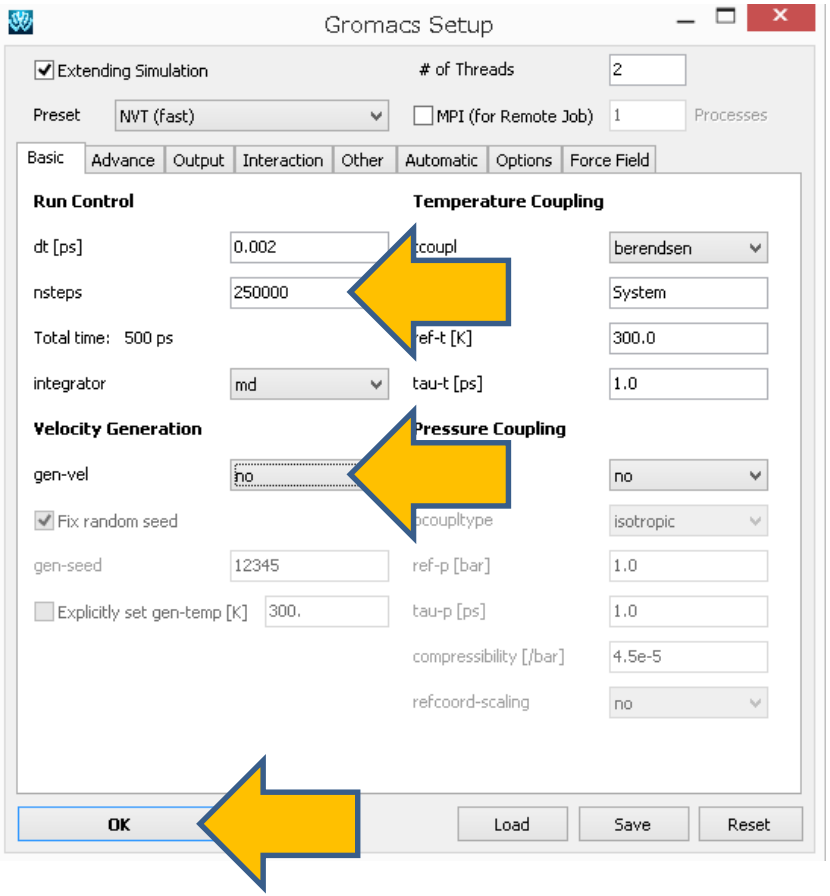
III. Product run

1. After the calculation, click **MD** | **Gromacs** | **Keywords Setup**.
2. Set **nsteps** to **250000**, **gen-vel** to **no**, then click **OK**.
3. Click **MD** | **Gromacs** | **Start Gromacs**.



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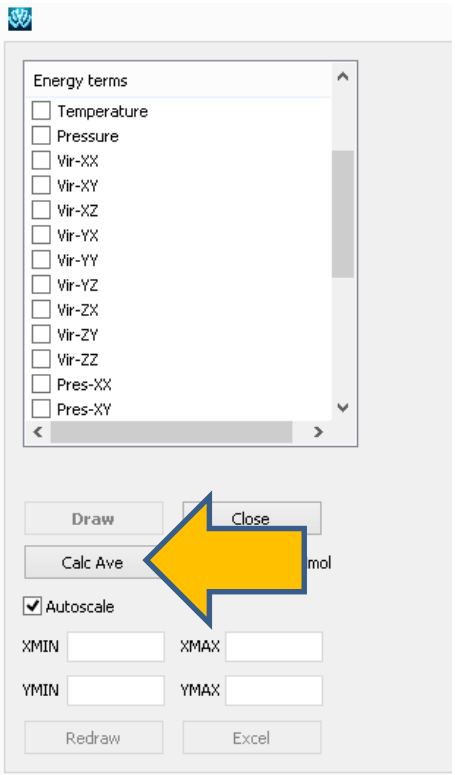
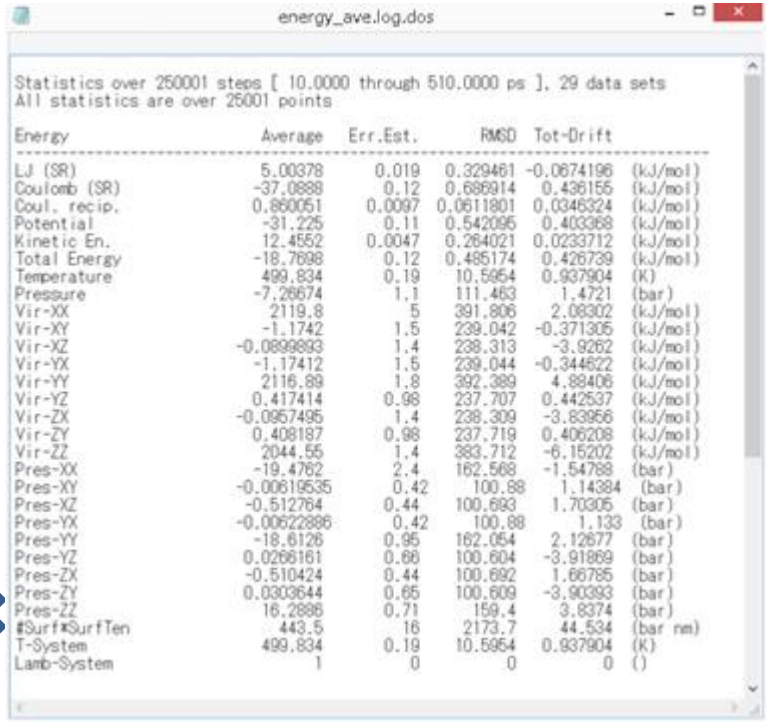
IV. Analyze

1. Click **MD** | **Gromacs** | **Energy Plot**.
2. Open the **.edr** file selected by default.
3. Click **Calc Ave**, then open the **.gro** file selected by default.

[Pres-ZZ] indicates vapor pressure（vapor-liquid pressure, the unit is bar）,
[#Surf*SurfTen] indicates the product of number of interfaces (2 in this case) multiplied by surface tension（the unit is bar*nm）.





Reference: R. Sakamaki *et al.*, J. Chem. Phys., 134, 124708 (2011).

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IV. Analyze

1. Click **MD** | **Gromacs** | **Density Profile**.
2. Open default files and repeat 3 times.
3. In the **Density** tab under **Group**, check box for **0:System**.
4. Click **Draw** to draw Density distribution toward the z axis.

If you need the density of liquid or gas phase respectively, click **Excel** to obtain csv file. Try distribution fitting configurations on various graphing software.