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Winmostar tutorial
LAMMPS
Polymer Annealing
V8.007

X-Ability Co., Ltd.

question@winmostar.com

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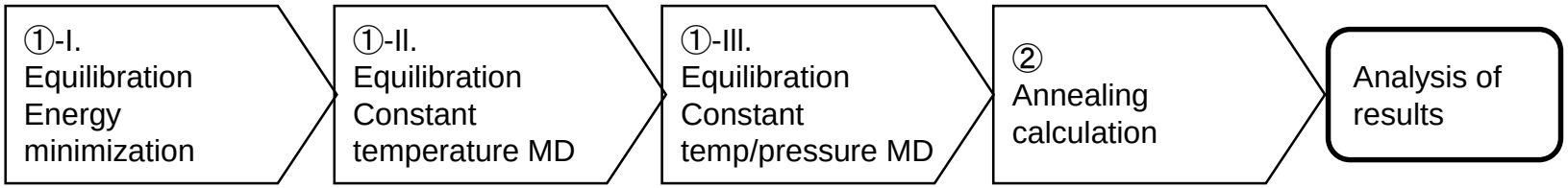
Summary

- 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.

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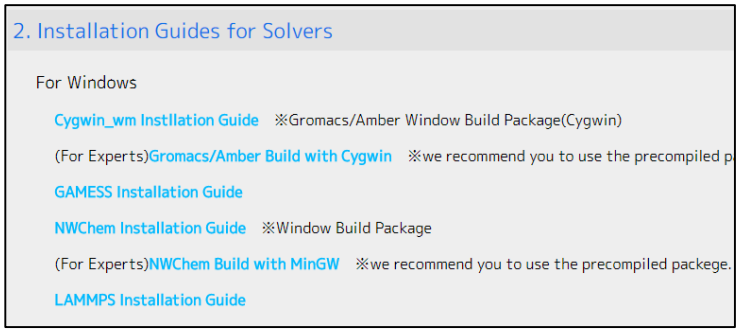
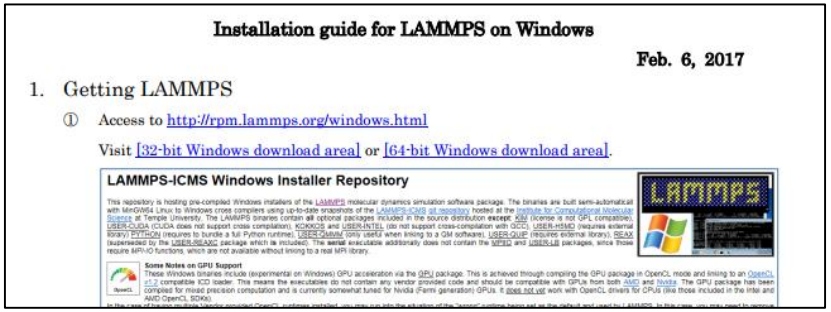
Configuration

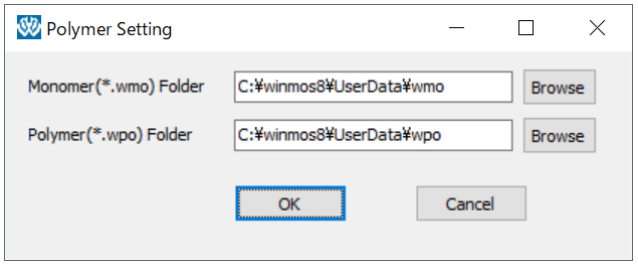
Set up LAMMPS and Cygwin in advance.

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





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



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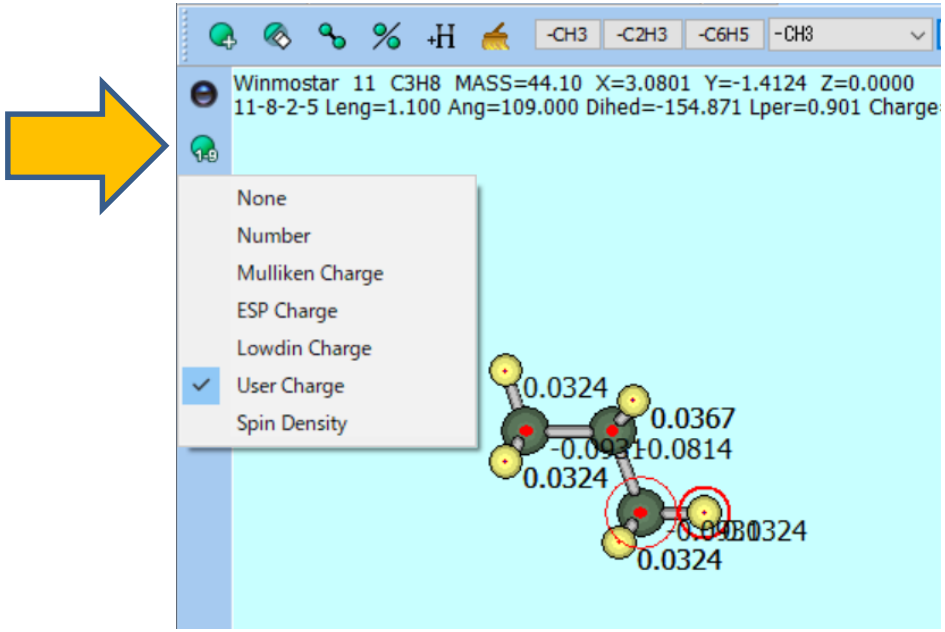
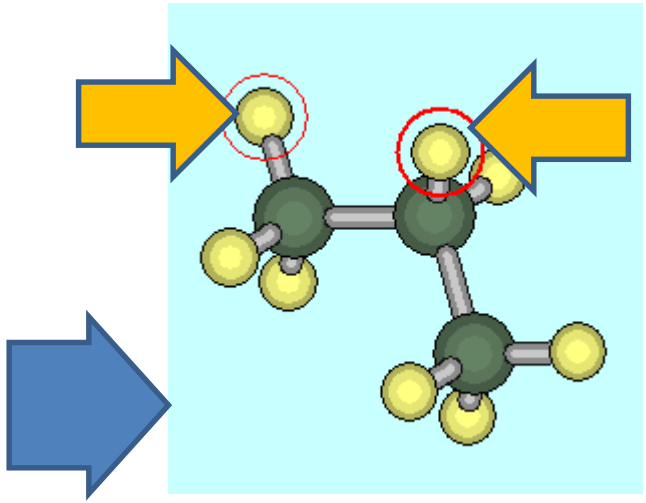
I. Register a monomer

This tutorial will describe how to model a polypropane.

1. Model a monomer of polypropyrene (propane, C_3H_8) on the main window.
2. Click **MD** | **Assign Charges** | **By Acpype** | **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.





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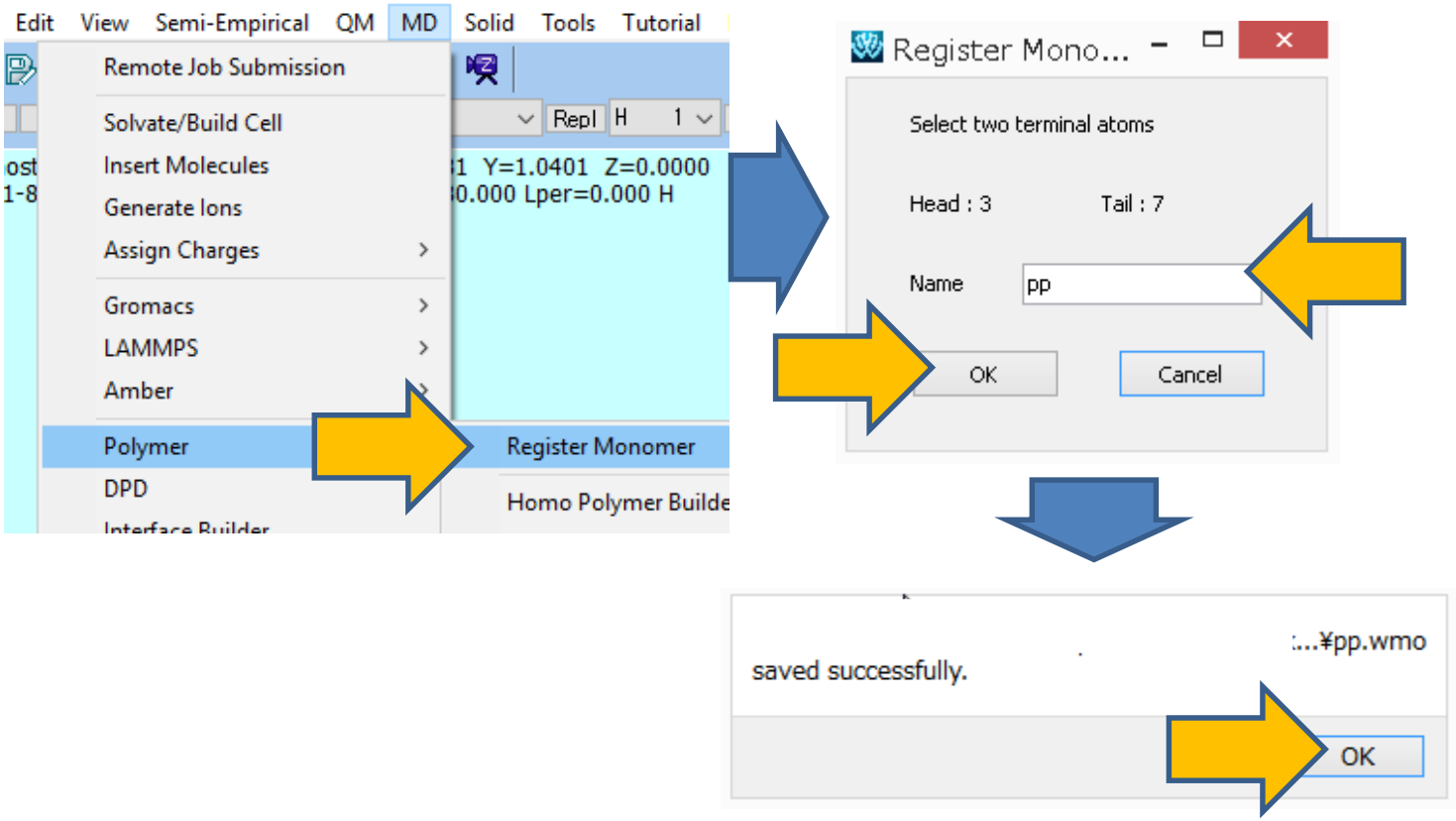
I. Register a monomer

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



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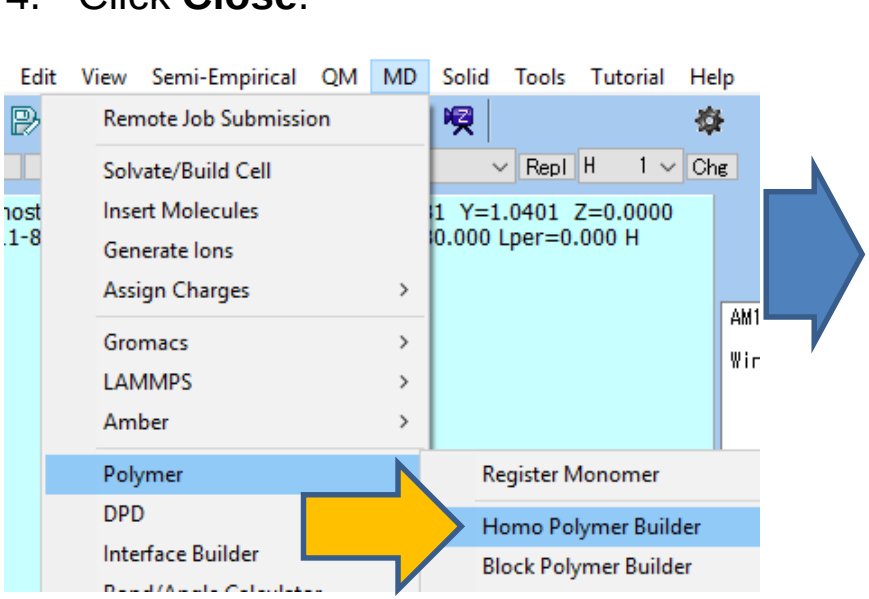
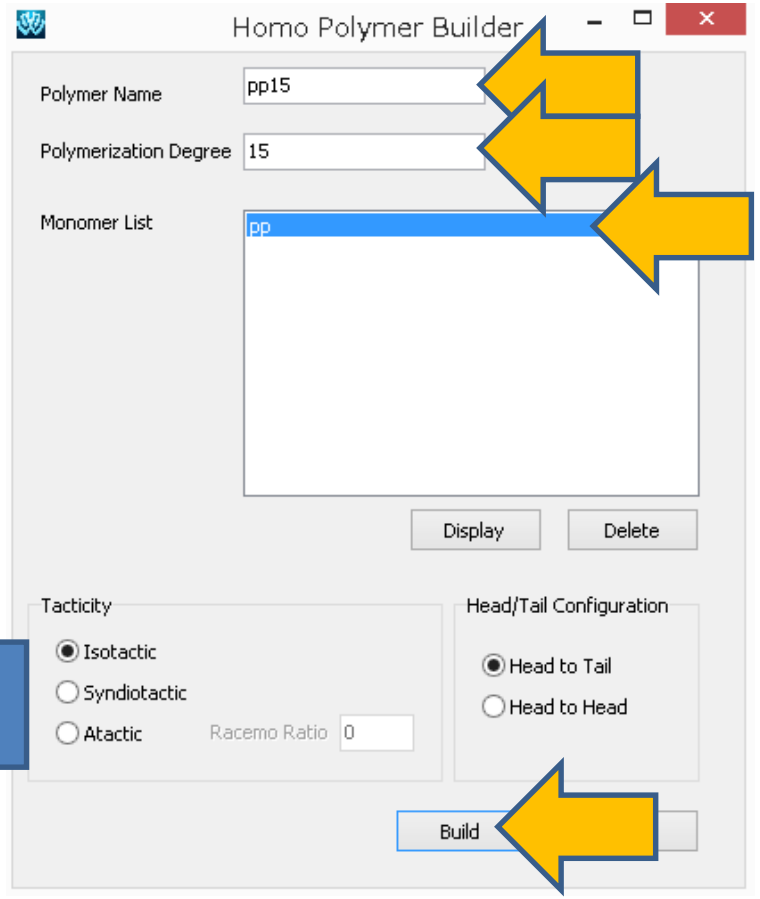
II. Define a polymer

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**.





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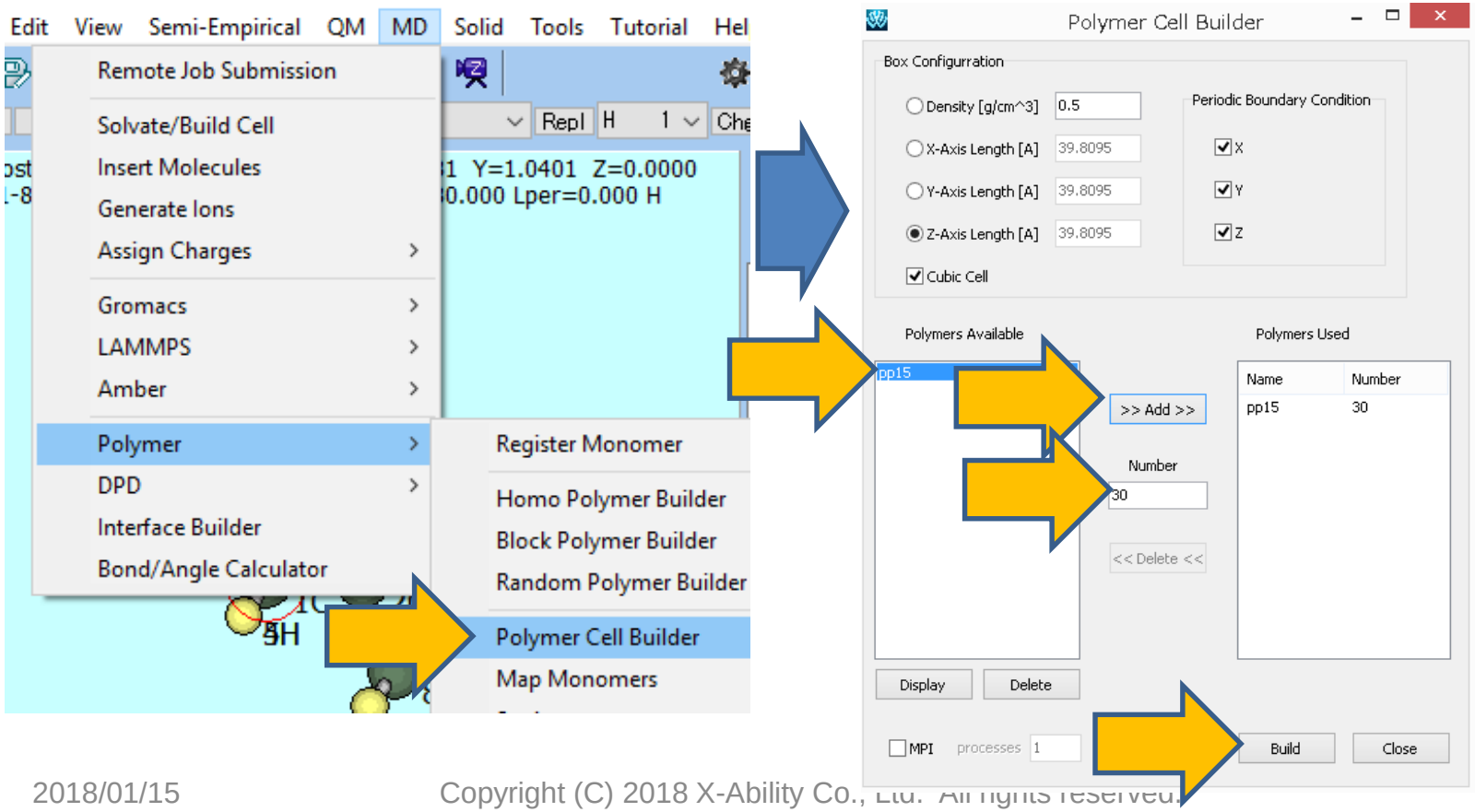
III. Build a simulation cell

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**.



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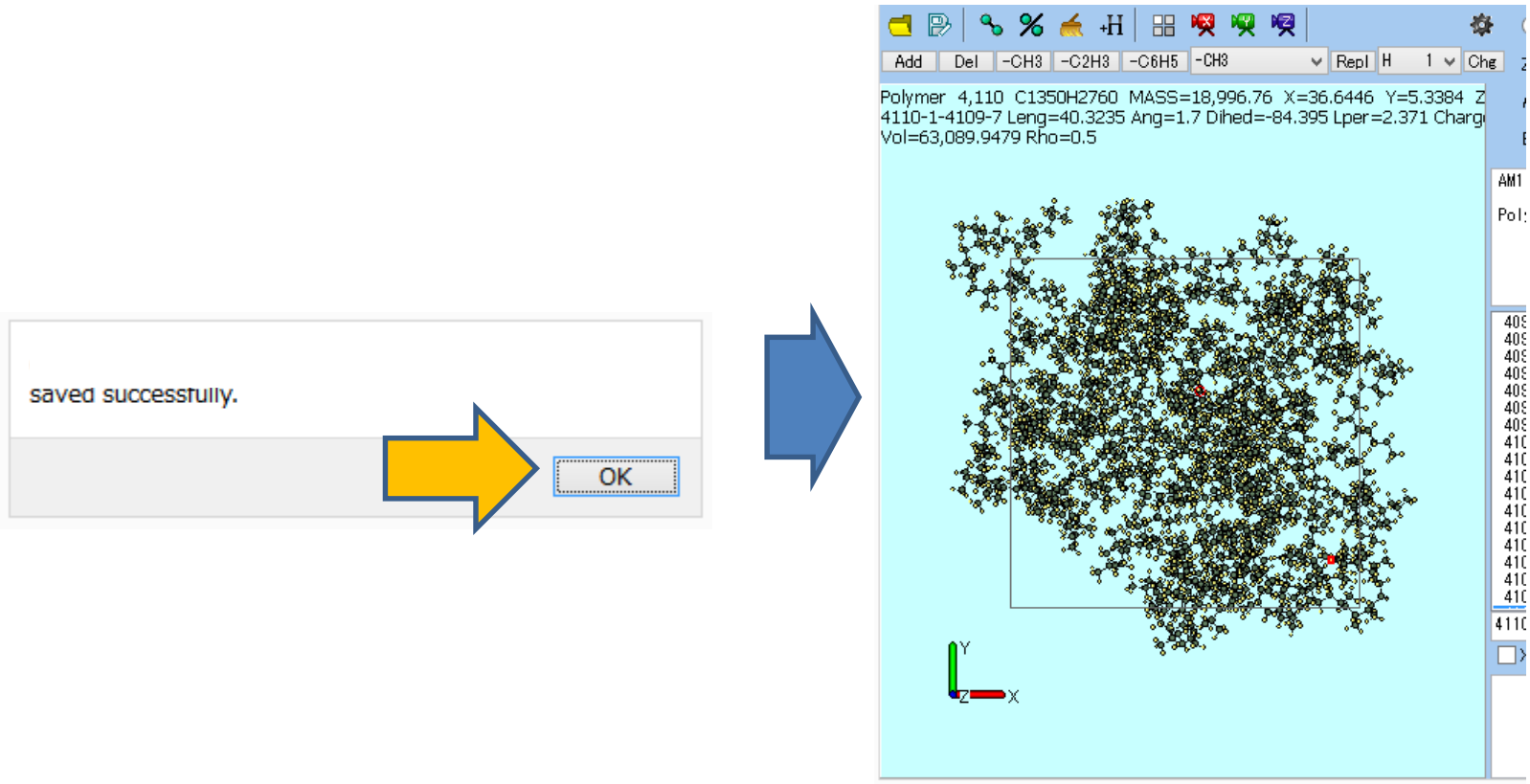
III. Build a simulation cell

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



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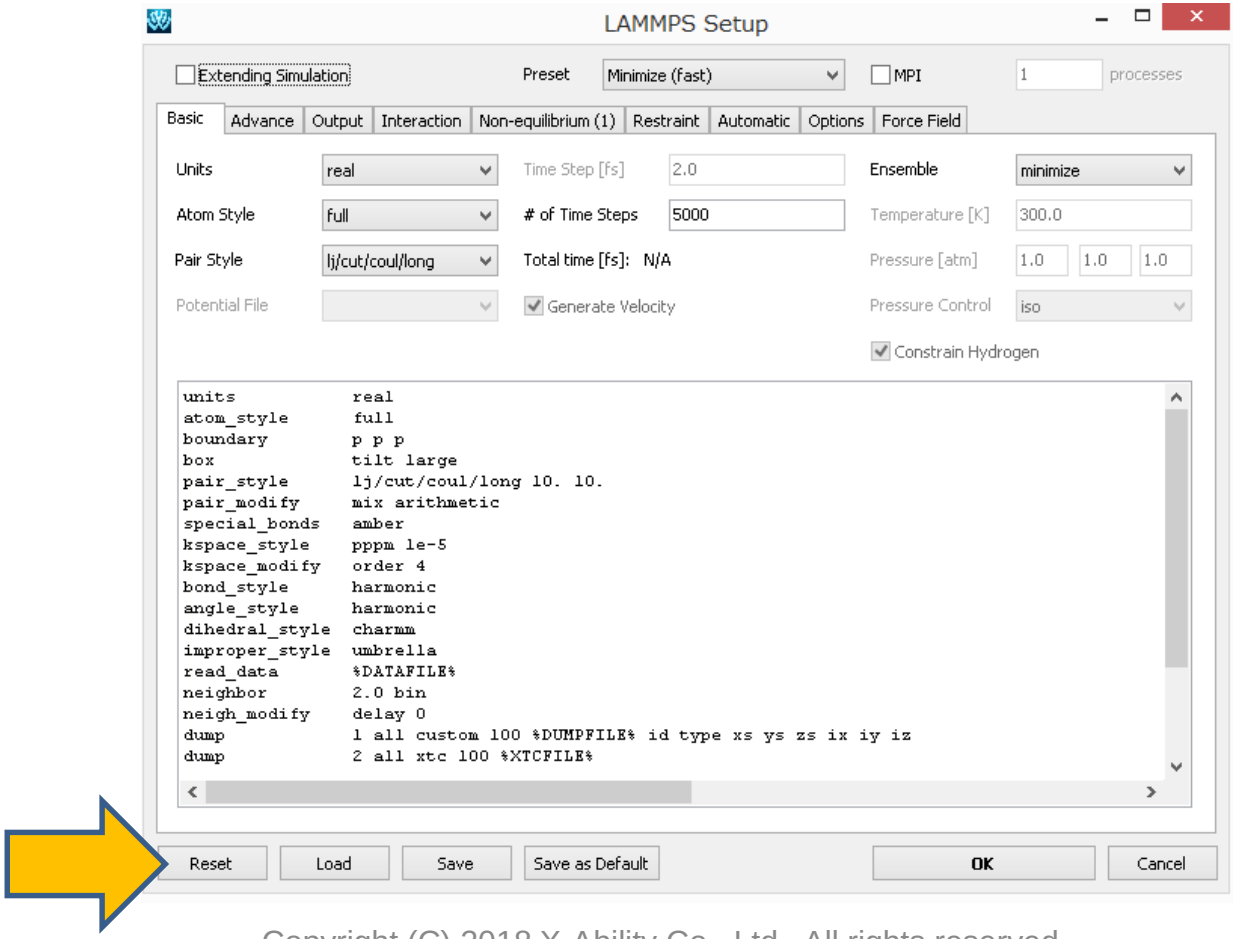
IV. Equilibration

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



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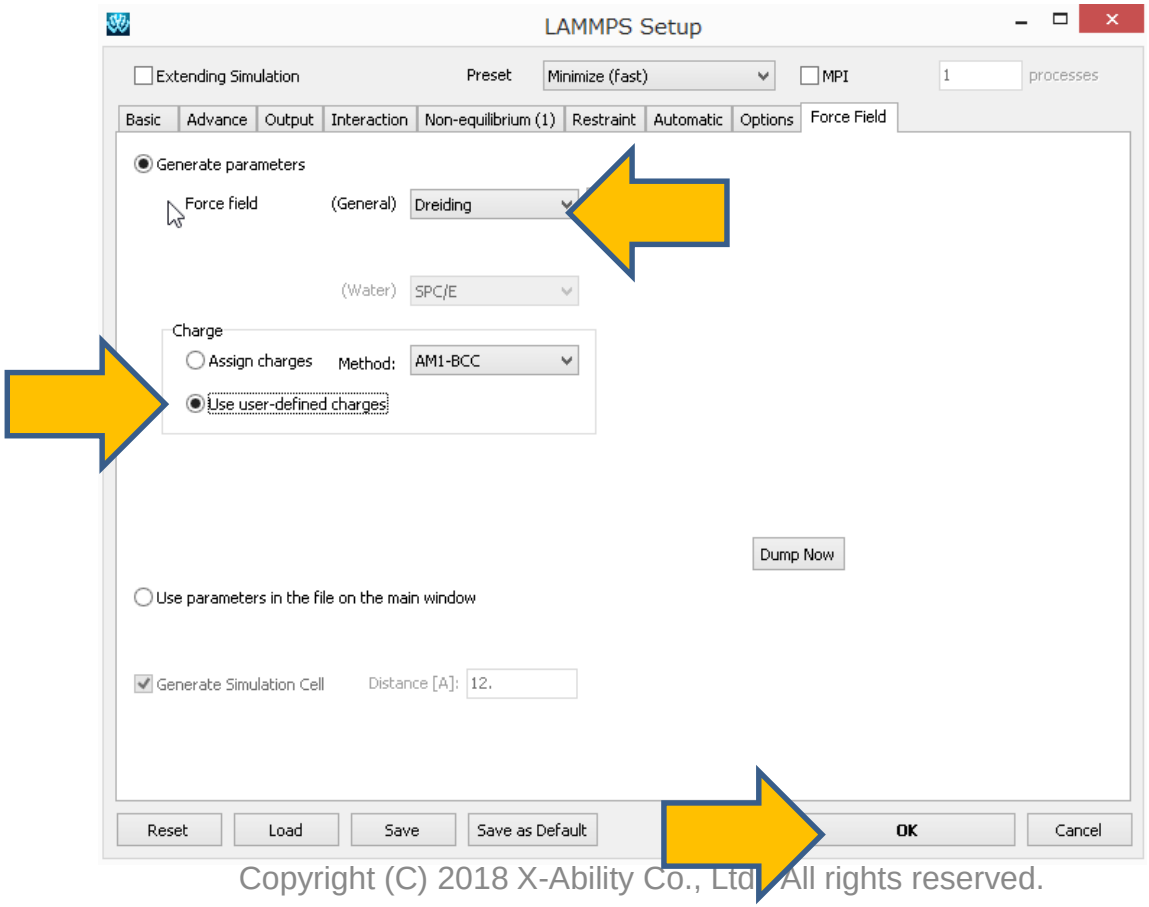
IV. Equilibration

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**.



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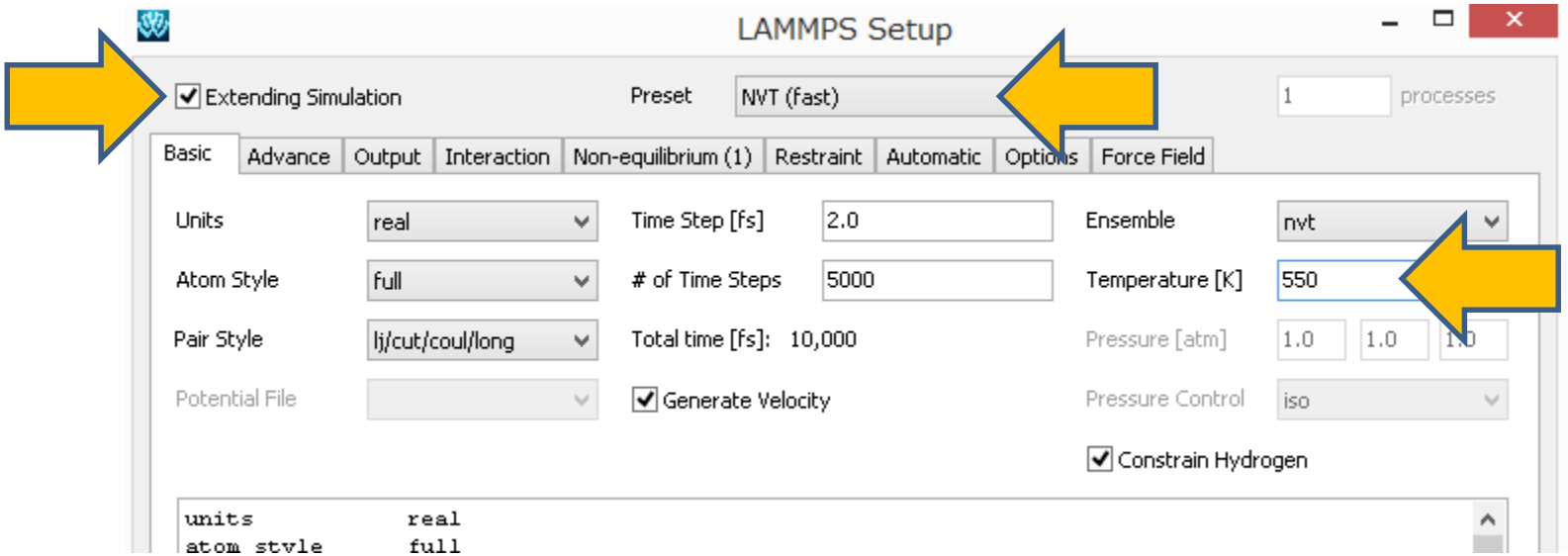
IV. Equilibration

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**.



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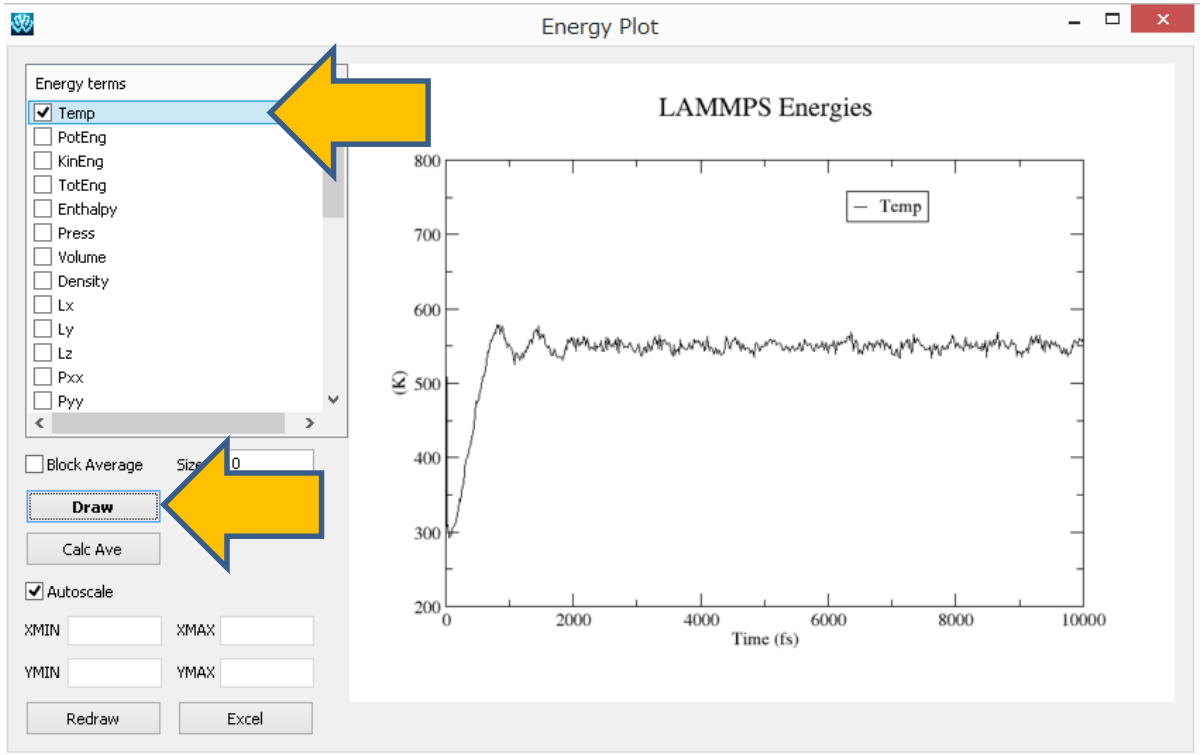
IV. Equilibration

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.



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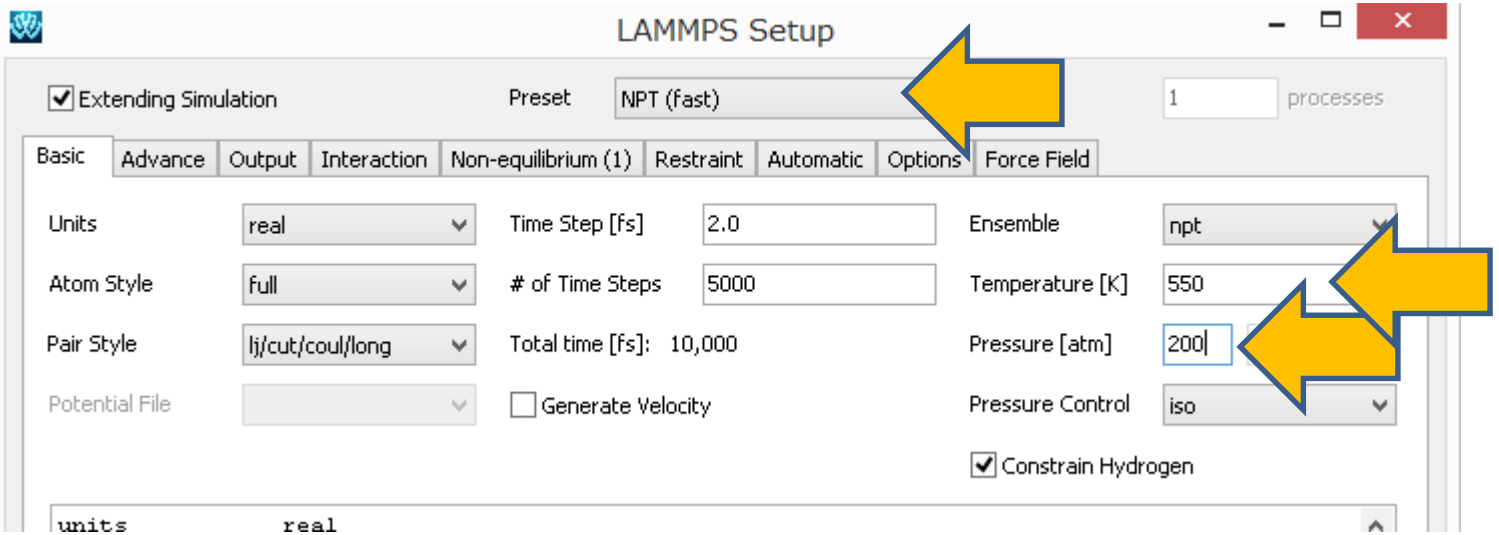
IV. Equilibration

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**.



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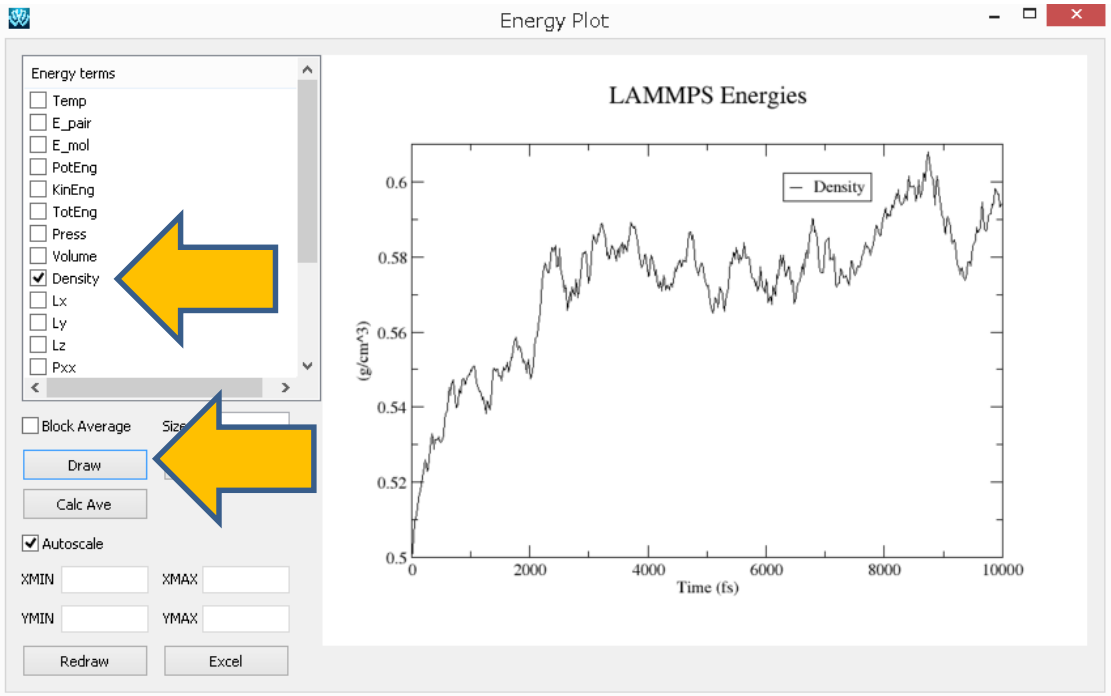
IV. Equilibration

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).



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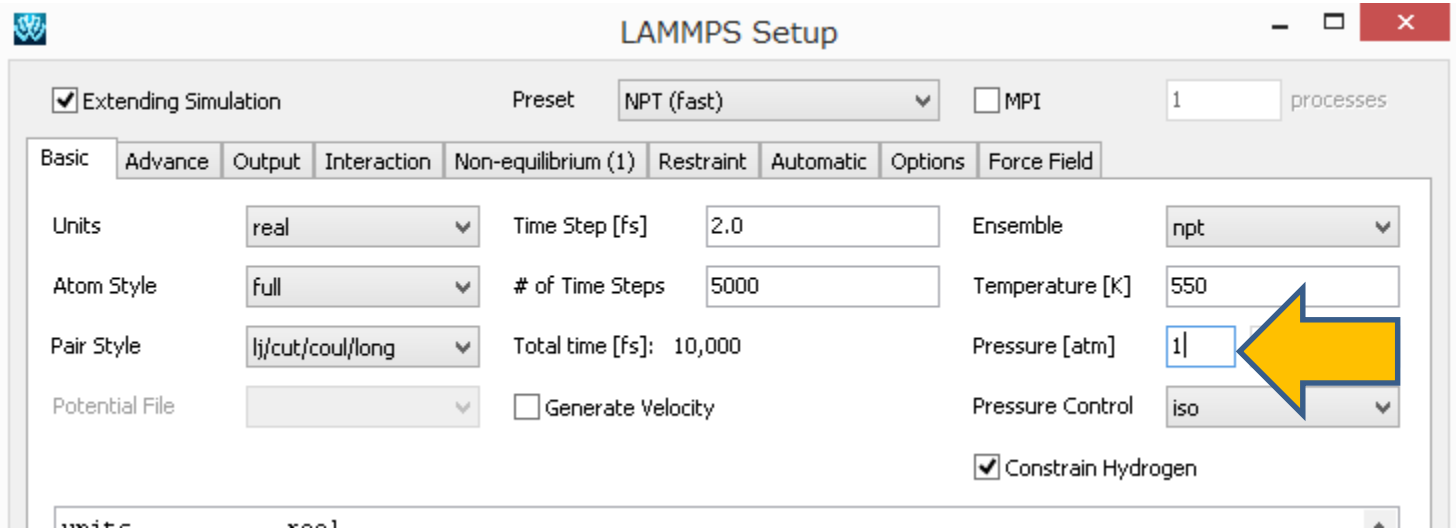
IV. Equilibration

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



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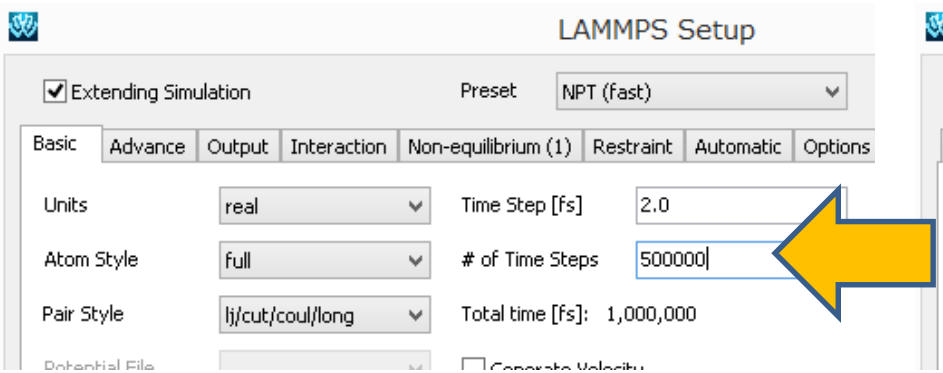
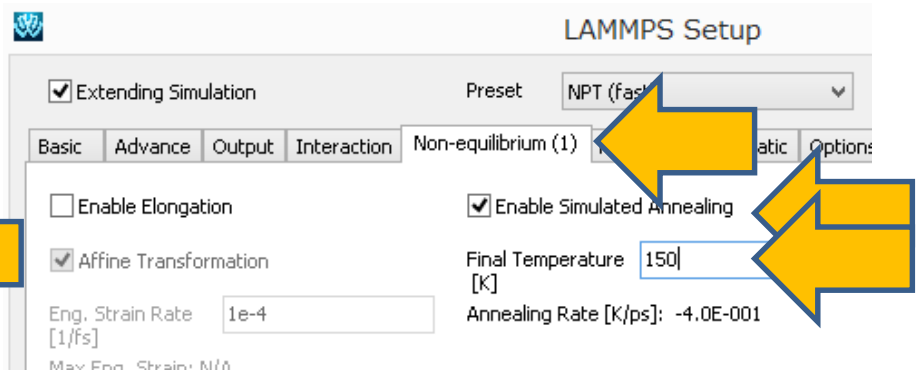
V. Annealing Calculation

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 **c**lick **OK**.
4. Click **MD** | **LAMMPS** | **Start LAMMPS**.





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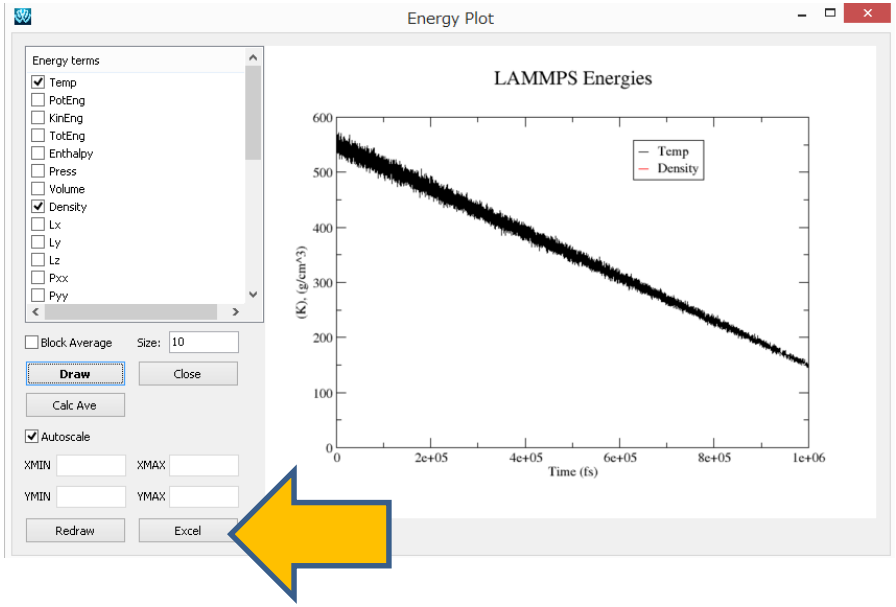
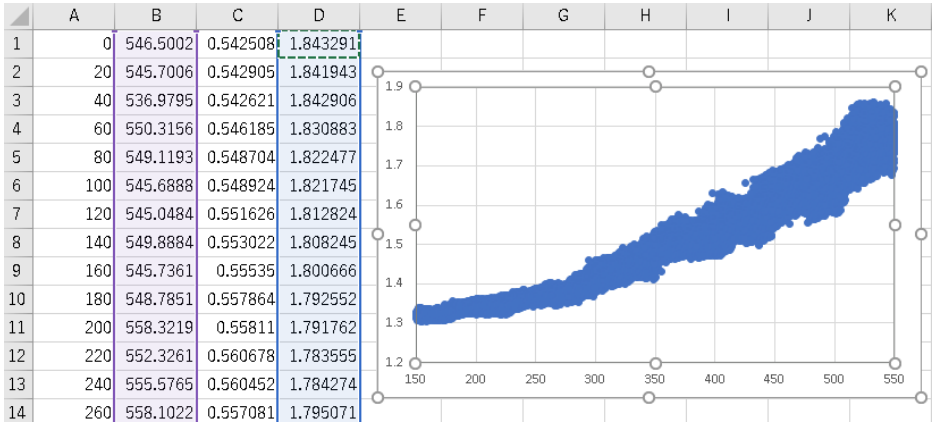
V. Annealing Calculation

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.





	A	B	C	D
1	0	546.5002	0.542508	1.843291
2	20	545.7006	0.542905	1.841943
3	40	536.9795	0.542621	1.842906
4	60	550.3156	0.546185	1.830883
5	80	549.1193	0.548704	1.822477
6	100	545.6888	0.548924	1.821745
7	120	545.0484	0.551626	1.812824
8	140	549.8884	0.553022	1.808245
9	160	545.7361	0.55535	1.800666
10	180	548.7851	0.557864	1.792552
11	200	558.3219	0.55811	1.791762
12	220	552.3261	0.560678	1.783555
13	240	555.5765	0.560452	1.784274
14	260	558.1022	0.557081	1.795071