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Winmostar Tutorial
LAMMPS
Basics

V7.003

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Note

- The simulation steps required are depend on the 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.

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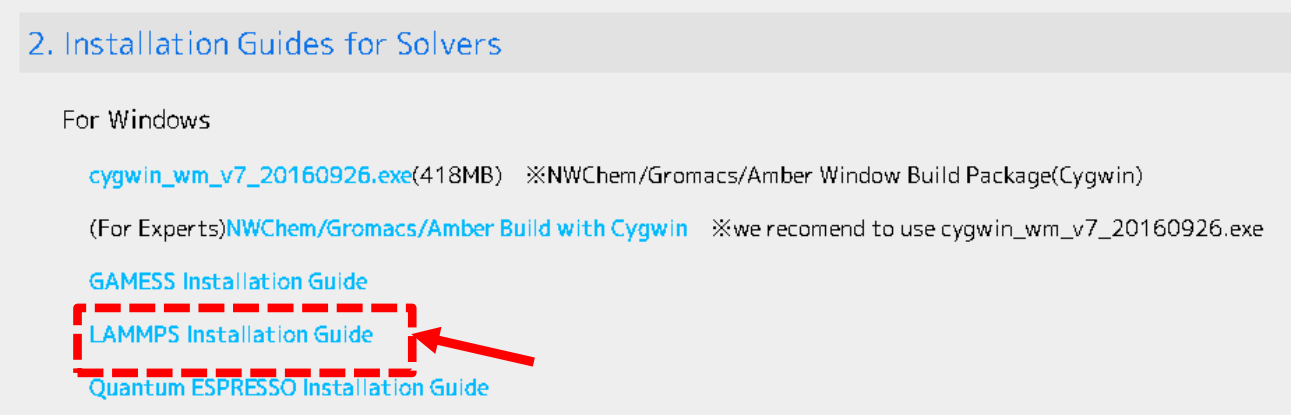
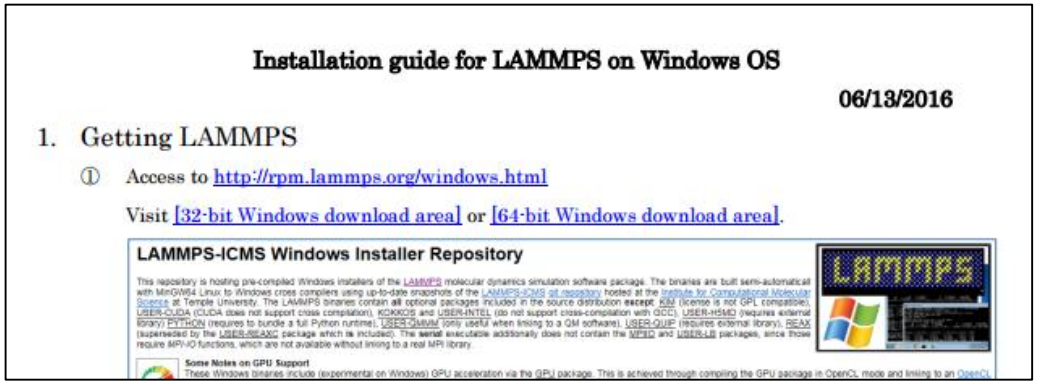
I. Configure

You must set up both LAMMPS and Cygwin ahead.

- Set up LAMMPS by following **LAMMPS Installation Guide** located at https://winmostar.com/en/manual_en.html.




Installation guide for LAMMPS on Windows OS

06/13/2016

1. Getting LAMMPS

① Access to http://rpm.lammps.org/windows.html

Visit [32-bit Windows download area] or [64-bit Windows download area].

LAMMPS-ICMS Windows Installer Repository

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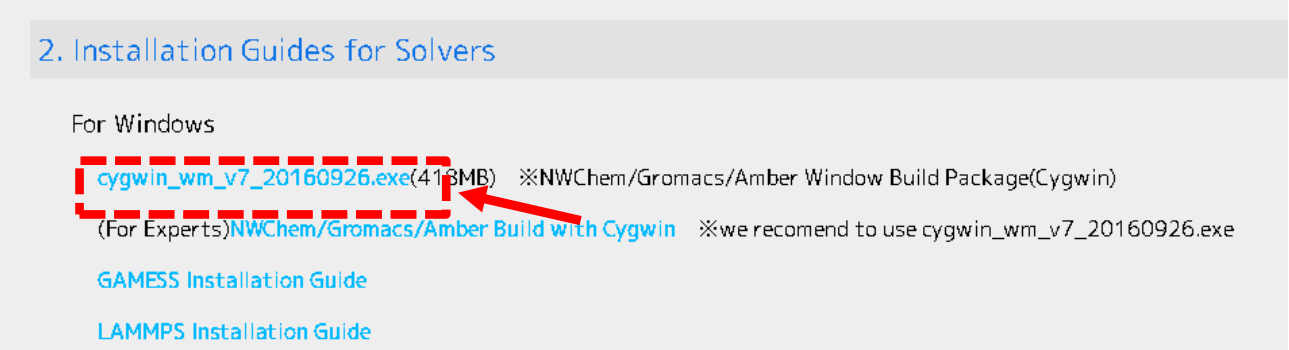
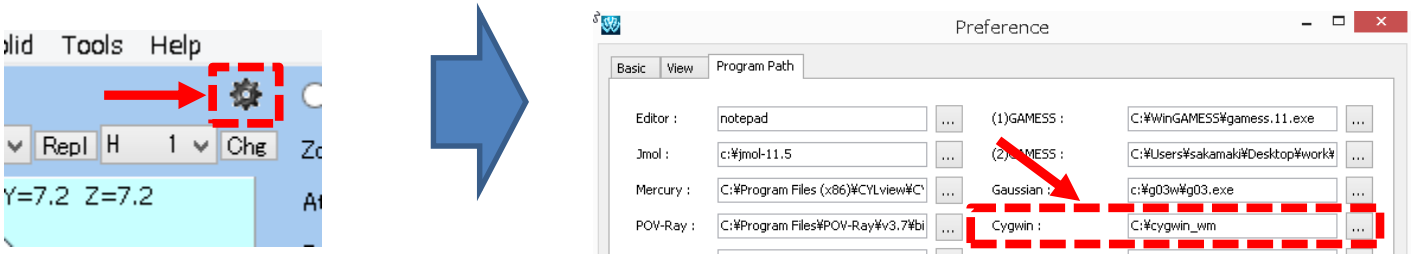
I. Configure

You must set up both LAMMPS and Cygwin ahead.

- Obtain the installer for Cygwin, which contains the several 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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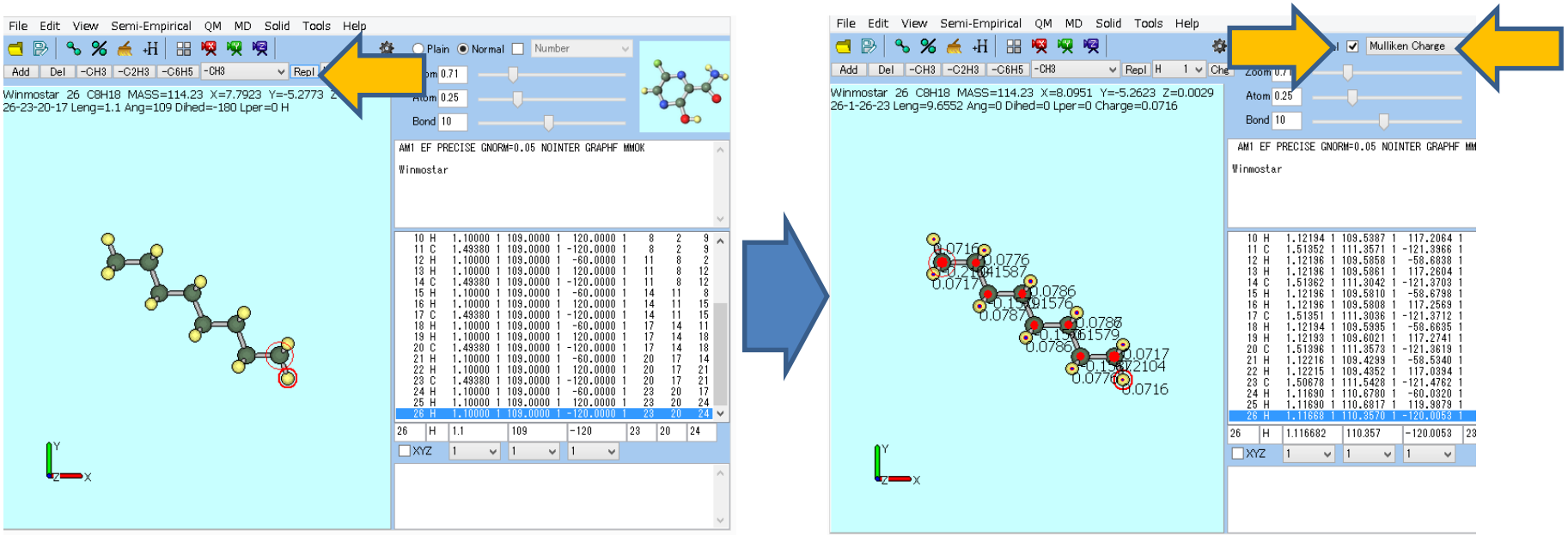
II. Define a molecule

Select **File | New** and click the **Repl** button eight times to obtain n-octane.
Execute MOPAC at **Semi-Empirical | MOPAC | Start (1)MOP6W70**.
Point charges obtained from MOPAC can be seen when click the checkbox at top left side of the main window and select **Mulliken Charge**.
Finally, save this molecule with .mol2 format at **File | Save as**.



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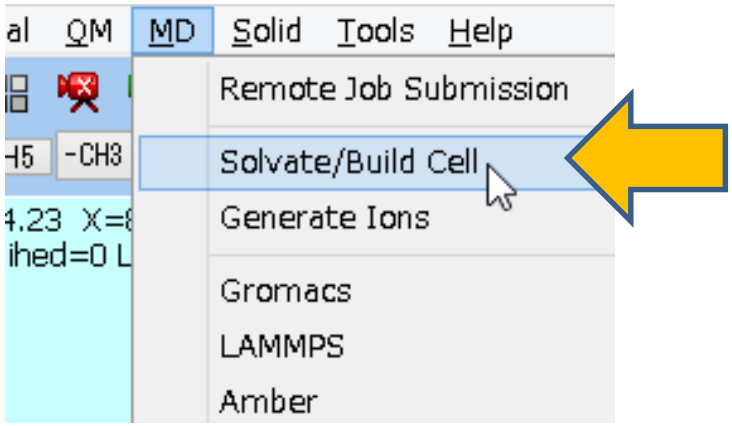
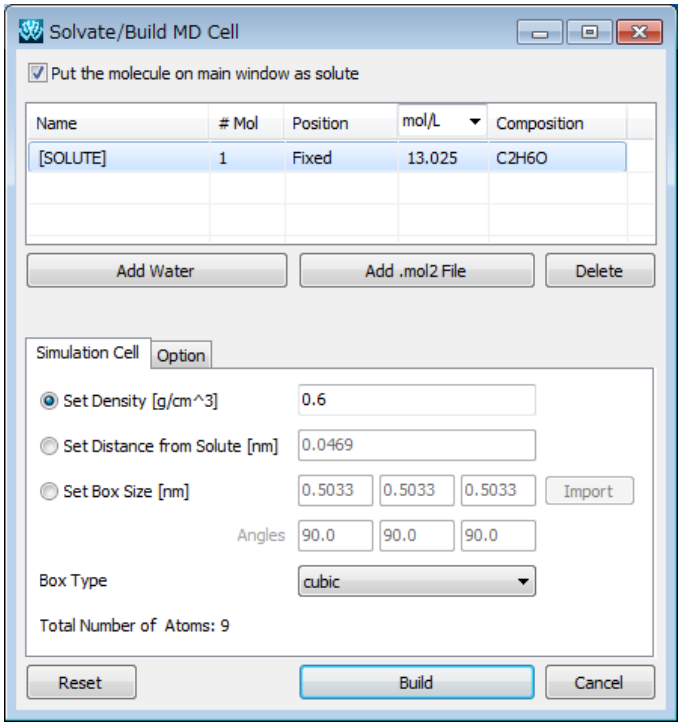
III. Build a simulation cell

Select **MD | Solvate/Build Cell**.





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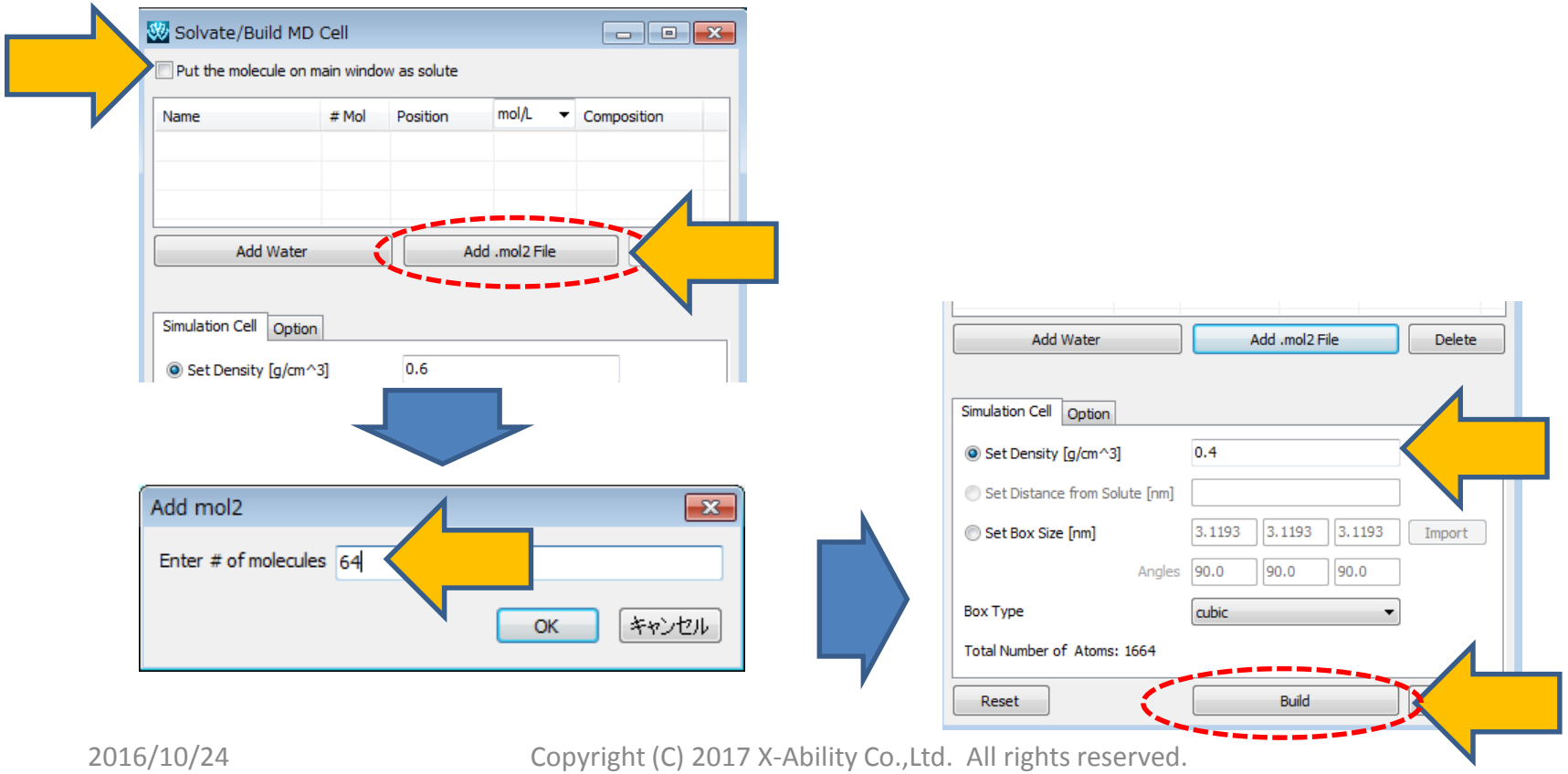
III. Build a simulation cell

Uncheck **Put the molecule on main window as solute**. Click the **Add .mol2 File** button and select the file saved at the last step. Enter the number of molecules and click **OK**. Finally, enter the density and click **Build**.



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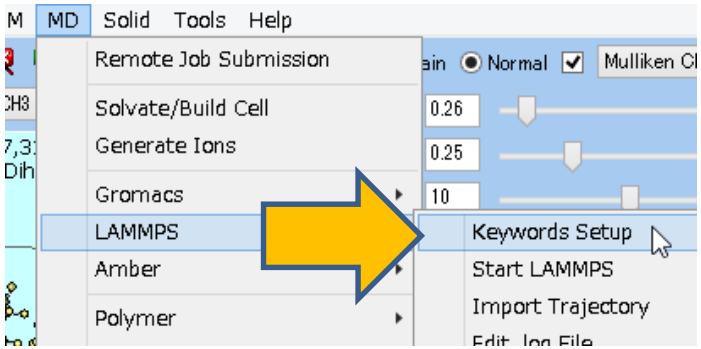
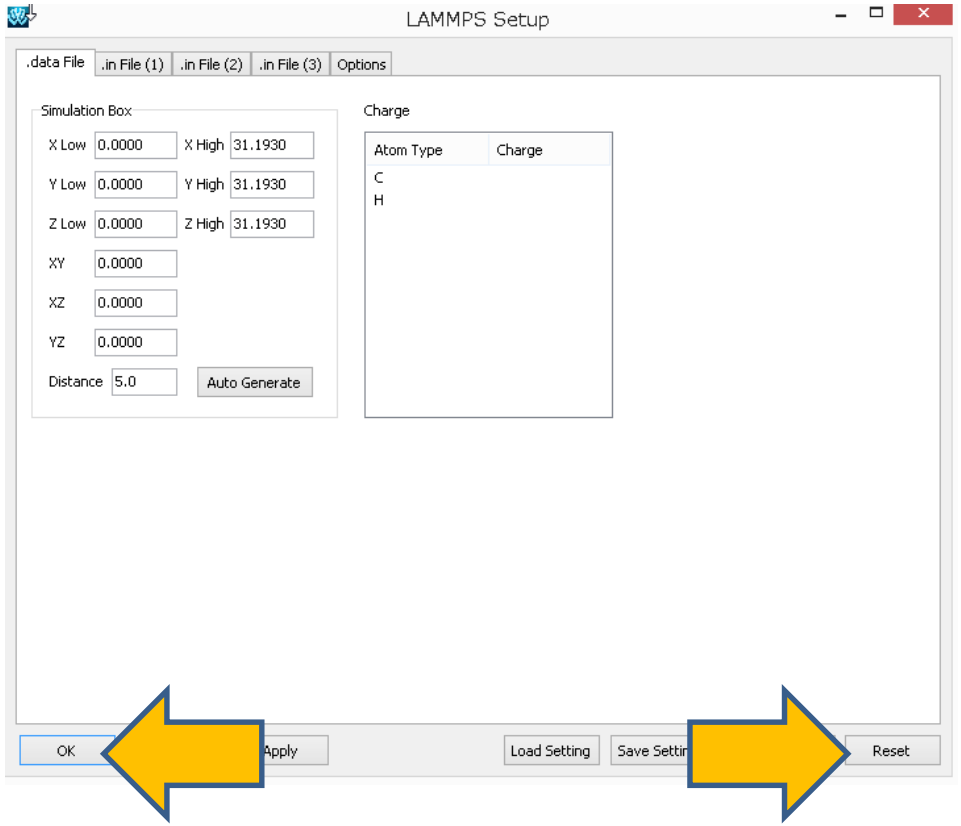
IV. Execute energy minimization

Select **MD | LAMMPS | Keywords Setup**. Click the **Reset** button, then click **OK**.





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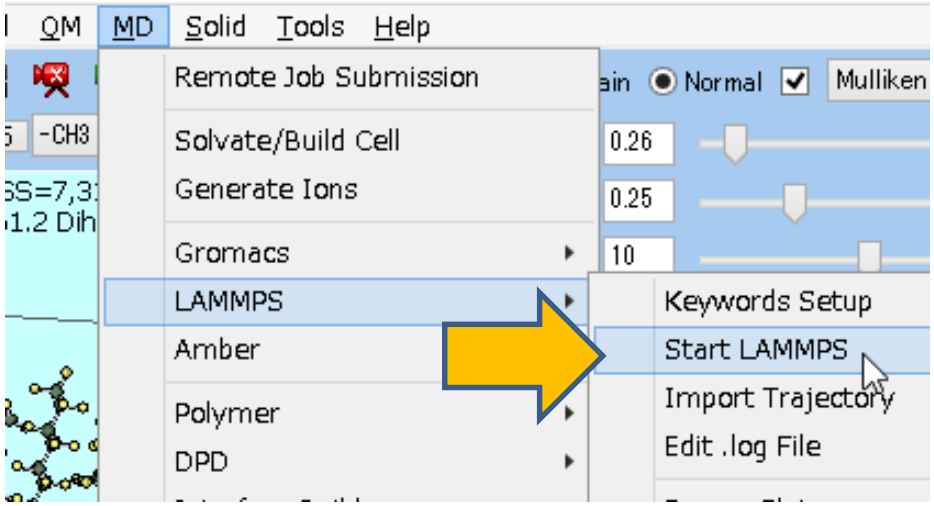
IV. Execute energy minimization

Select **MD | LAMMPS | Start LAMMPS**. After entering the name for LAMMPS .data file, LAMMPS will start.



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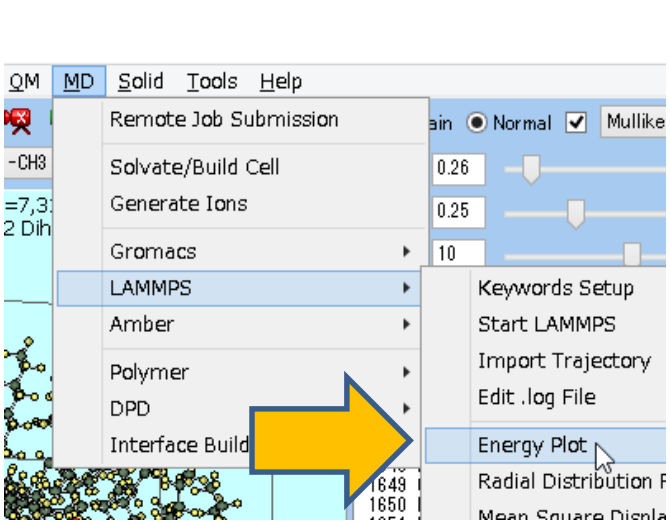
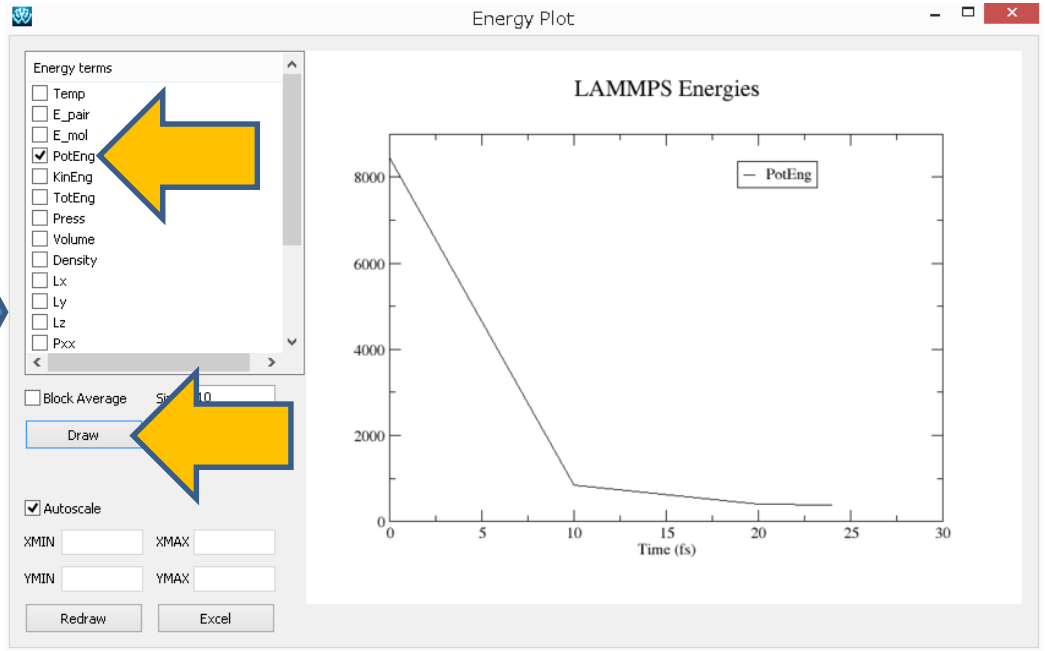
IV. Execute energy minimization

Select **MD | LAMMPS | Energy Plot** and open the file selected by default.
Check **PotEng** in **Energy term** and click **Draw**.





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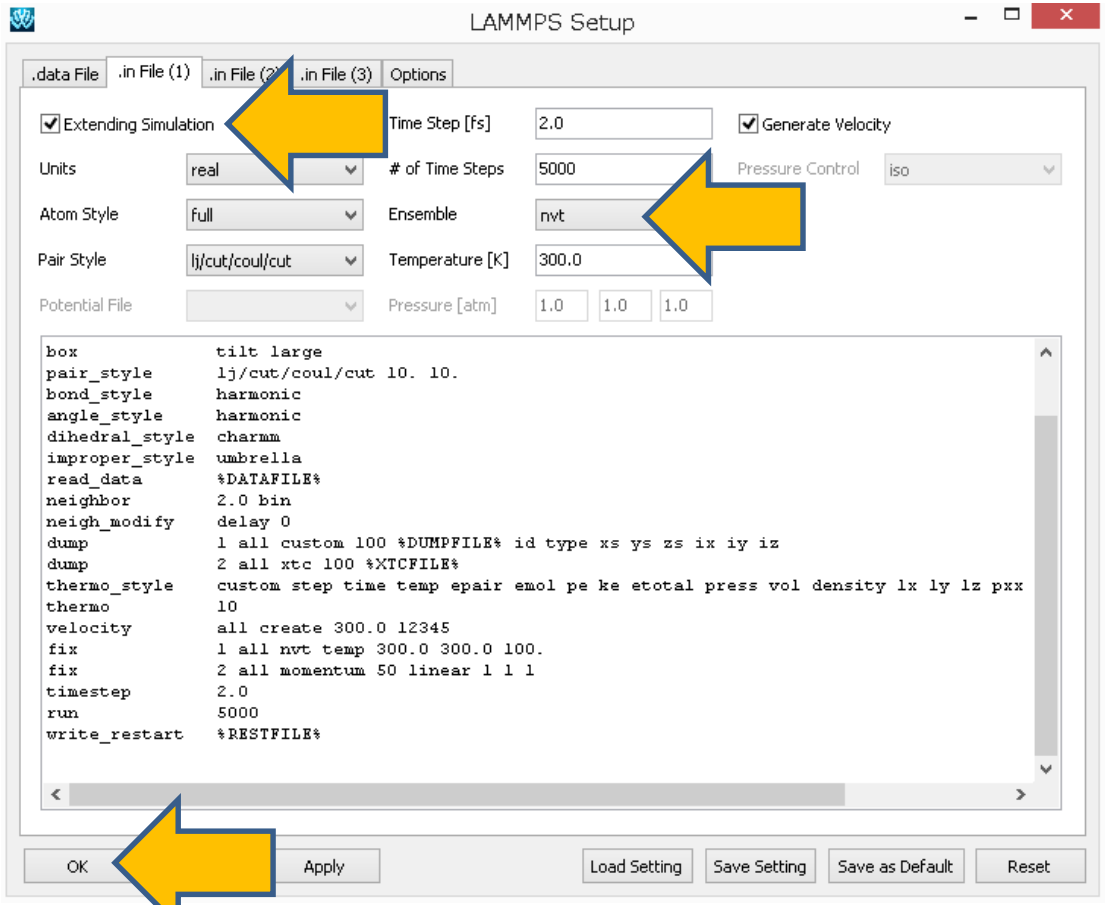
V. Execute an *NVT* MD simulation

Open the **.in File (1)** tab at **MD | LAMMPS | Keywords Setup**. Check **Extending Simulation** and set **Ensemble** to **nvt**. Then, click **OK**.



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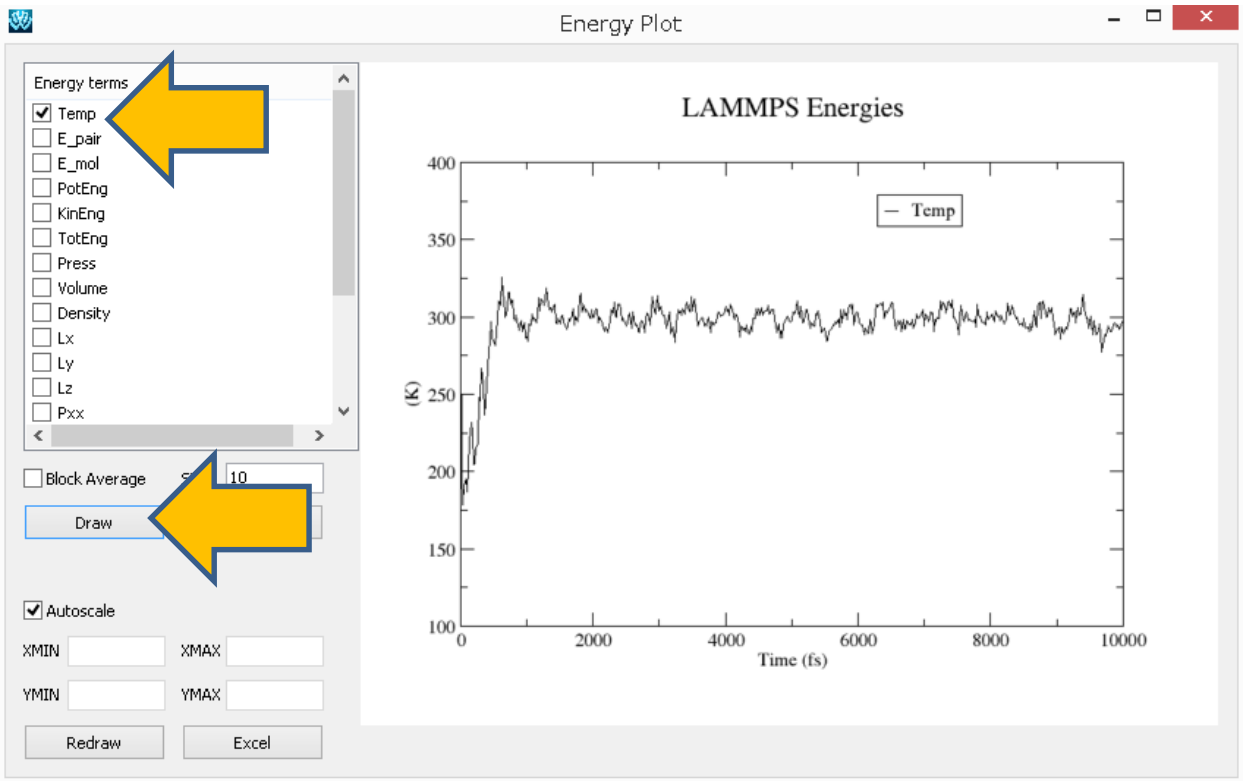
V. Execute an *NVT* MD simulation

Select **MD | LAMMPS | Start LAMMPS**. After the simulation is successfully finished, go to **MD | LAMMPS | Energy Plot** and draw the time evolution of the temperature (Temp).



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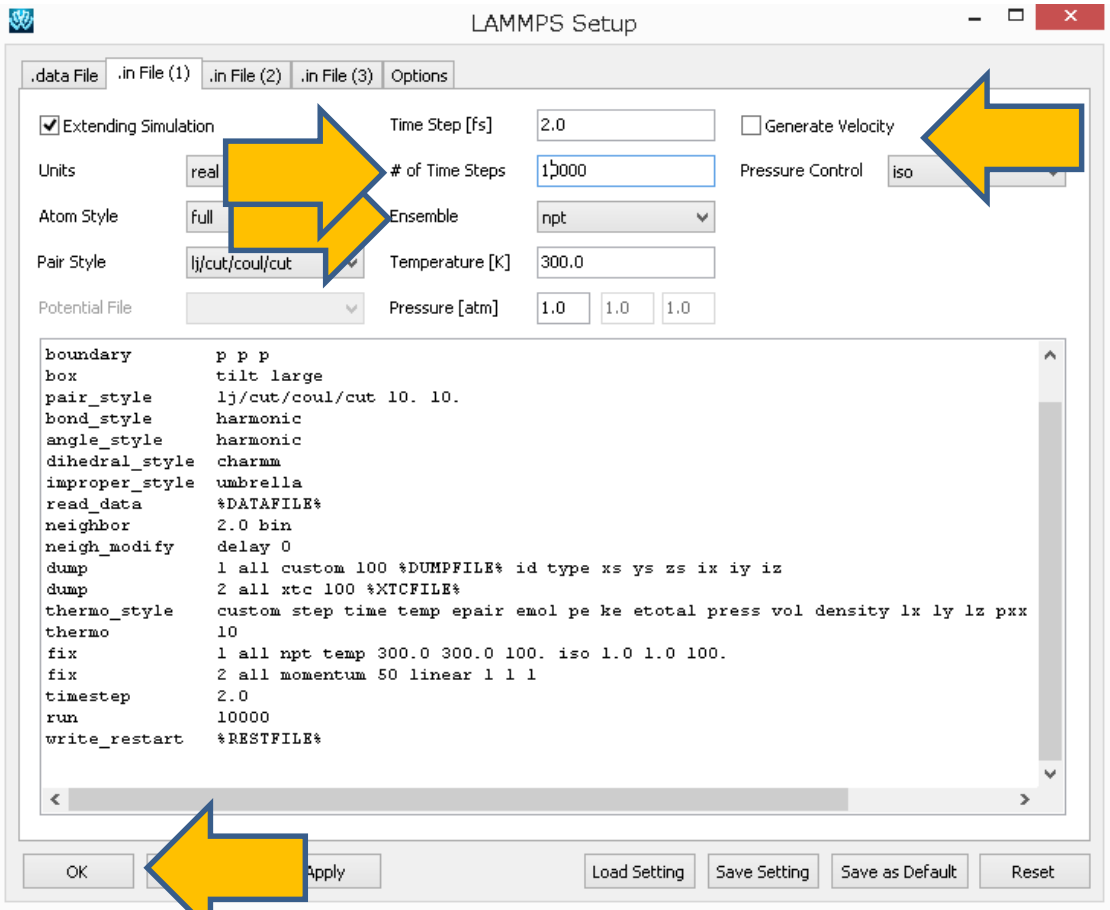
VI. Execute an *NPT* MD simulation

Select **MD | LAMMPS | Keywords Setup**. Set **# of Time Steps** and **Ensemble** to **10000** and **npt**, respectively. Uncheck **Generate Velocity** and click **OK**.



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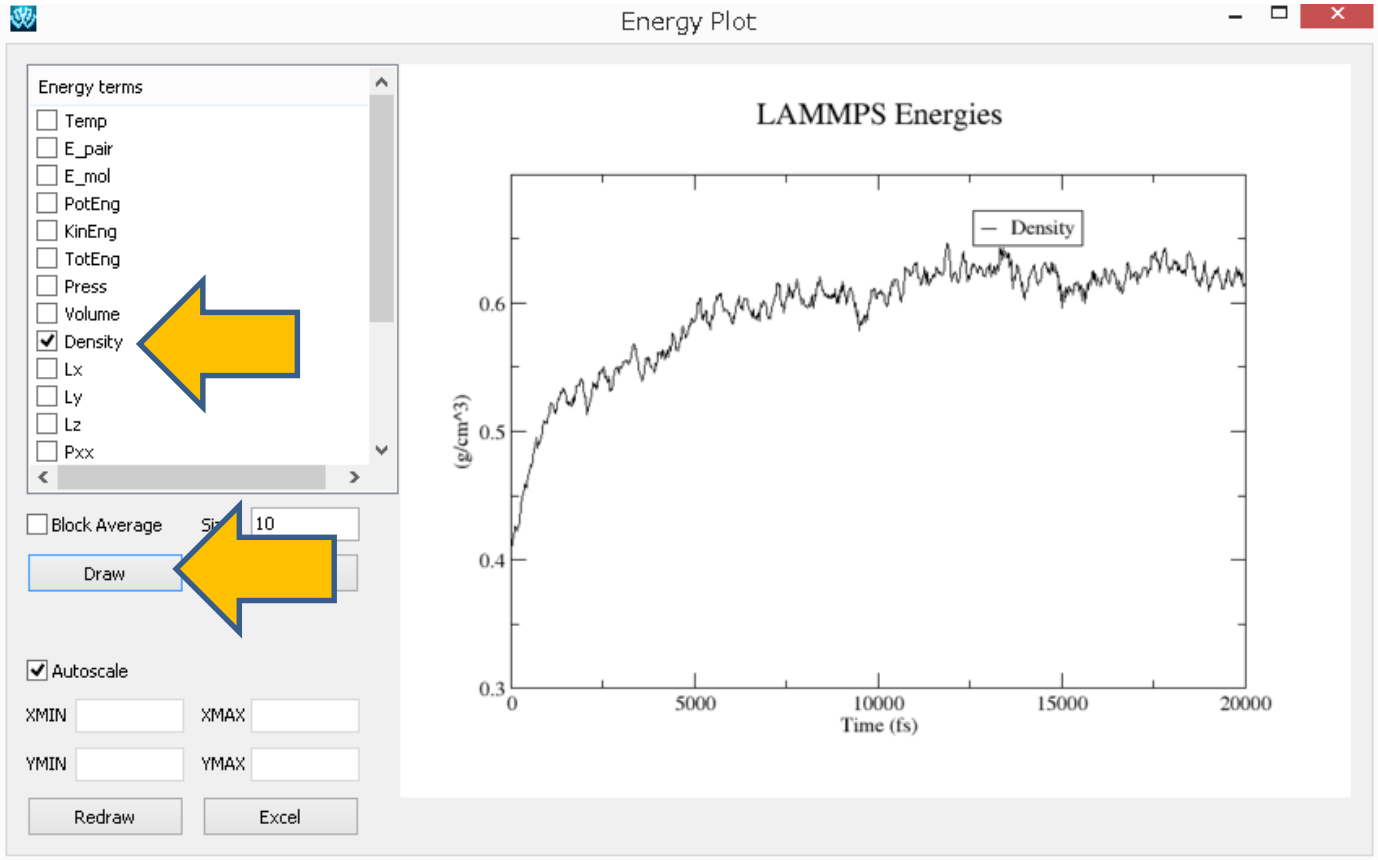
VI. Execute an *NPT* MD simulation

Start LAMMPS again. See the time evolution of the density at **MD | LAMMPS | Energy Plot**.



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VI. Execute an *NPT* MD simulation

Select **MD | LAMMPS | Import Trajectory** and open the data and dump files selected by default. On **Animation** window, click the **|>**(Play) button to start an animation or click the **3D** button to launch Winmostar 3D Viewer.