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Winmostar tutorial
LAMMPS
Polymer modeling
V7.021

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Note

- 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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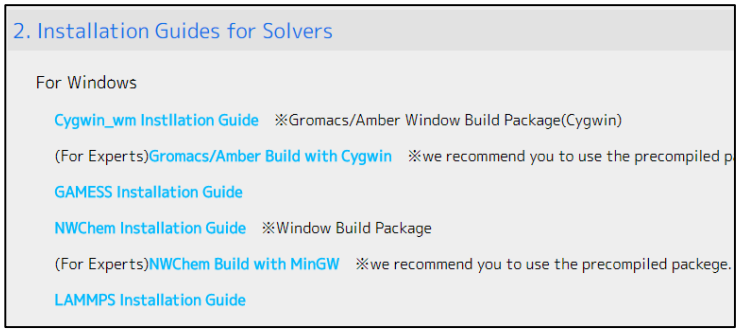
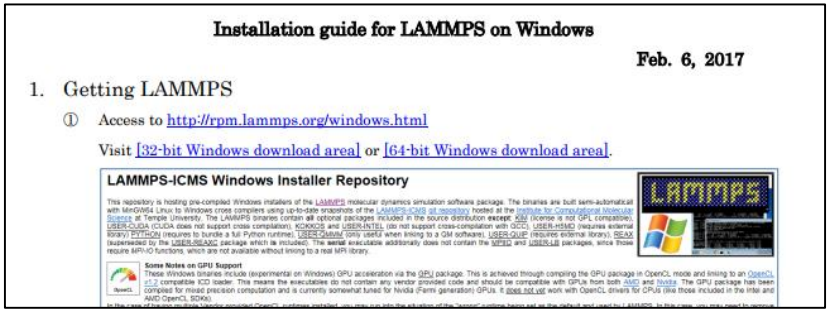
Configure

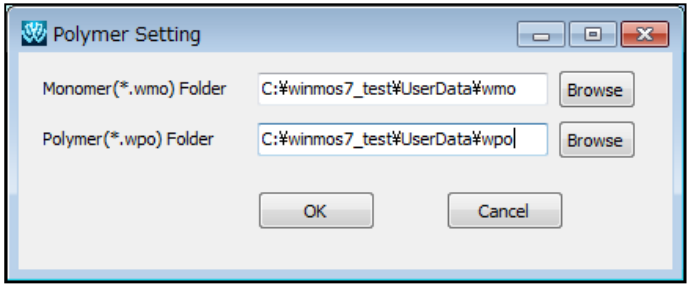
Set up LAMMPS and Cygwin in advance.

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





- Configuration of polymer tool
  Click **MD** | **Polymer** | **Setting.** 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. Uncheck **User Charge** to hide charge information**.**
4. Click two hydrogens to be the end points of the monomer.

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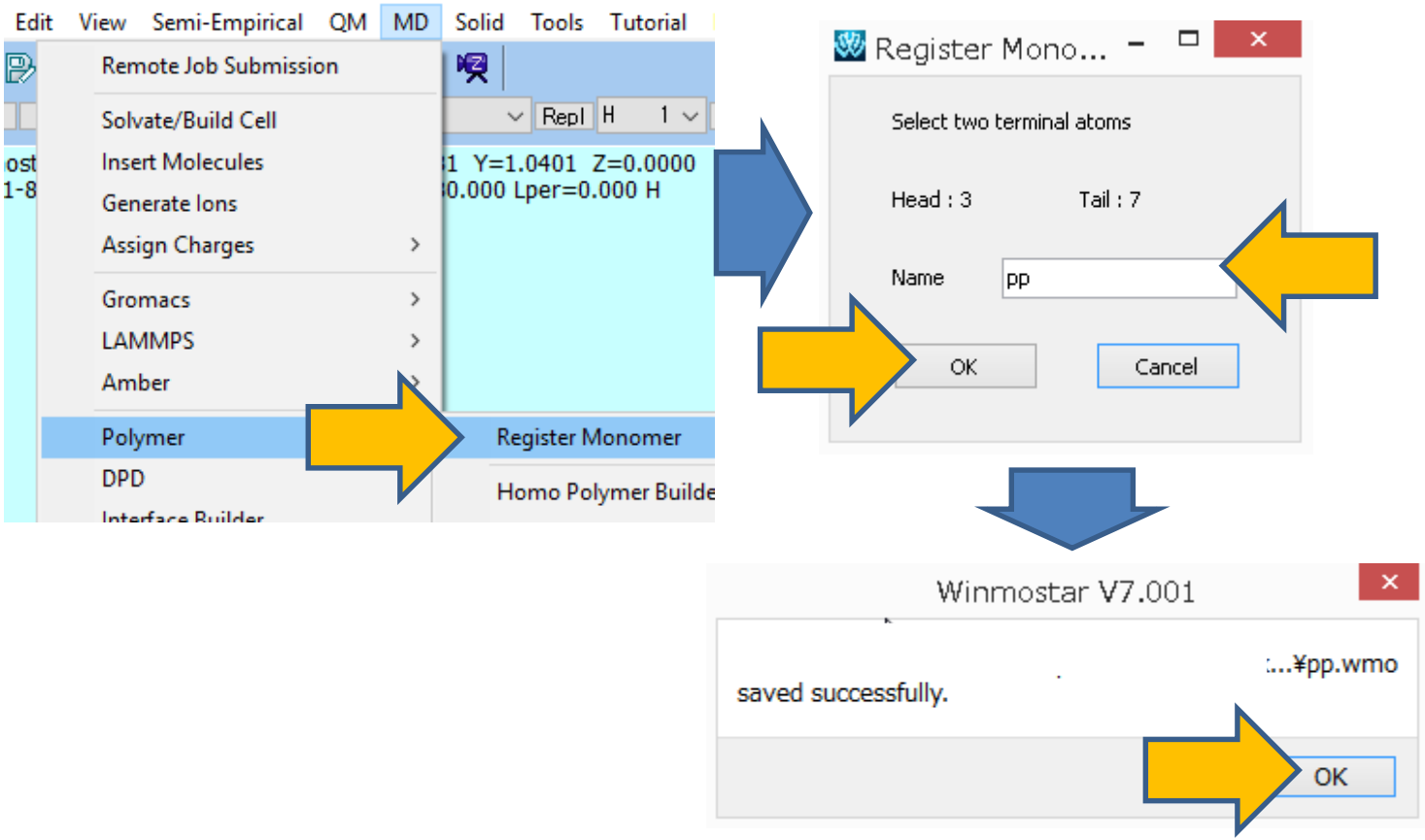
I. Register a monomer

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



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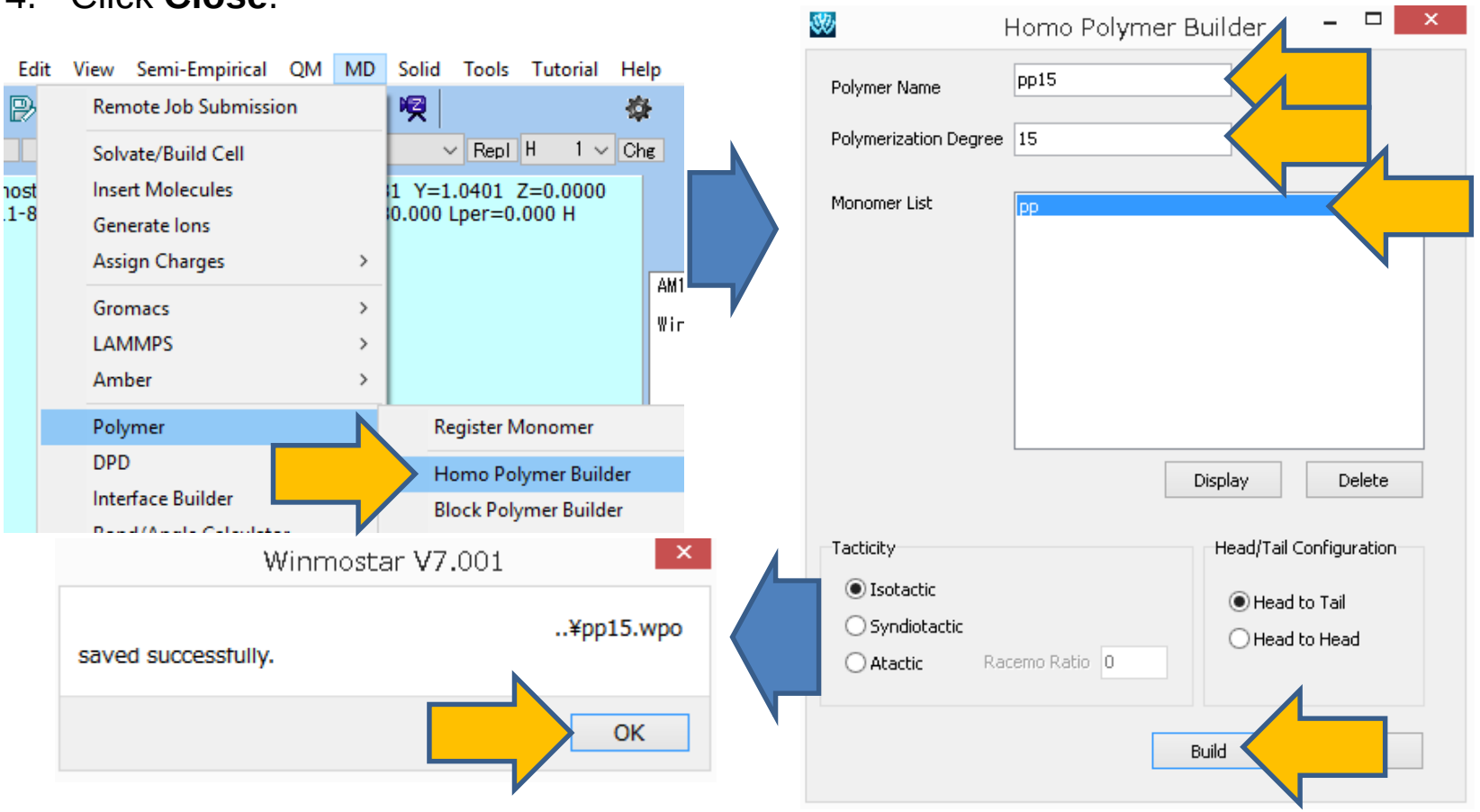
II. Define a polymer

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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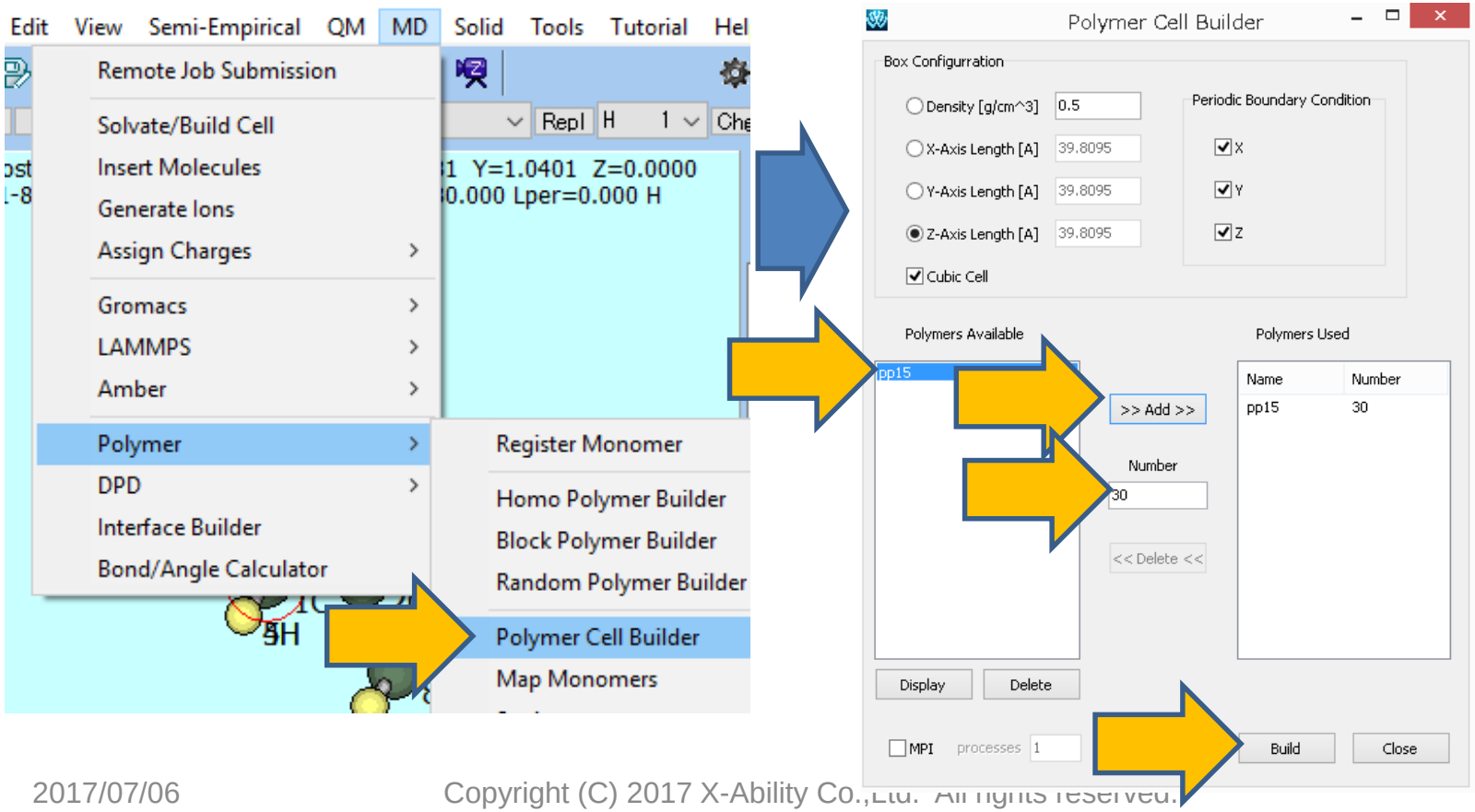
III. Build a simulation cell

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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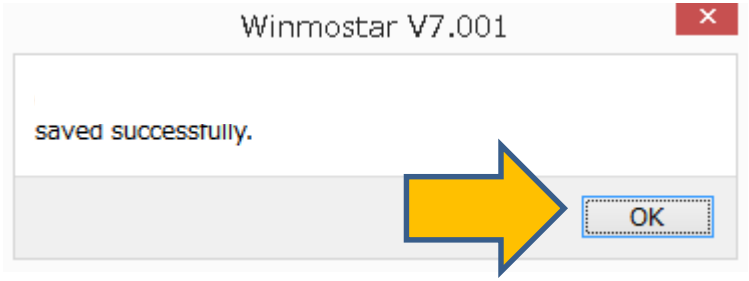
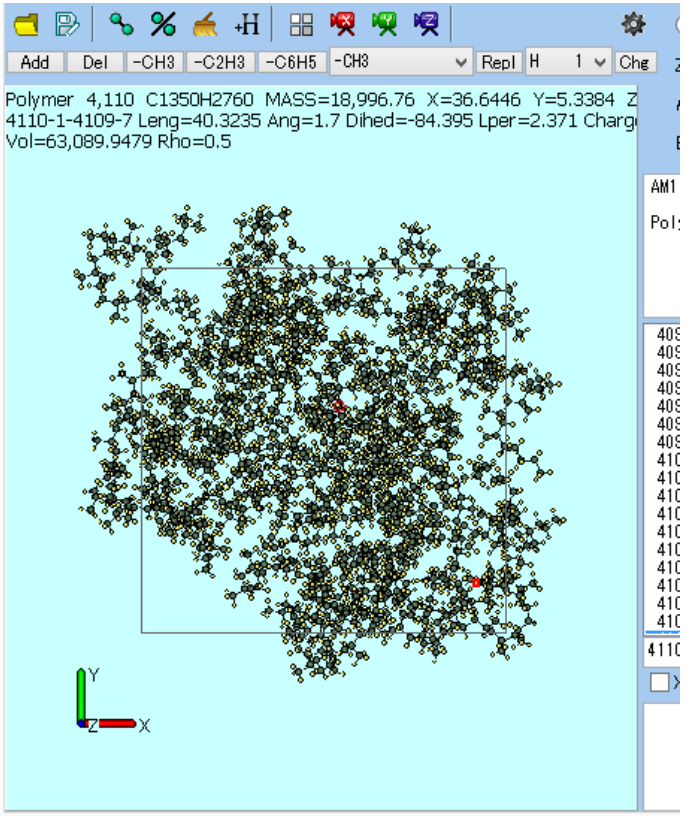
III. Build a simulation cell

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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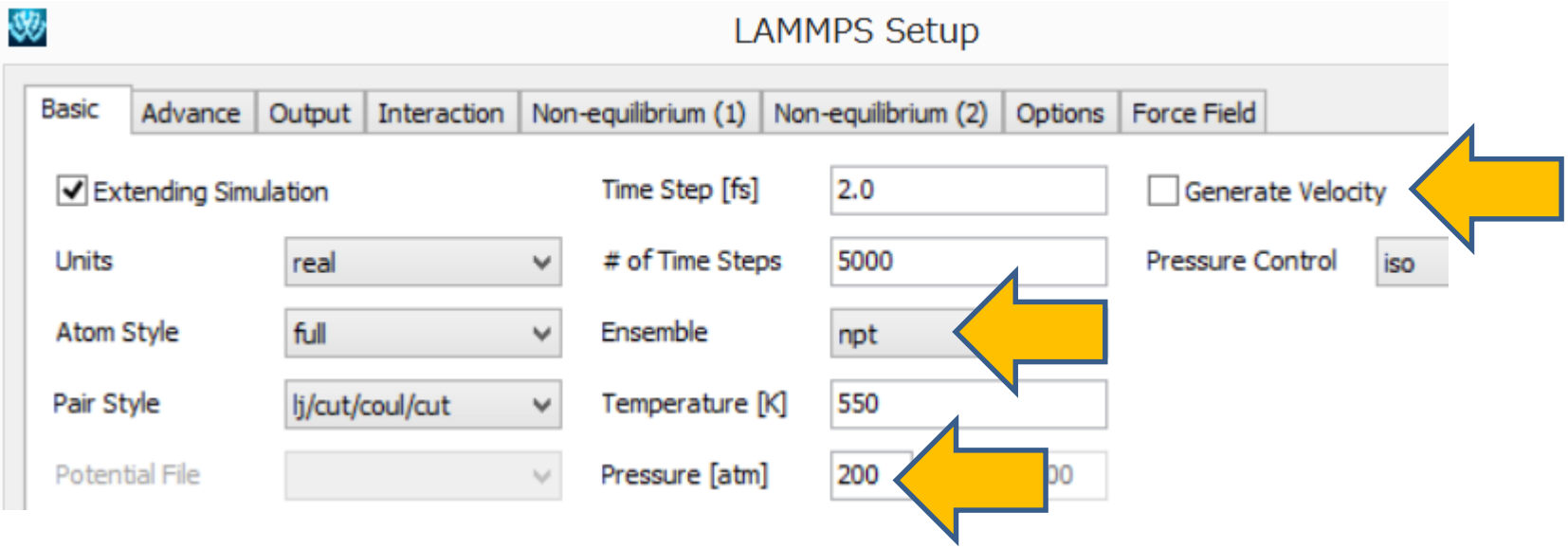
IV. Execute simulations
1. Equilibration (*NPT*, high pressure)

1. Click **MD** | **LAMMPS** | **Keywords Setup**.
2. On **Basic** tab, uncheck **Generate Velocity**,
   set **Ensemble** to **npt**, **Pressure** to **200**, then click **OK**.
3. Click **MD** | **LAMMPS** | **Start LAMMPS**.



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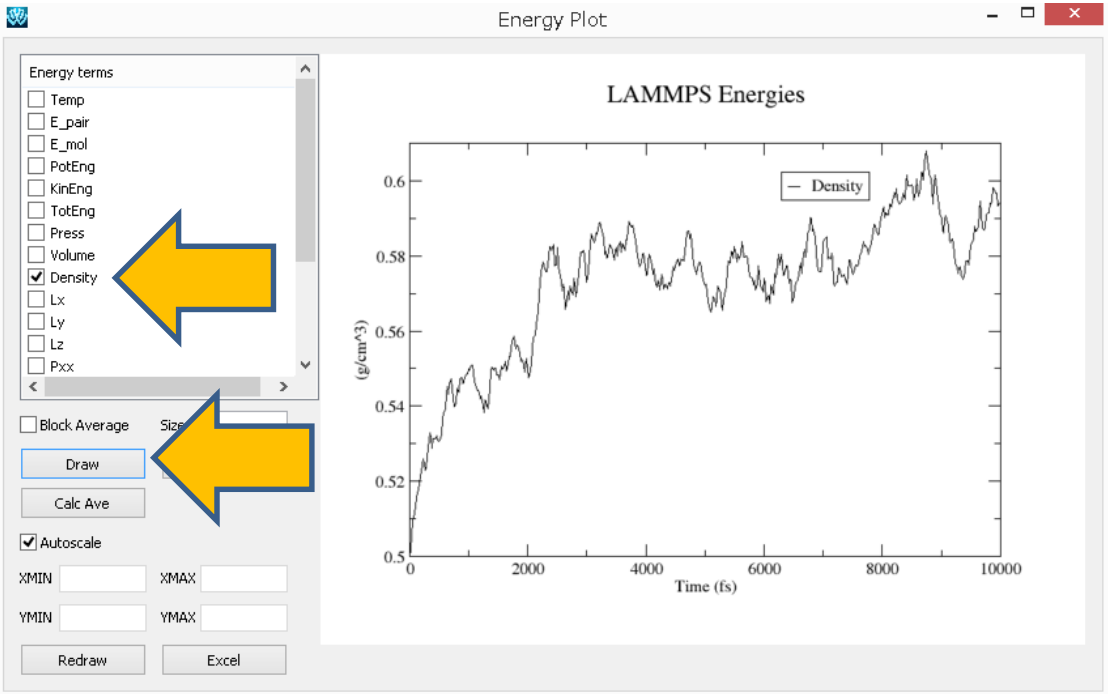
IV. Execute simulations

1. Equilibration (*NPT*, high pressure)

1. Click **MD** | **LAMMPS** | **Energy plot**. Open the default file.
2. On **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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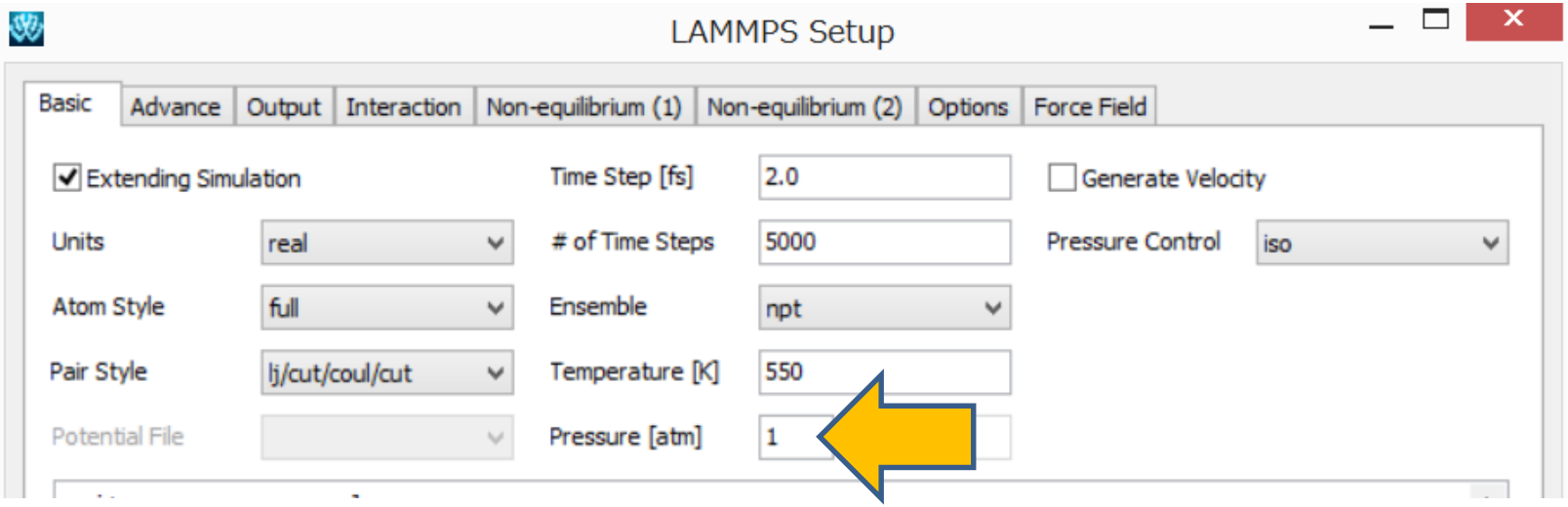
IV. Execute simulations
1. Equilibration (*NPT*, low pressure)

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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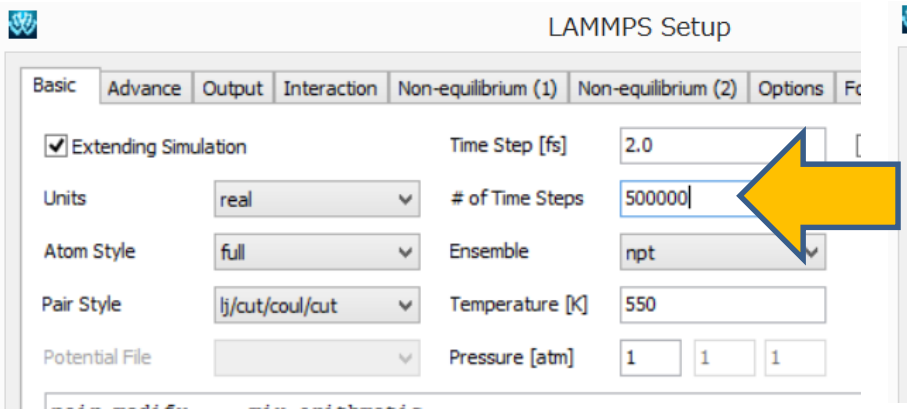
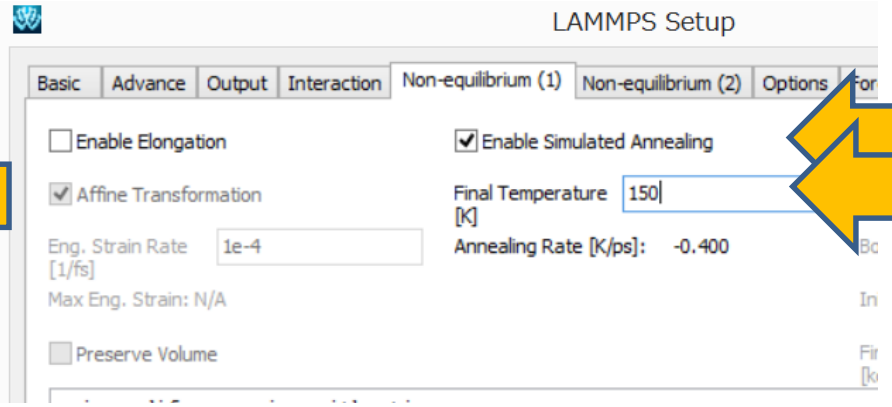
IV. Execute simulations
2. Annealing calculation

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

1. Click **MD** | **LAMMPS** | **Keywords Setup.**
2. On **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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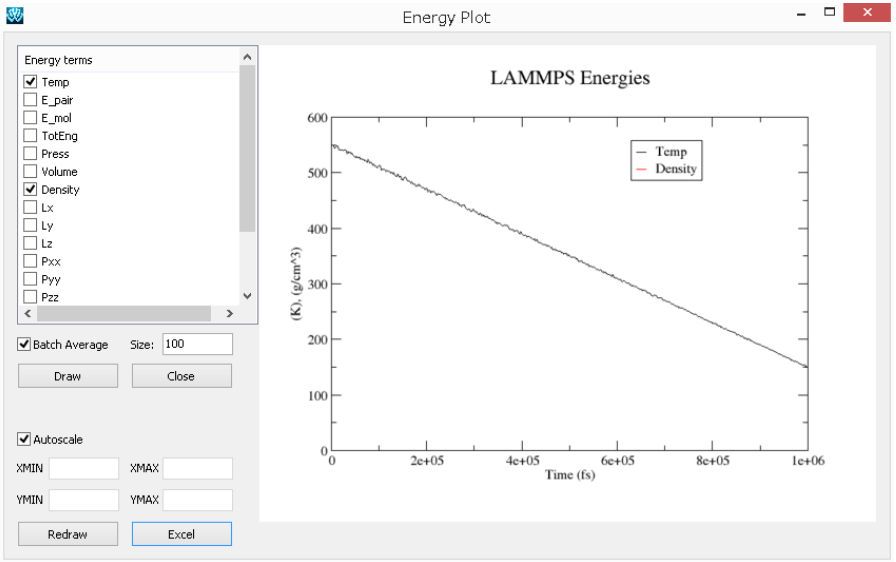
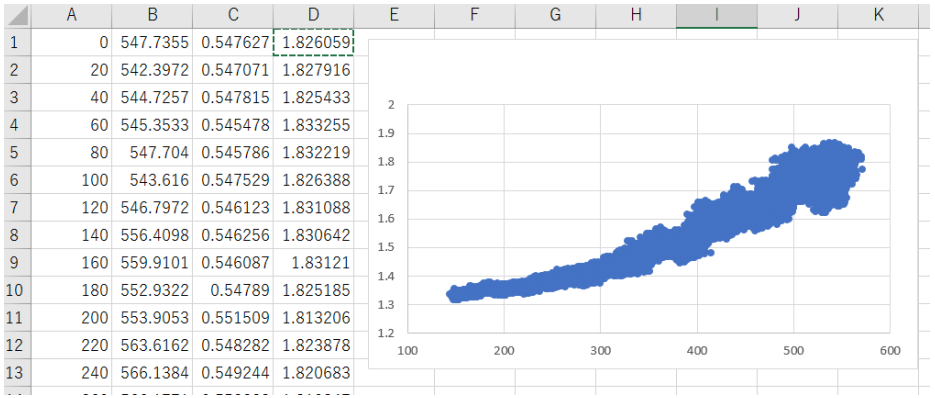
IV. Execute simulations
2. Annealing calculation

1. Click **MD | LAMMPS | Energy plot**. Then open the file selected by default.
2. On **Energy Terms**, check **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 280 – 300K) on this curve for a given distribution fitting.





	A	B	C	D
1	0	547.7355	0.547627	1.826059
2	20	542.3972	0.547071	1.827916
3	40	544.7257	0.547815	1.825433
4	60	545.3533	0.545478	1.833255
5	80	547.704	0.545786	1.832219
6	100	543.616	0.547529	1.826388
7	120	546.7972	0.546123	1.831088
8	140	556.4098	0.546256	1.830642
9	160	559.9101	0.546087	1.83121
10	180	552.9322	0.54789	1.825185
11	200	553.9053	0.551509	1.813206
12	220	563.6162	0.548282	1.823878
13	240	566.1384	0.549244	1.820683