

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.

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.

2. Installation Guides for Solvers

For Windows

[cygwin_wm_v7_20160926.exe](#)(418MB) ※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](#)

[Quantum ESPRESSO Installation Guide](#)

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

This repository is hosting pre-compiled Windows installers of the LAMMPS molecular dynamics simulation software package. The binaries are built semi-automatically with MinGW64 Linux-to-Windows cross compilers using up-to-date snapshots of the LAMMPS-ICMS git repository, hosted at the Institute for Computational Molecular Science at Temple University. The LAMMPS binaries contain all optional packages included in the source distribution except [GPU](#) (license is not GPL compatible), [LAMMPS_CUDA](#) (CUDA does not support cross-compiler), [ICMSMPI2](#) and [LAMMPS-INTSL](#) (do not support cross-compiler with GCC), [LAMMPS-MSMD](#) (requires external library), [PYTHON](#) (requires to bundle a full Python runtime), [LAMMPS-OSQAR](#) (only useful when linking to a GM software), [LAMMPS-QUIP](#) (requires external library), [REAX](#) (supported by the [LAMMPS-REACT](#) package which it includes). The [serial](#) executable additionally does not contain the [WPKI](#) and [LAMMPS-LE](#) packages, since those require GPU functions, which are not available without linking to a real GPU library.

Some Notes on GPU Support

These Windows binaries include (experimental) on Windows GPU acceleration via the GPU package. This is achieved through compiling the GPU package in OpenCL mode and linking to an OpenCL



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.

2. Installation Guides for Solvers

For Windows

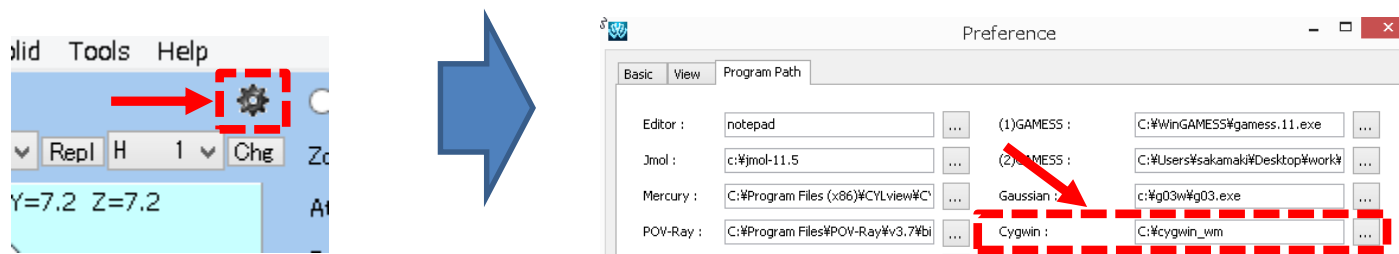
cygwin_wm_v7_20160926.exe(413MB) ※NWChem/Gromacs/Amber Window Build Package(Cygwin)

(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.



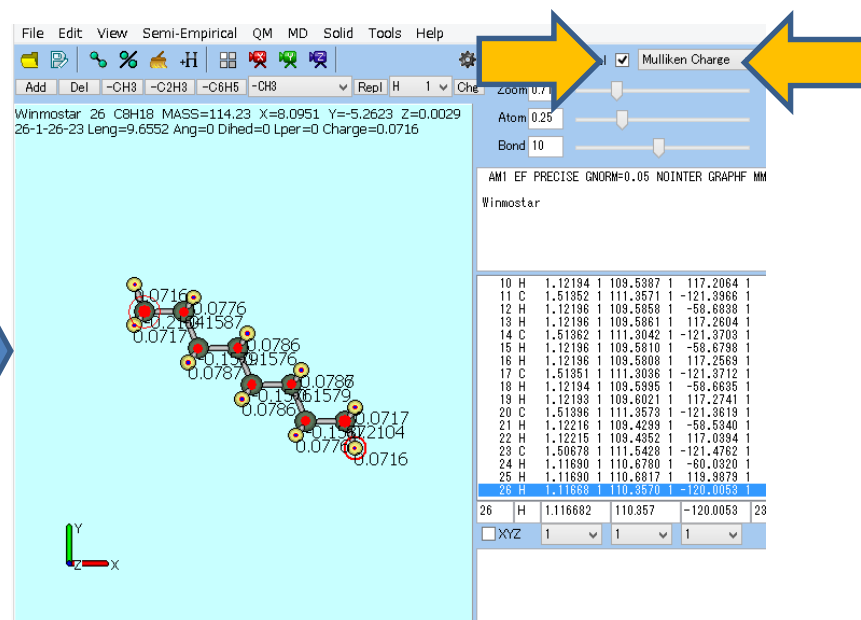
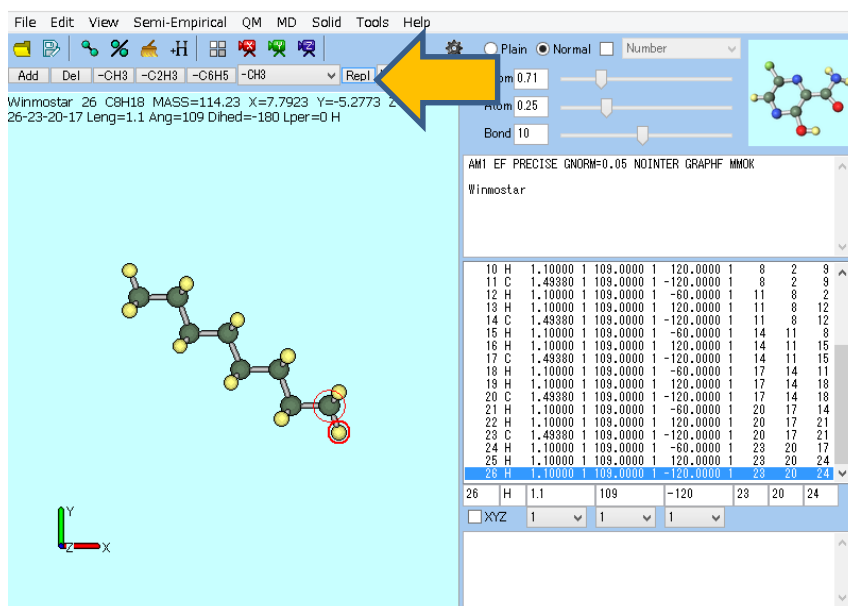
II. Define a molecule

Select **File | New** and click the **Repl** button eight times to obtain n-octane.

Execute MOPAC at **Semi-Empirical | MOPAC | Start (1)MOP6W70**.

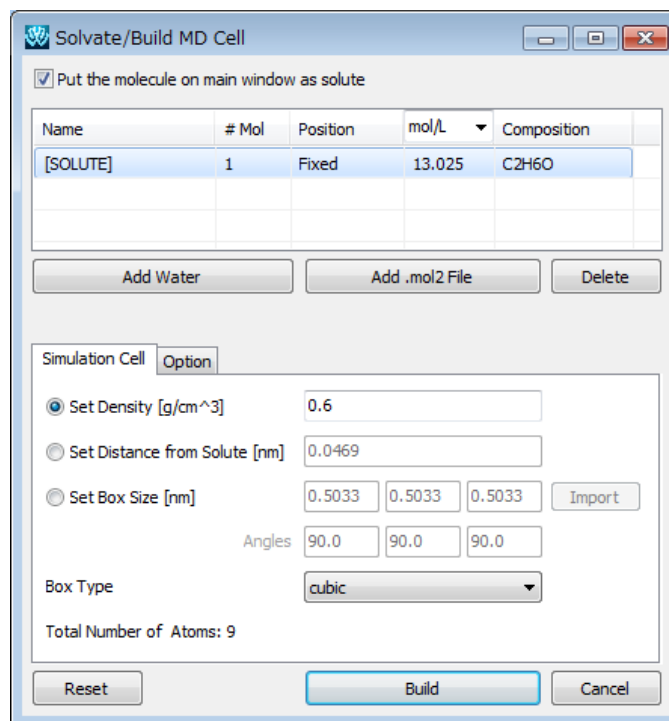
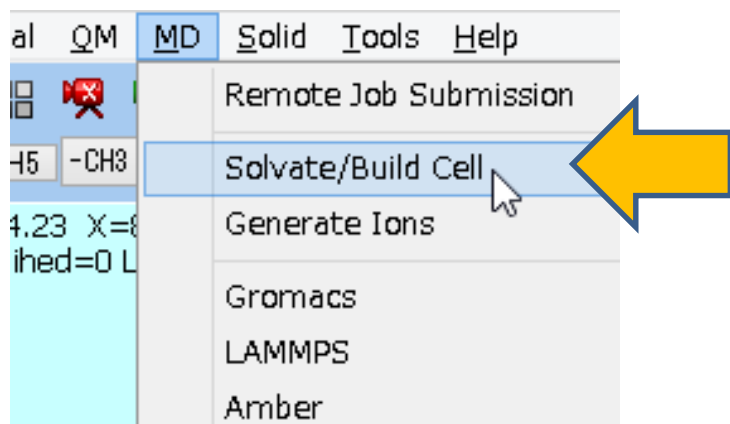
Point charges obtained from MOPAC can be seen when click the checkbox at top left side of the main window and select **Mulliken Charge**.

Finally, save this molecule with **.mol2** format at **File | Save as**.



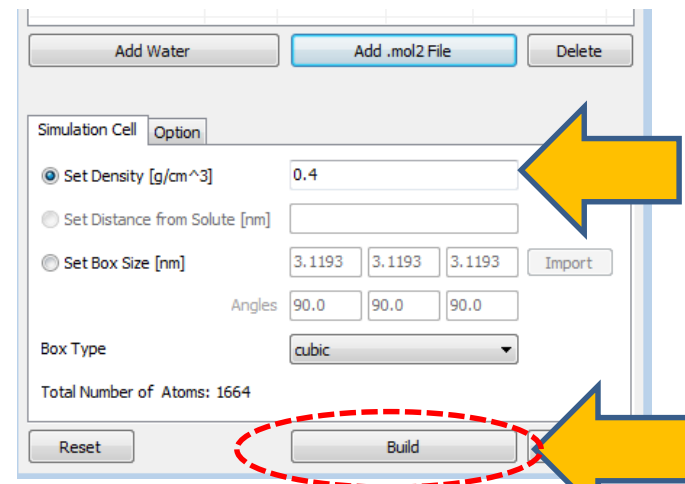
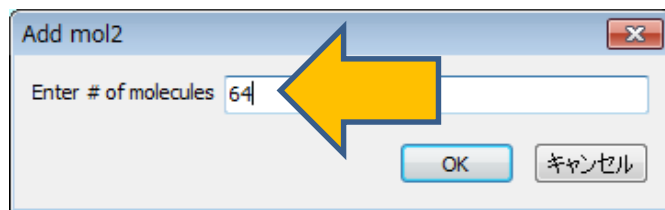
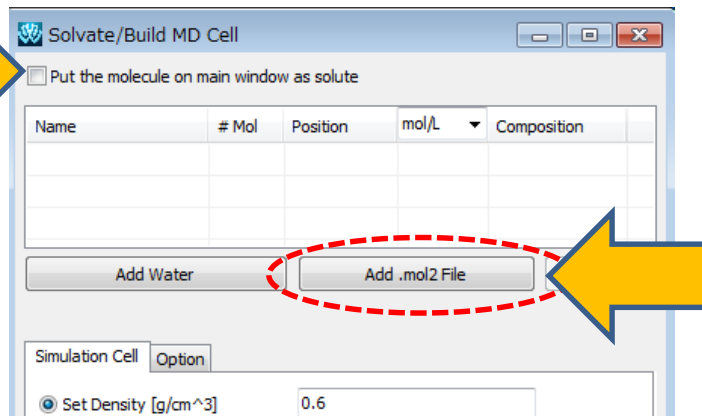
III. Build a simulation cell

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



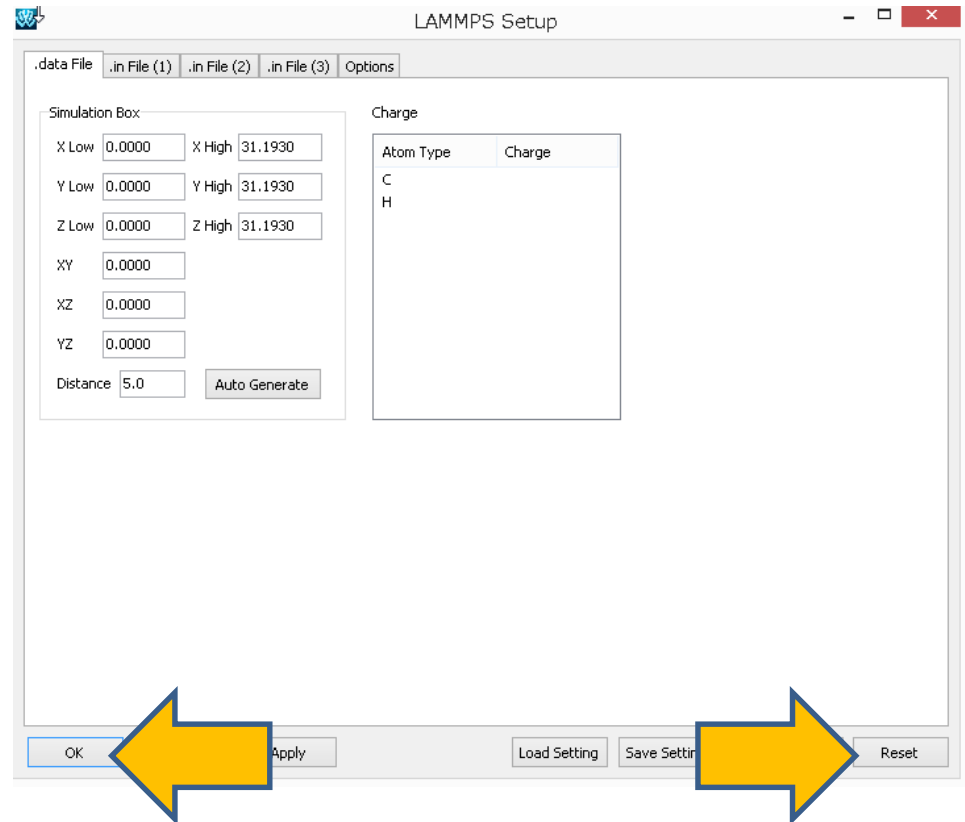
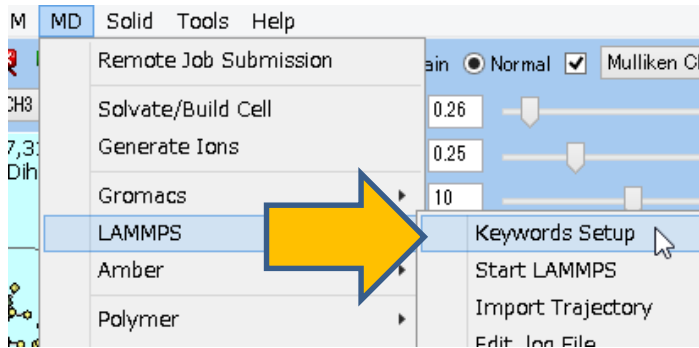
III. Build a simulation cell

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**.



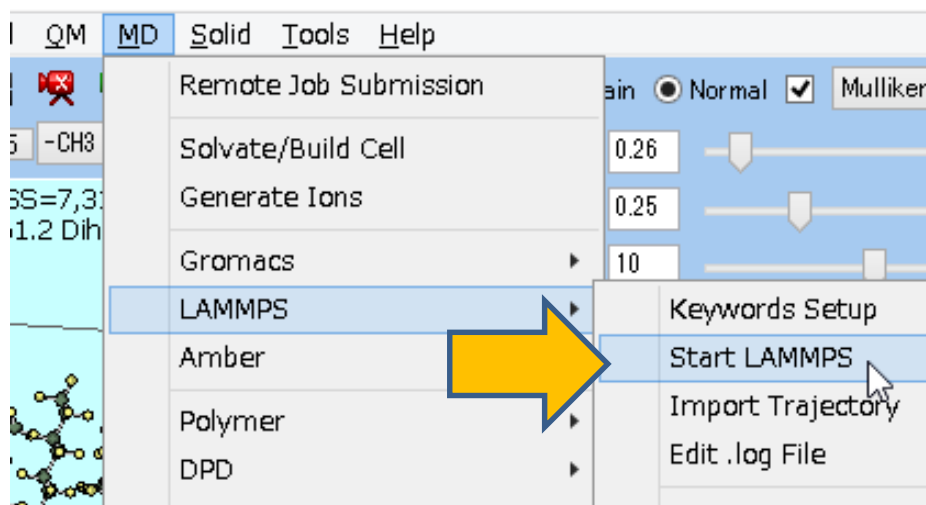
IV. Execute energy minimization

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



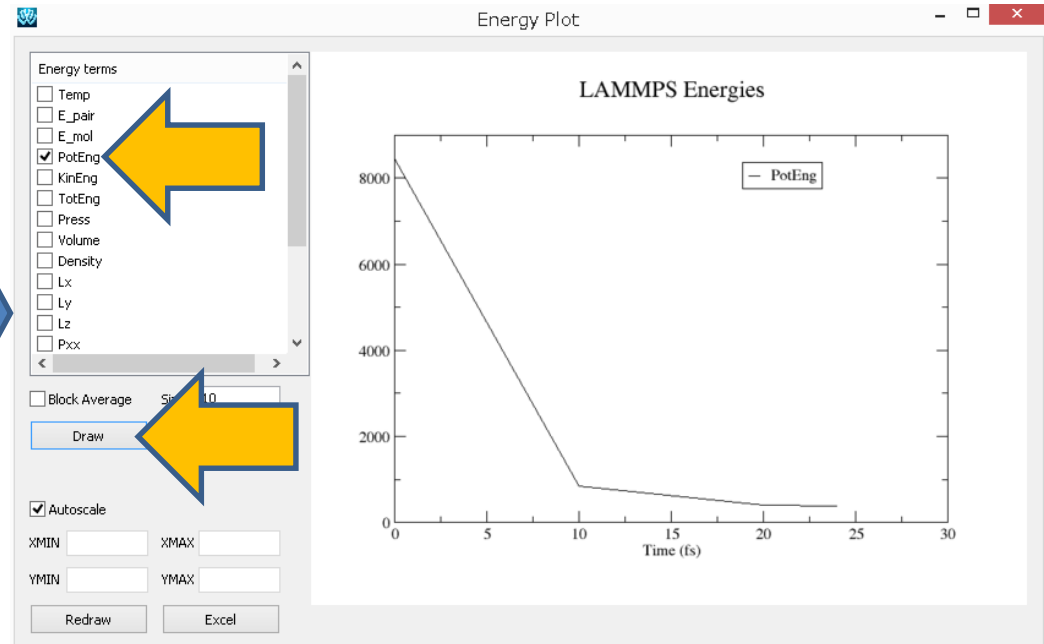
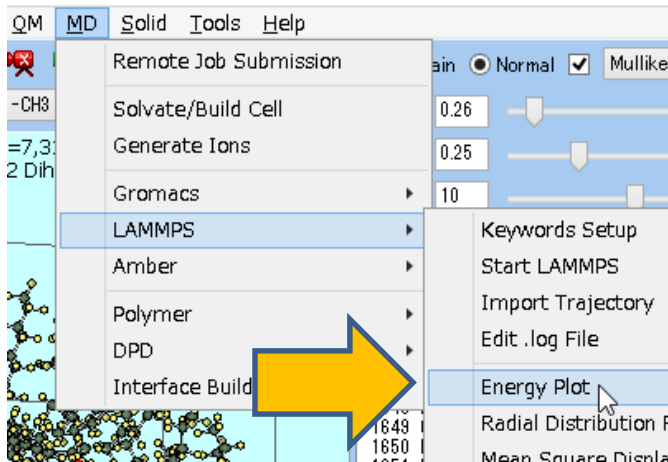
IV. Execute energy minimization

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



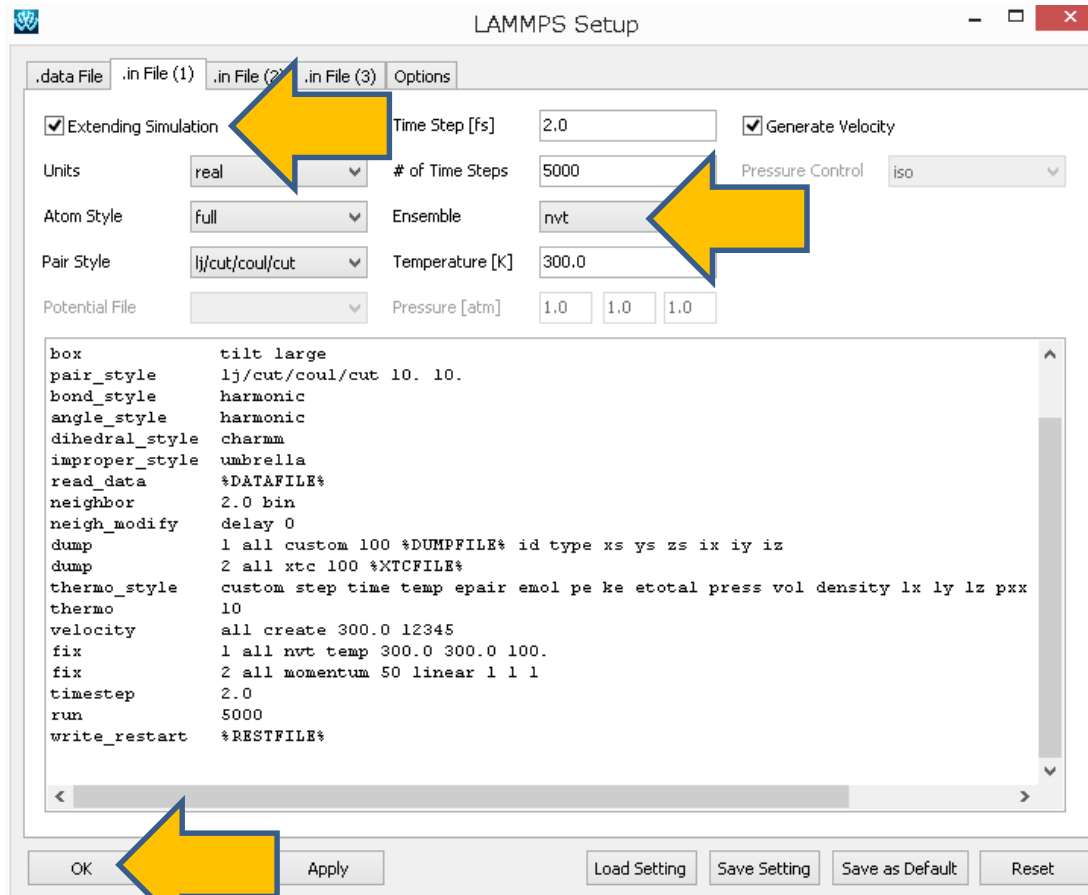
IV. Execute energy minimization

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



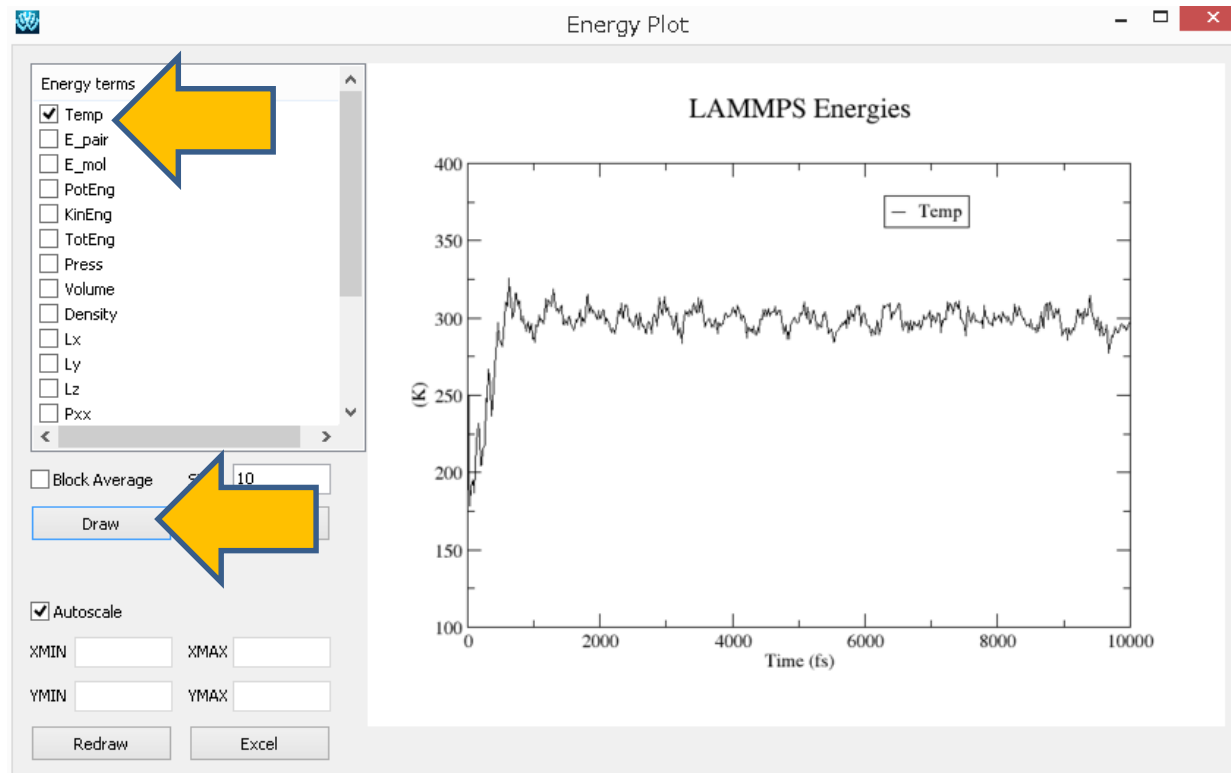
V. Execute an *NVT* MD simulation

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



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).



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**.

The screenshot shows the LAMMPS Setup dialog box with the following settings:

- Extending Simulation
- Units: real
- Atom Style: full
- Pair Style: lj/cut/coul/cut
- Potential File: (empty)
- Time Step [fs]: 2.0
- # of Time Steps: 10000
- Ensemble: npt
- Temperature [K]: 300.0
- Pressure [atm]: 1.0, 1.0, 1.0
- Generate Velocity
- Pressure Control: iso

The bottom section of the dialog contains the following keywords:

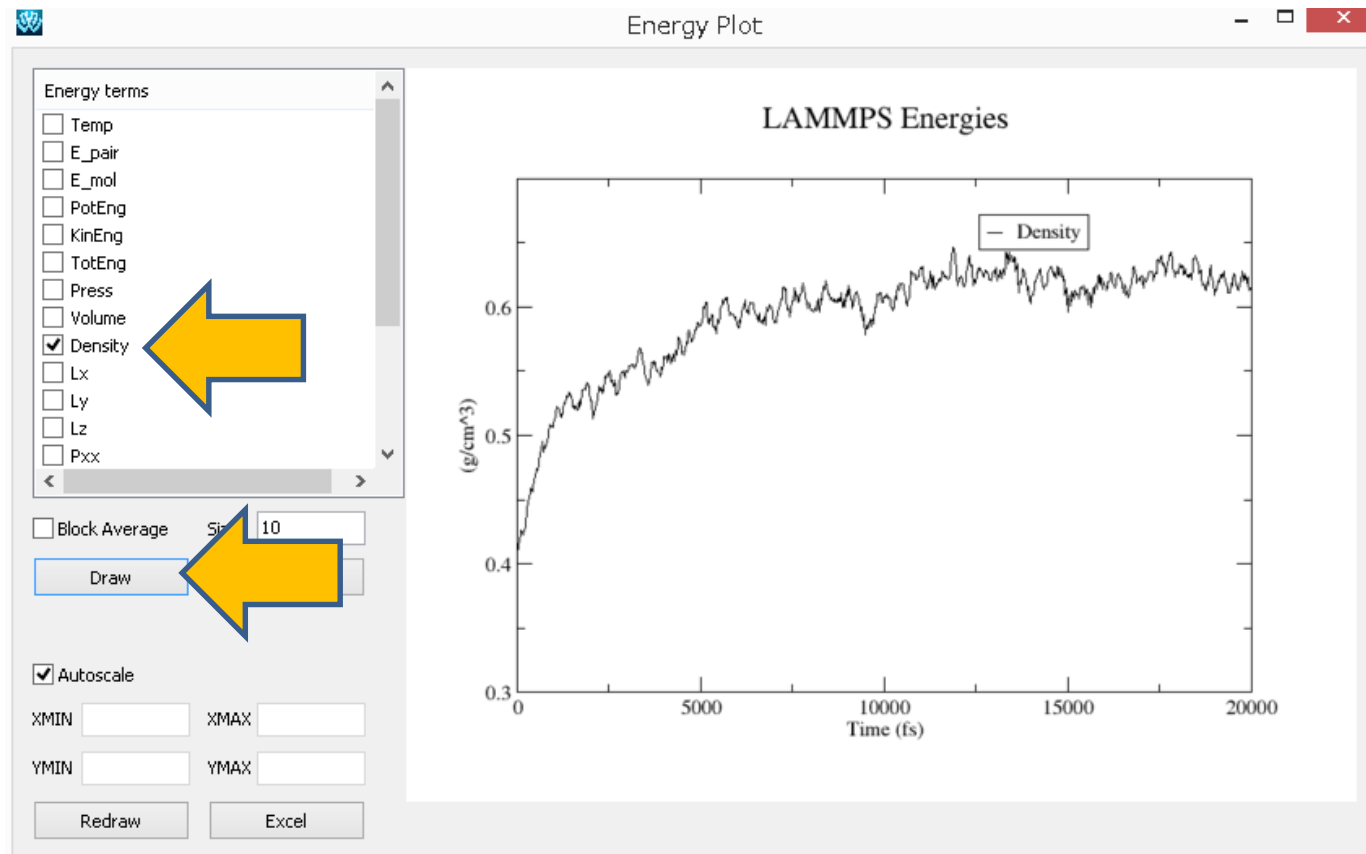
```

boundary      p p p
box           tilt large
pair_style    lj/cut/coul/cut 10. 10.
bond_style    harmonic
angle_style   harmonic
dihedral_style charmm
improper_style umbrella
read_data     %DATAFILE%
neighbor      2.0 bin
neigh_modify  delay 0
dump          1 all custom 100 %DUMPFIL% id type xs ys zs ix iy iz
dump          2 all xtc 100 %XTCFIL%
thermo_style  custom step time temp epair emol pe ke etotal press vol density lx ly lz pxx
thermo        10
fix           1 all npt temp 300.0 300.0 100. iso 1.0 1.0 100.
fix           2 all momentum 50 linear 1 1 1
timestep      2.0
run           10000
write_restart %RESTARTFILE%
  
```

At the bottom of the dialog, there are buttons for OK, Apply, Load Setting, Save Setting, Save as Default, and Reset. Yellow arrows in the original image point to the # of Time Steps, Ensemble, Generate Velocity checkbox, and the OK button.

VI. Execute an *NPT* MD simulation

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



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.

