

Winmostar tutorial
LAMMPS
Polymer Annealing
V8.007

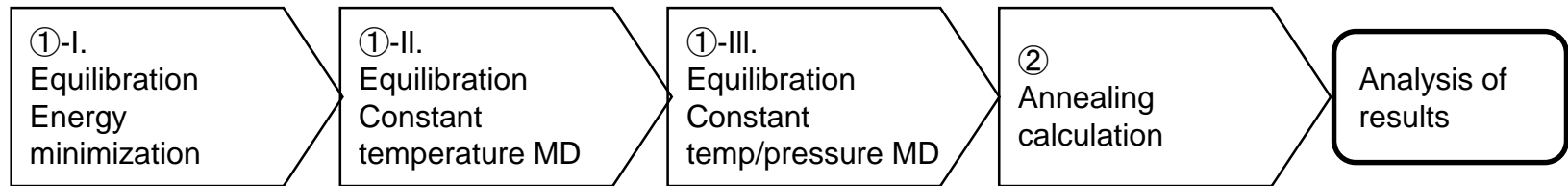
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Summary

- In this tutorial we will calculate glass transition temperature from the cooling process of polypropylene melt.
- Processing flow is described below. To reduce steps for equilibration, we will first regulate at high pressure (200 atm) then revert to constant pressure for constant temperature/pressure MD.



Notes:

- Steps required for equilibration will vary depending on the molecule and initial density.
- The method for interaction calculations and/or the force field and/or charges also affect the simulation results.
- The polymerization degree (the length of chain) , and rate of temperature reduction (and/or incalescence) also affect the simulation results.
- For the purpose of this tutorial, we will not show complete equilibration steps for polymers.

Configuration

Set up LAMMPS and Cygwin in advance.

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 Installation Guide](#) ※Gromacs/Amber Window Build Package(Cygwin)

(For Experts)Gromacs/Amber Build with Cygwin ※we recommend you to use the precompiled package

[GAMESS Installation Guide](#)

[NWChem Installation Guide](#) ※Window Build Package

(For Experts)NWChem Build with MinGW ※we recommend you to use the precompiled package.

[LAMMPS Installation Guide](#)

Installation guide for LAMMPS on Windows

Feb. 6, 2017

1. Getting LAMMPS

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

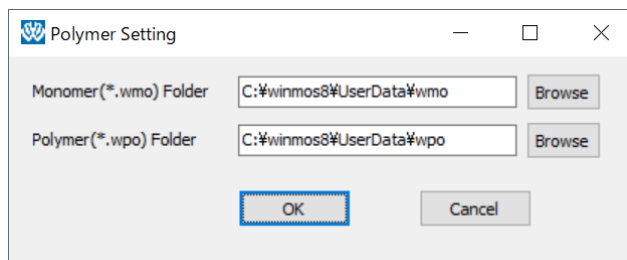
Visit [\[32-bit Windows download area\]](#) or [\[64-bit Windows download area\]](#).

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 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 (because it is not GPU accelerated). OPENGL (OPENGL does not support cross-compilation), KOKOS and OPENMPI (do not support cross-compilation with GCC), USE_EXTERNAL_BINARY (requires to bundle a full Python runtime), USE_CUDA (requires external binaries), USE_GPU (requires external binaries), GPU (requires for the USE_CUDA package which is included). The serial executable additionally does not contain the MPI and USE_MPI packages, since those require MPIV2 functions, which are not available without linking to a real MPI library.

Some Notes on GPU Support
These Windows binaries include (experimentally on Windows) GPU acceleration via the GPU package. This is achieved through compiling the GPU package in OpenCL mode and linking to an OpenCL (v2.2) compatible ICD loader. This means the executables do not contain any vendor provided code and should be compatible with GPUs from both AMD and NVIDIA. The GPU package has been compiled for mixed precision computation and is currently somewhat tuned for Nvidia (Fermi generation) GPUs. It does not yet work with OpenCL drivers for GPUs like those included in the Intel and AMD OpenCL ICDs.

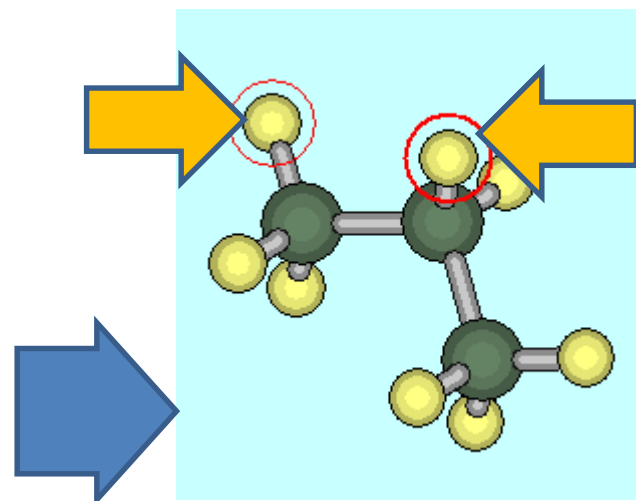
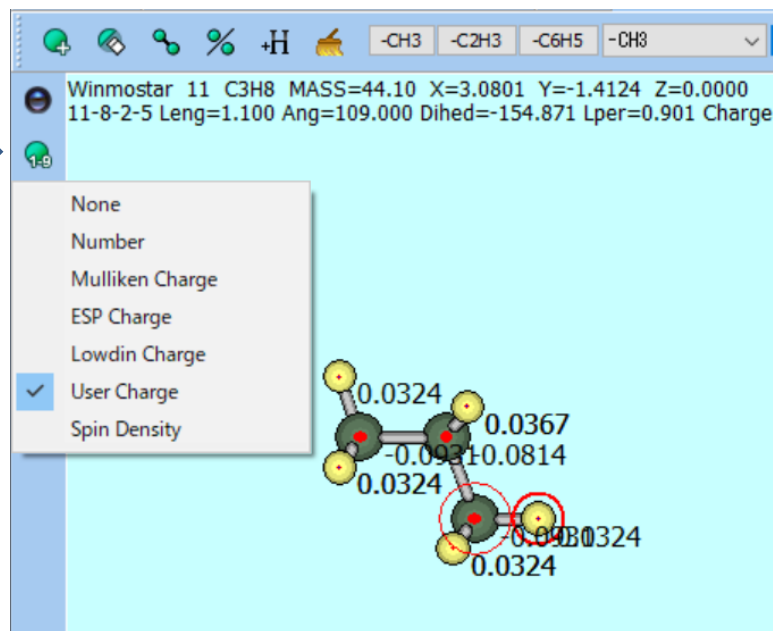
- Configuration of polymer tool
Click **MD | Polymer | Settings**. Set folders for monomer files (extension **.wmo**) and polymer files (extension **.wpo**) as need.



I. Register a monomer

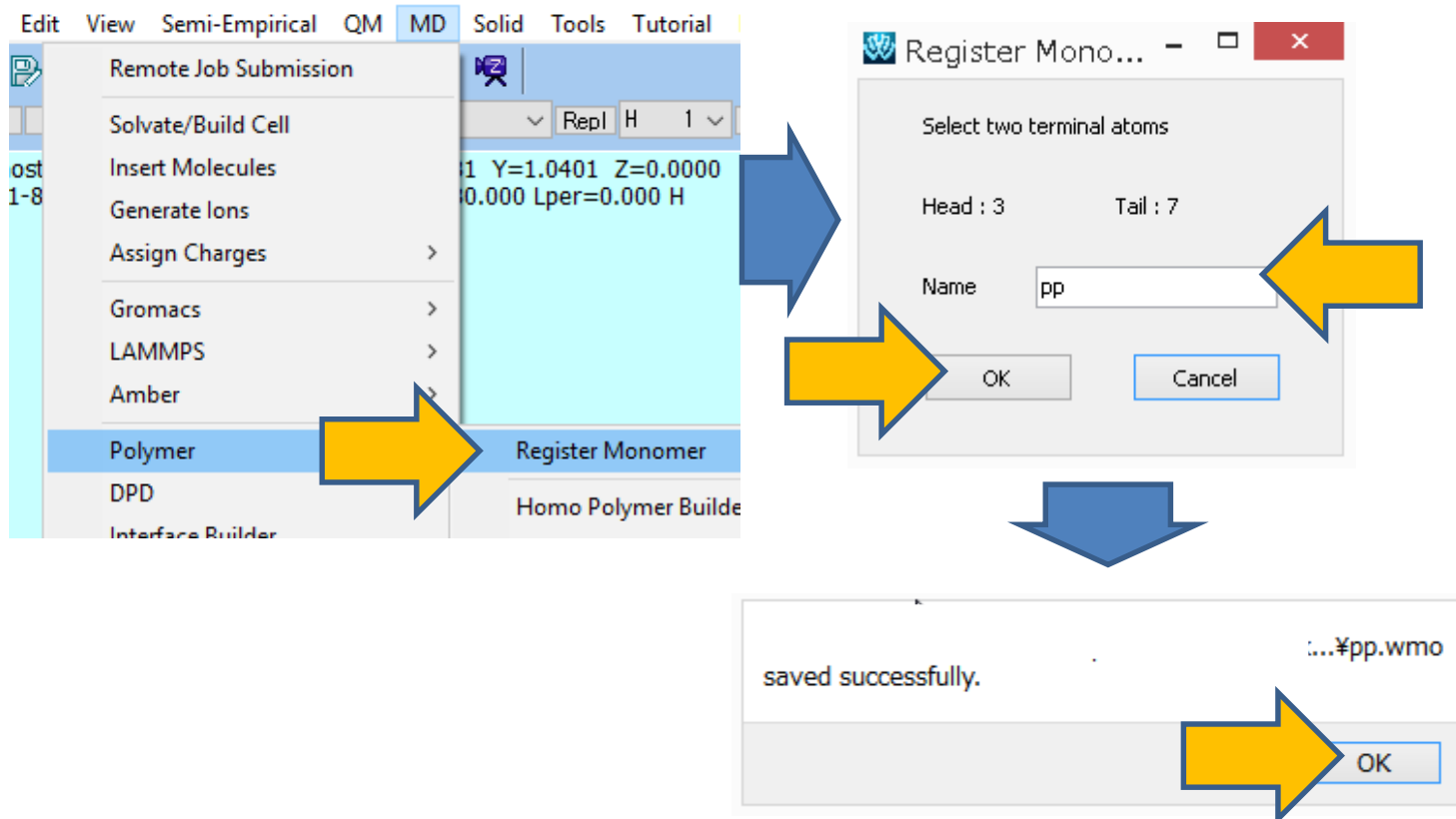
This tutorial will describe how to model a polypropylene.

1. Model a monomer of polypropylene (propane, C_3H_8) on the main window.
2. Click **MD | Assign Charges | By Actype | Execute**.
3. Use **annotation button** to the left of the main window to hide charge information.
4. Click two hydrogens to be the end points of the monomer.



I. Register a monomer

1. Click **MD | Polymer | Register Monomer**.
2. Set **Name** to **pp**, and click **OK**.
3. Click **OK** on the dialog.



II. Define a polymer

1. Click **MD | Polymer | Homo Polymer Builder**.
2. Set **Polymer Name** to **pp15**, **Polymerization Degree** to **15**, Select **pp** in **Monomer List**.
3. Click **Build**.
4. Click **Close**.

The image shows a sequence of four screenshots illustrating the steps to define a polymer in the software:

- Step 1:** The 'MD' menu is open, and 'Homo Polymer Builder' is selected.
- Step 2:** The 'Homo Polymer Builder' dialog box is shown with 'Polymer Name' set to 'pp15', 'Polymerization Degree' set to '15', and 'pp' selected in the 'Monomer List'.
- Step 3:** A 'Build' button is highlighted in the dialog box.
- Step 4:** A confirmation dialog box shows 'saved successfully.' for the file '..¥pp15.wpo' with an 'OK' button.

III. Build a simulation cell

1. Click **MD | Polymer | Polymer Cell Builder**.
2. Set **Polymers Available** to **pp15**, **Number** to **30**, and click **>> Add >>**.
3. Click **Build**. Save as **pp15_30.mol2**.

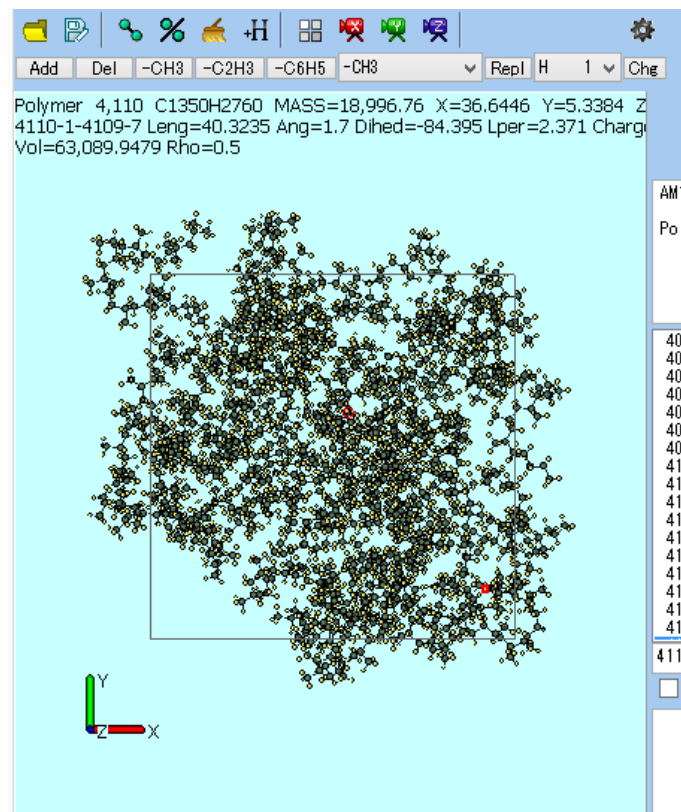
The screenshot illustrates the software interface for building a simulation cell. The 'MD' menu is open, and the 'Polymer Cell Builder' option is selected. The 'Polymer Cell Builder' dialog box is shown with the following settings:

- Box Configuration:**
 - Density [g/cm³]: 0.5
 - X-Axis Length [Å]: 39.8095
 - Y-Axis Length [Å]: 39.8095
 - Z-Axis Length [Å]: 39.8095 (selected)
 - Cubic Cell
- Periodic Boundary Condition:**
 - X
 - Y
 - Z
- Polymers Available:**
 - pp15 (selected)
- Polymers Used:**

Name	Number
pp15	30
- Number:** 30
- Buttons:** >> Add >> (highlighted), << Delete <<, Display, Delete, Build (highlighted), Close

III. Build a simulation cell

1. Click **OK** on the dialog, then the simulation cell will be displayed on the window.
2. Click **Close** to close **Polymer Cell Builder**.



IV. Equilibration

1. Click **MD | LAMMPS | Keywords Setup**.
2. Click **Reset**.

LAMMPS Setup

Extending Simulation: Preset: Minimize (Fast) MPI 1 processes

Basic Advance Output Interaction Non-equilibrium (1) Restraint Automatic Options Force Field

Units: real Time Step [fs]: 2.0 Ensemble: minimize

Atom Style: full # of Time Steps: 5000 Temperature [K]: 300.0

Pair Style: lj/cut/coul/long Total time [fs]: N/A Pressure [atm]: 1.0 1.0 1.0

Potential File: Generate Velocity Pressure Control: iso

Constrain Hydrogen

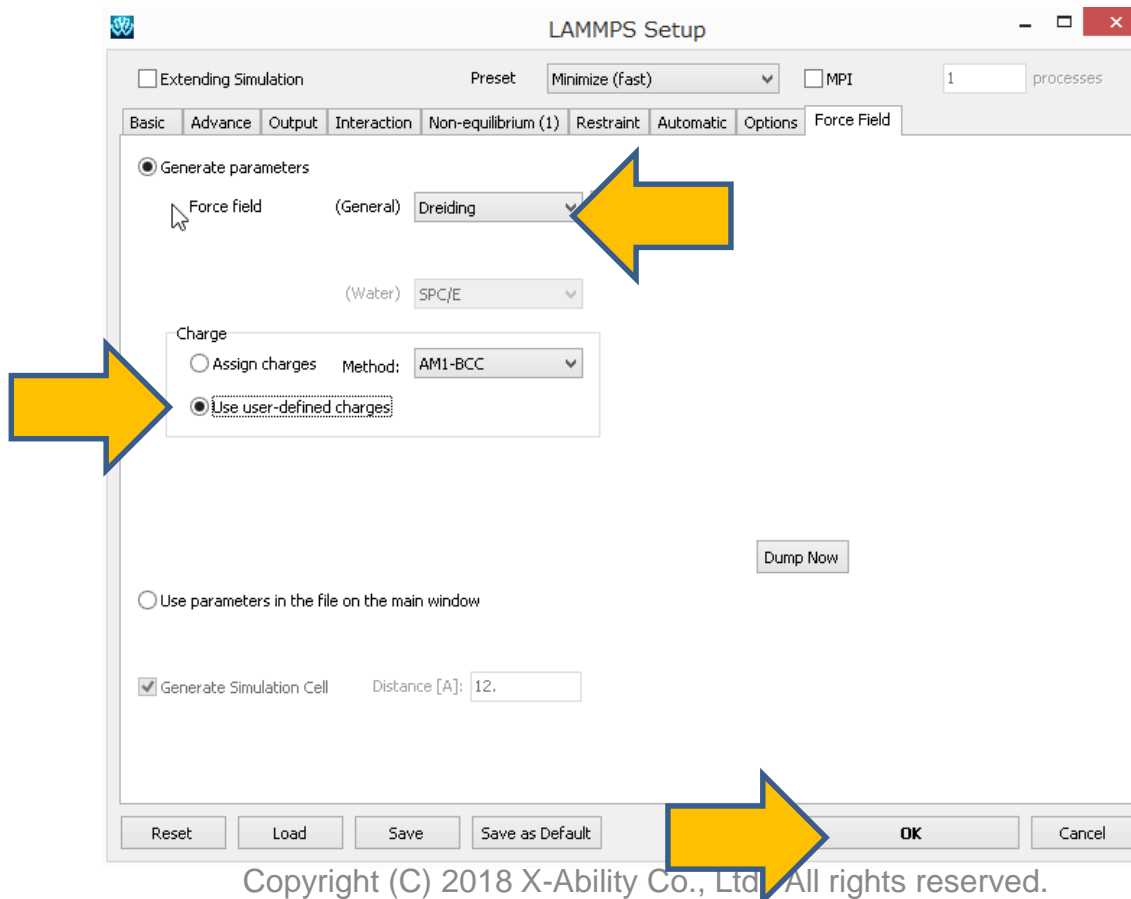
```

units          real
atom_style     full
boundary       p p p
box            tilt large
pair_style     lj/cut/coul/long 10. 10.
pair_modify    mix arithmetic
special_bonds  amber
kspace_style   pppm 1e-5
kspace_modify  order 4
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 %DUMPPFILE% id type xs ys zs ix iy iz
dump          2 all xtc 100 %XTCFILE%
  
```

Reset Load Save Save as Default OK Cancel

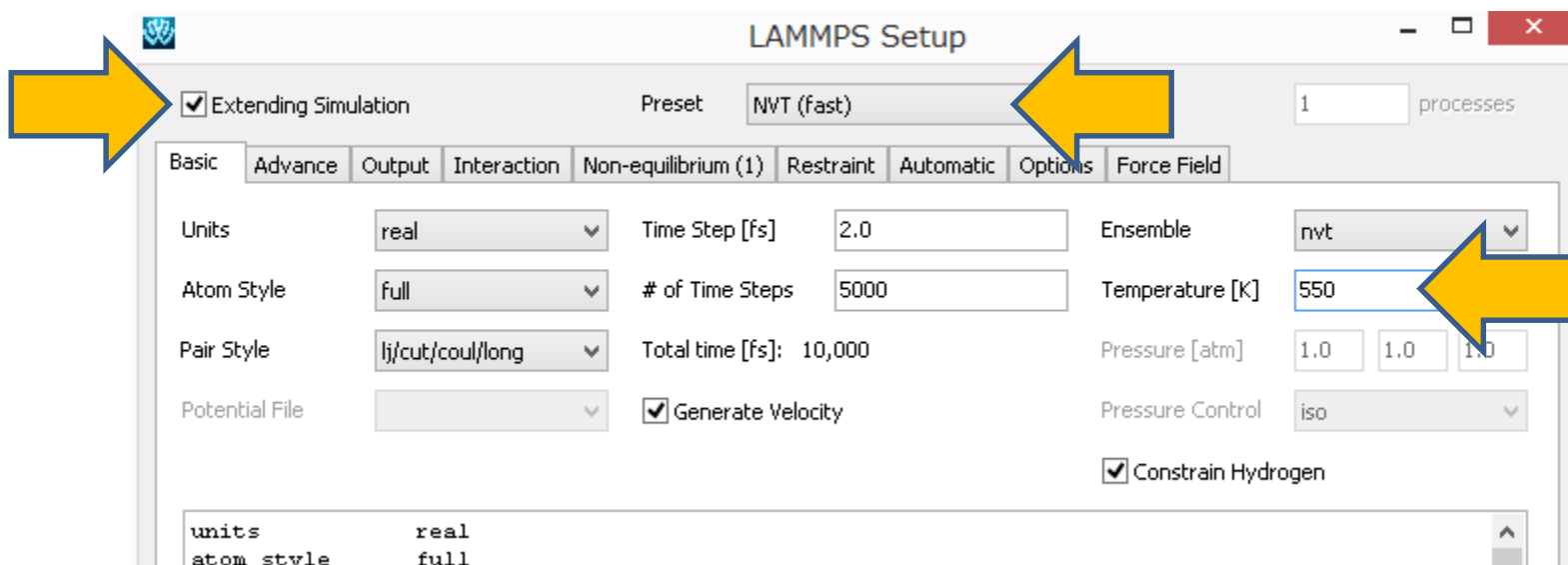
IV. Equilibration

1. Select the Force Field tab.
2. Set Force Field to Dreiding, Charge to Use user-defined charges, click OK.
3. Click **MD | LAMMPS | Start LAMMPS**.



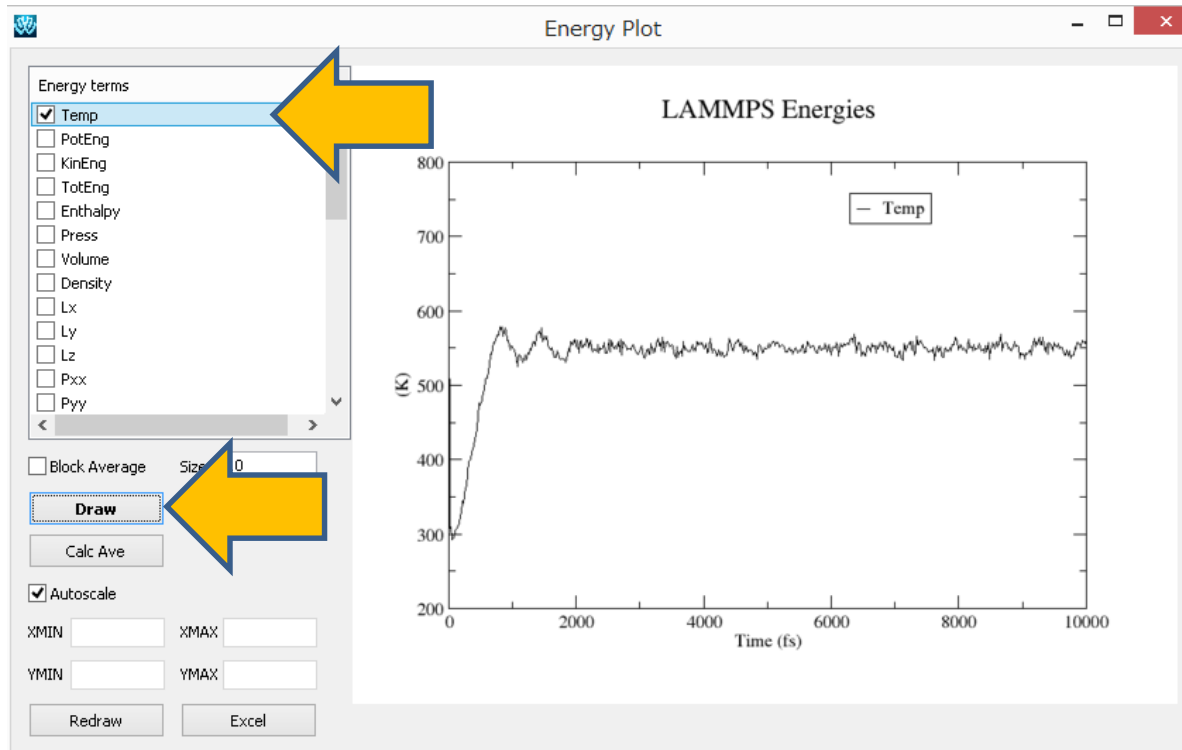
IV. Equilibration

1. Click **MD | LAMMPS | Keywords Setup** and check the box for **Extending Simulation**.
2. Set **Preset** to **NVT (fast)**, **Temperature** to **550**, then click **OK**.
3. Click **MD | LAMMPS | Start LAMMPS**.



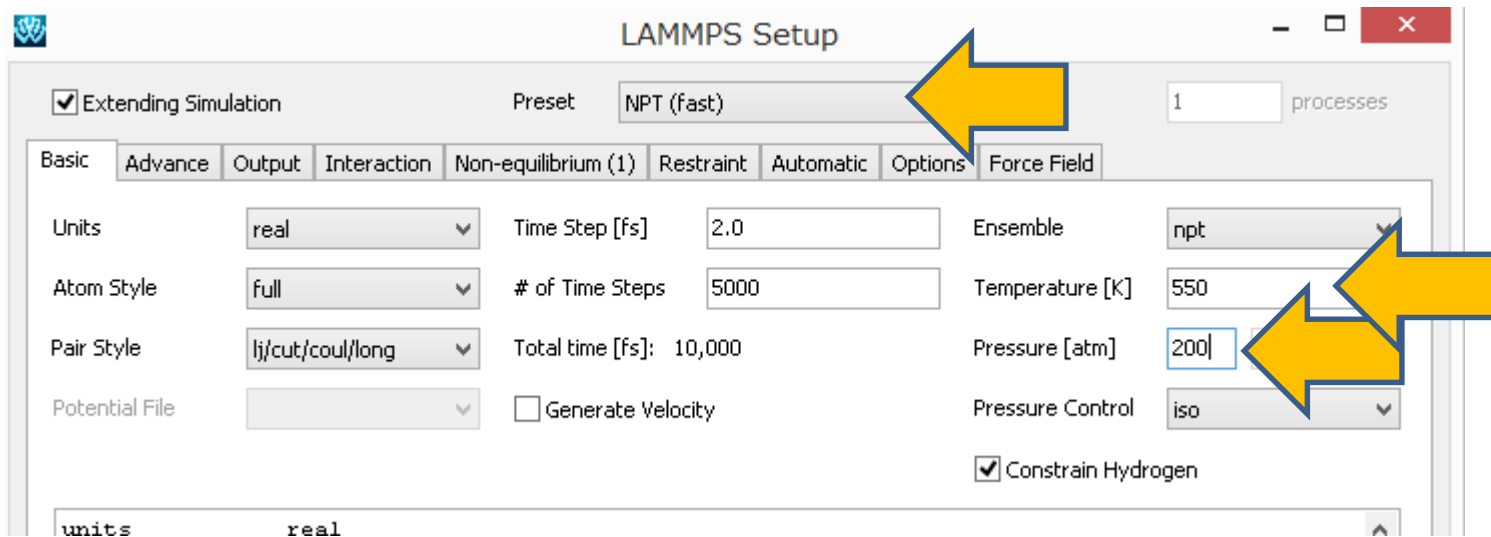
IV. Equilibration

1. Click **MD | LAMMPS | Energy plot**. Open the default file.
2. Under **Energy terms**, check **Temp**, then click **Draw**.
3. The graph will show convergence of temperature values to the target temperature. Click Close when done.



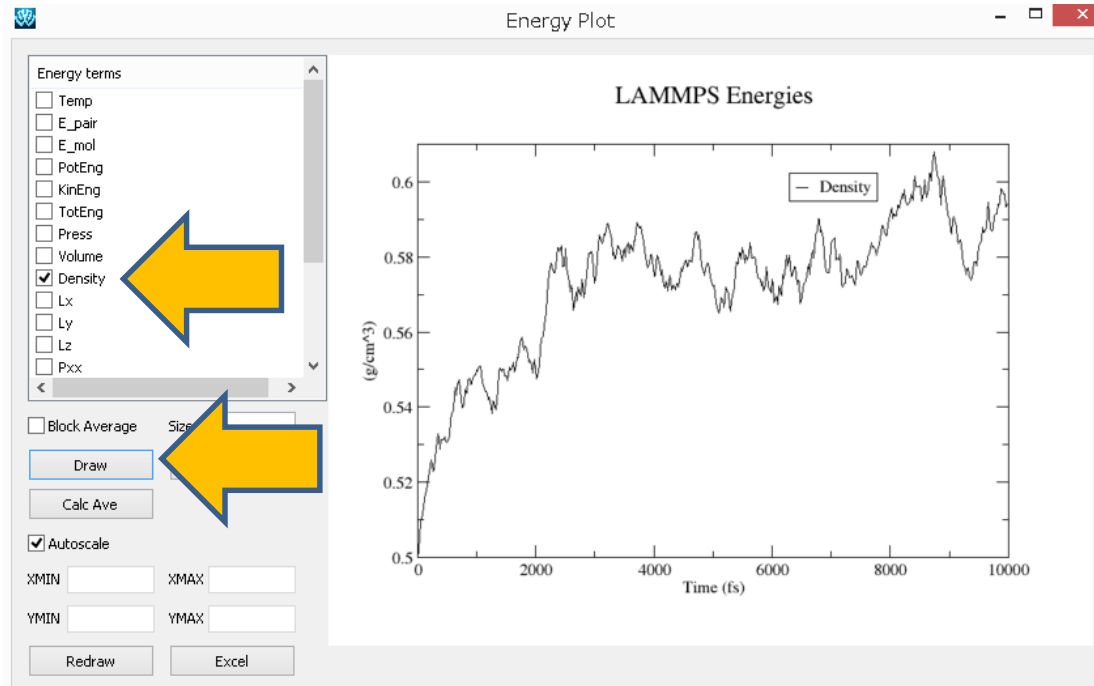
IV. Equilibration

1. Click **MD | LAMMPS | Keywords Setup**.
2. Set **Preset** to **NPT (fast)**, **Temperature** to **550**, **Pressure** to **200**, then click **OK**.
3. Click **MD | LAMMPS | Start LAMMPS**.



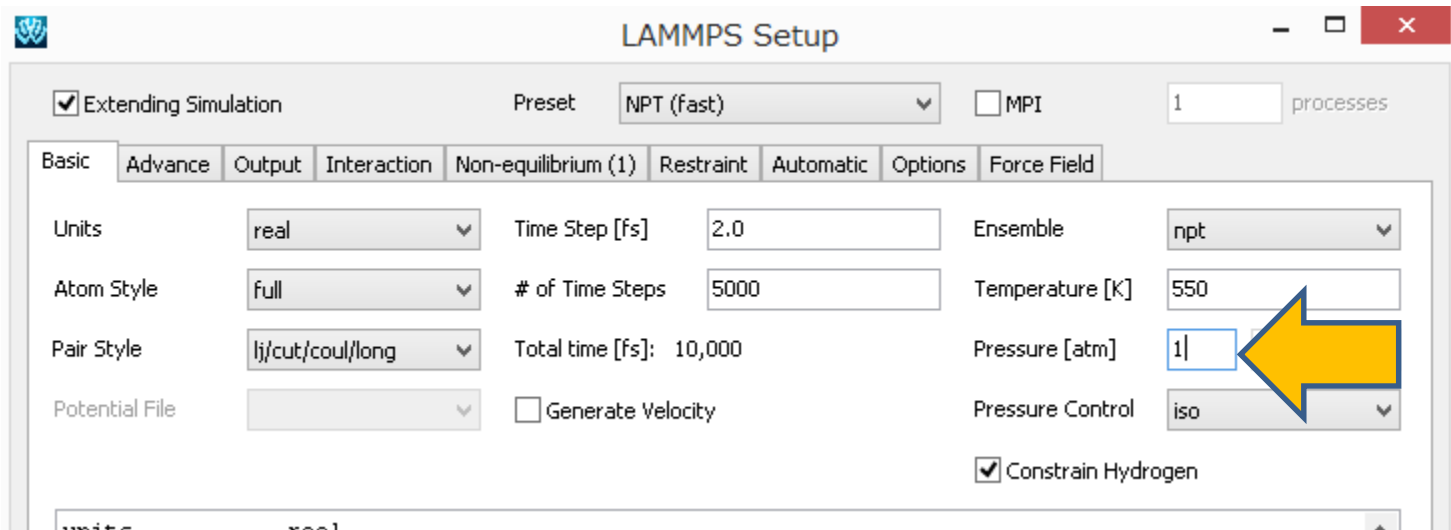
IV. Equilibration

1. Click **MD | LAMMPS | Energy plot**. Open the default file.
2. Under **Energy terms**, check **Density**, then click **Draw**.
3. The graph will show convergence of density values to a constant (although the convergence may be difficult to see with the given conditions, it serves the purpose of this tutorial).



IV. Equilibration

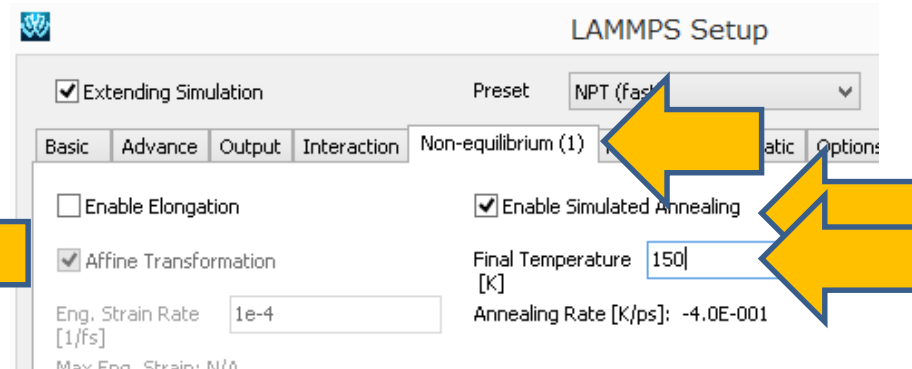
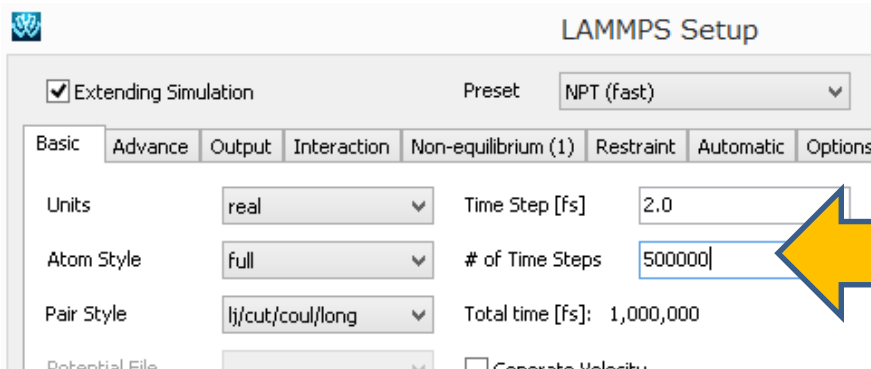
1. Click MD | **LAMMPS** | **Keywords Setup**.
2. On **Basic** tab, set **Pressure** to 1, click **OK**.
3. Click **MD** | **LAMMPS** | **Start LAMMPS**.



V. Annealing Calculation

Next, use simulated annealing in order to calculate glass-transition temperature.

1. Click **MD | LAMMPS | Keywords Setup**.
2. In the **Basic** tab, set **# of Time Steps** to **500000**
(set smaller value if you want to reduce calculation time.)
3. On **Non-equilibrium** tab, check **Enable Simulated Annealing**,
Set **Final Temperature** to **150**, then click **OK**.
4. Click **MD | LAMMPS | Start LAMMPS**.



V. Annealing Calculation

1. Click **MD | LAMMPS | Energy plot**. Then open the file selected by default.
2. Under **Energy Terms**, check boxes for **Temp** and **Density**, and click **Draw**.
3. Click **Excel**.

In the exported CSV file, plot column **B** on the X-axis and Column **C** on the Y-axis to get a Temperature-Specific Volume curve.

Estimations of glass transition temperatures can be found on inflection points (at around 250 – 300K) on this curve for a given distribution fitting.

