X-Ability
クロスアビリティ

Winmostar tutorial
LAMMPS
Elongation
V7.021

X-Ability Co,. Ltd.

question@winmostar.com

2017/7/6

X-Ability
クロスアビリティ

Contents

X-Ability
クロスアビリティ

Note

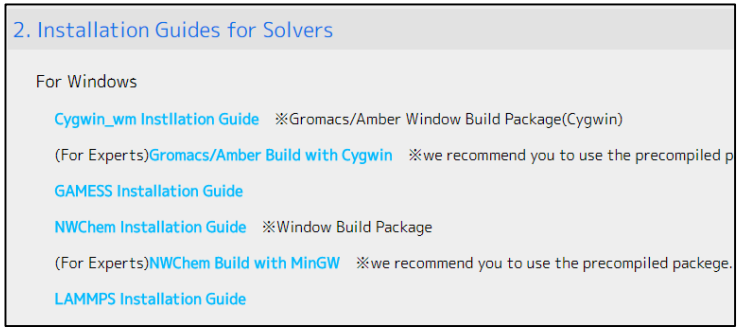
- Steps required for equilibration will vary depending on the molecule and initial density.
- The method for interaction calculations and/or the force field and/or charges also affect the simulation results.
- Degree of polymerization (chain length), number of molecules, elongation rate, pressure control, Poisson ratio will affect outcomes.
- For the purpose of this tutorial, we will not show complete equilibration steps for polymers.

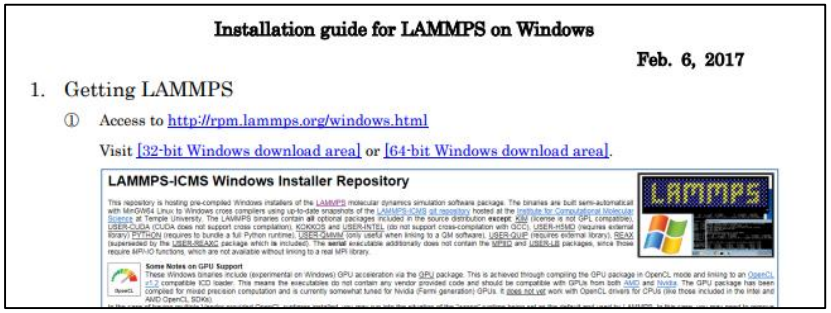
X-Ability
クロスアビリティ

Configure

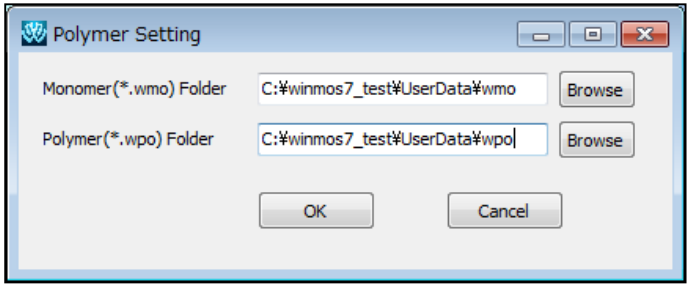
Set up LAMMPS and Cygwin in advance.

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.

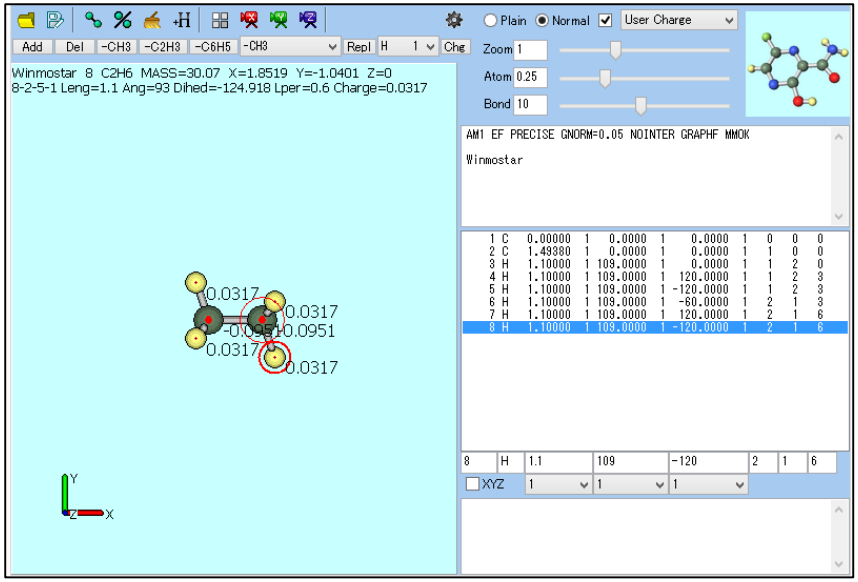


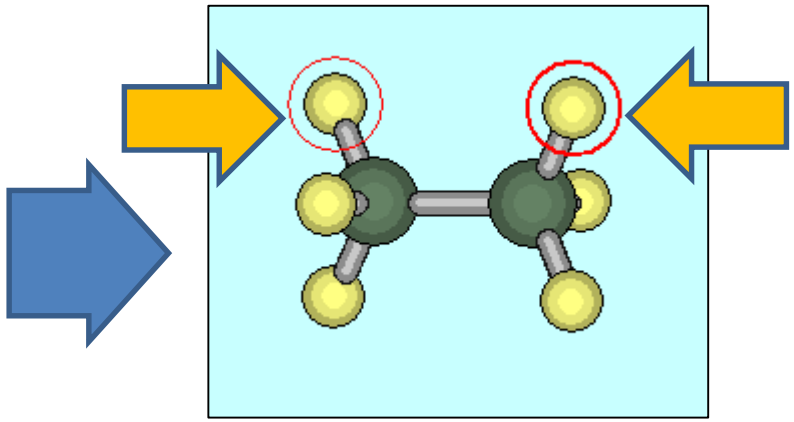
X-Ability
クロスアビリティ

I. Register a monomer

This tutorial will describe how to model a polyethylene.

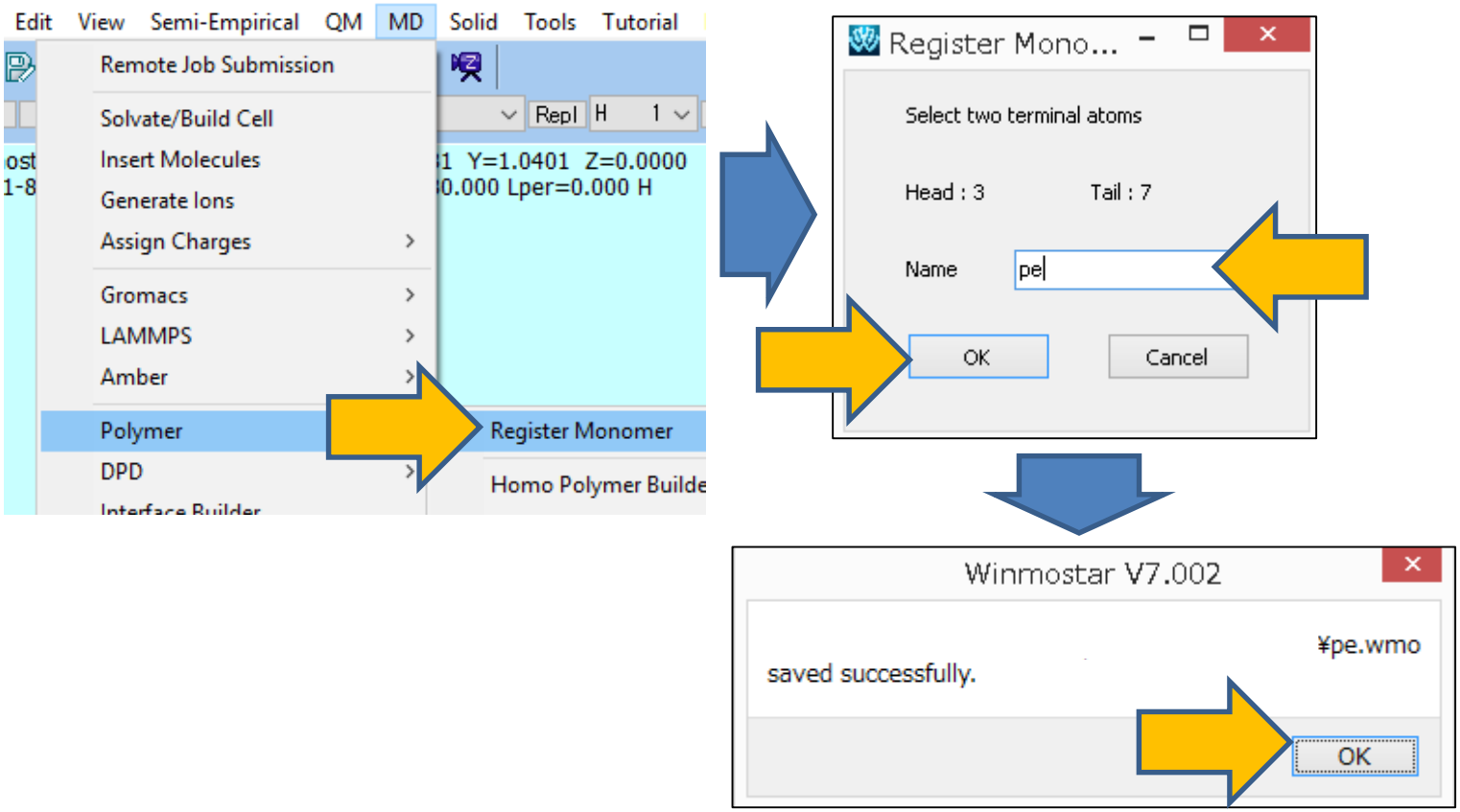
1. Model a monomer of polyethylene (ethane, C_2H_6) on the main window.
2. Click **MD** | **Assign Charges** | **By Acpype** | **Execute**.
3. Uncheck **User Charge** to hide charge information
4. Click two hydrogens to be the end point of the monomer.





I. Register a monomer

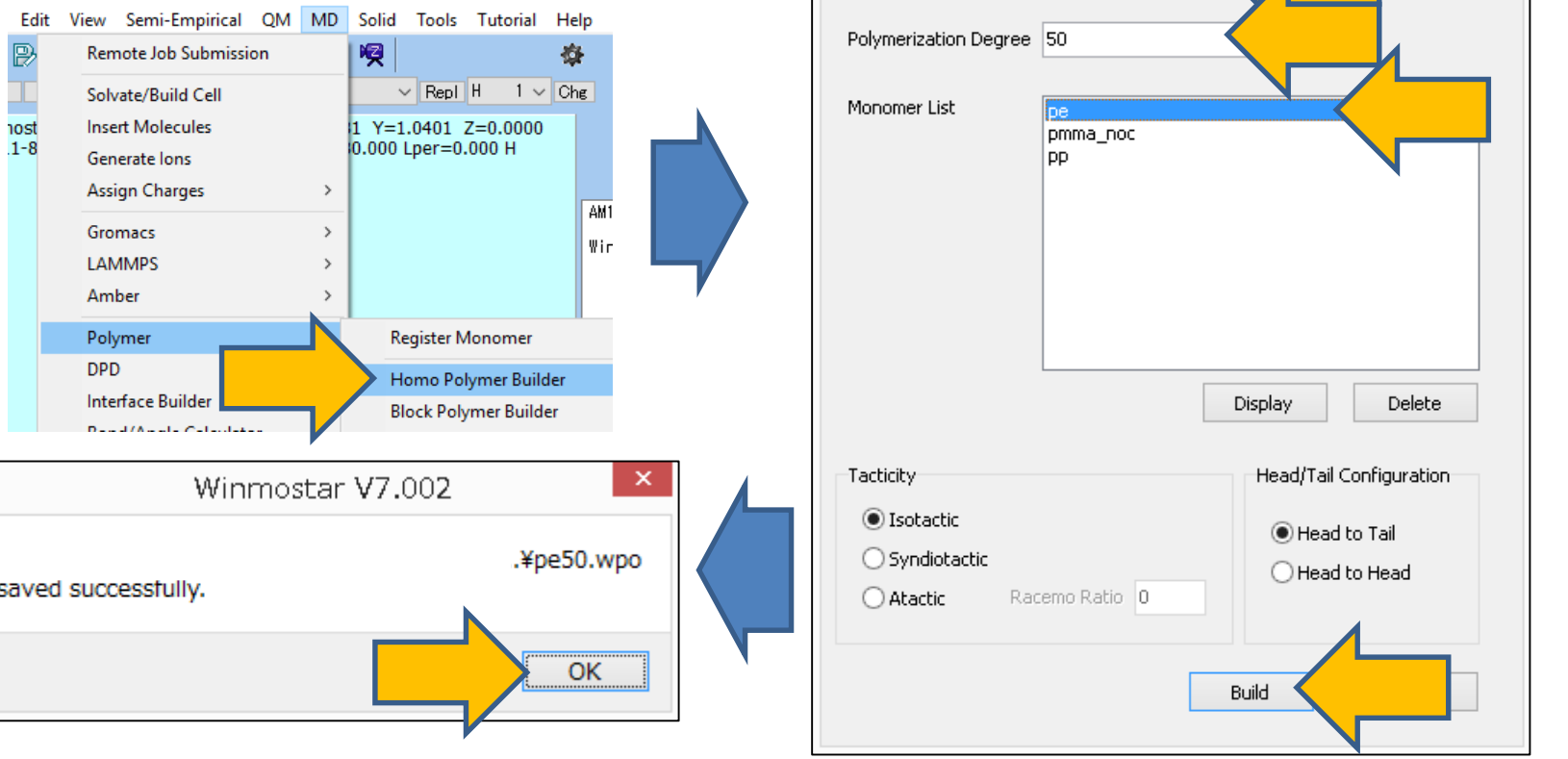
1. Click **MD** | **Polymer** | **Register Monomer**.
2. Set **Name** to **pe**, and click **OK**.
3. Click **OK** on the dialog.



X-Ability
クロスアビリティ

II. Define a polymer

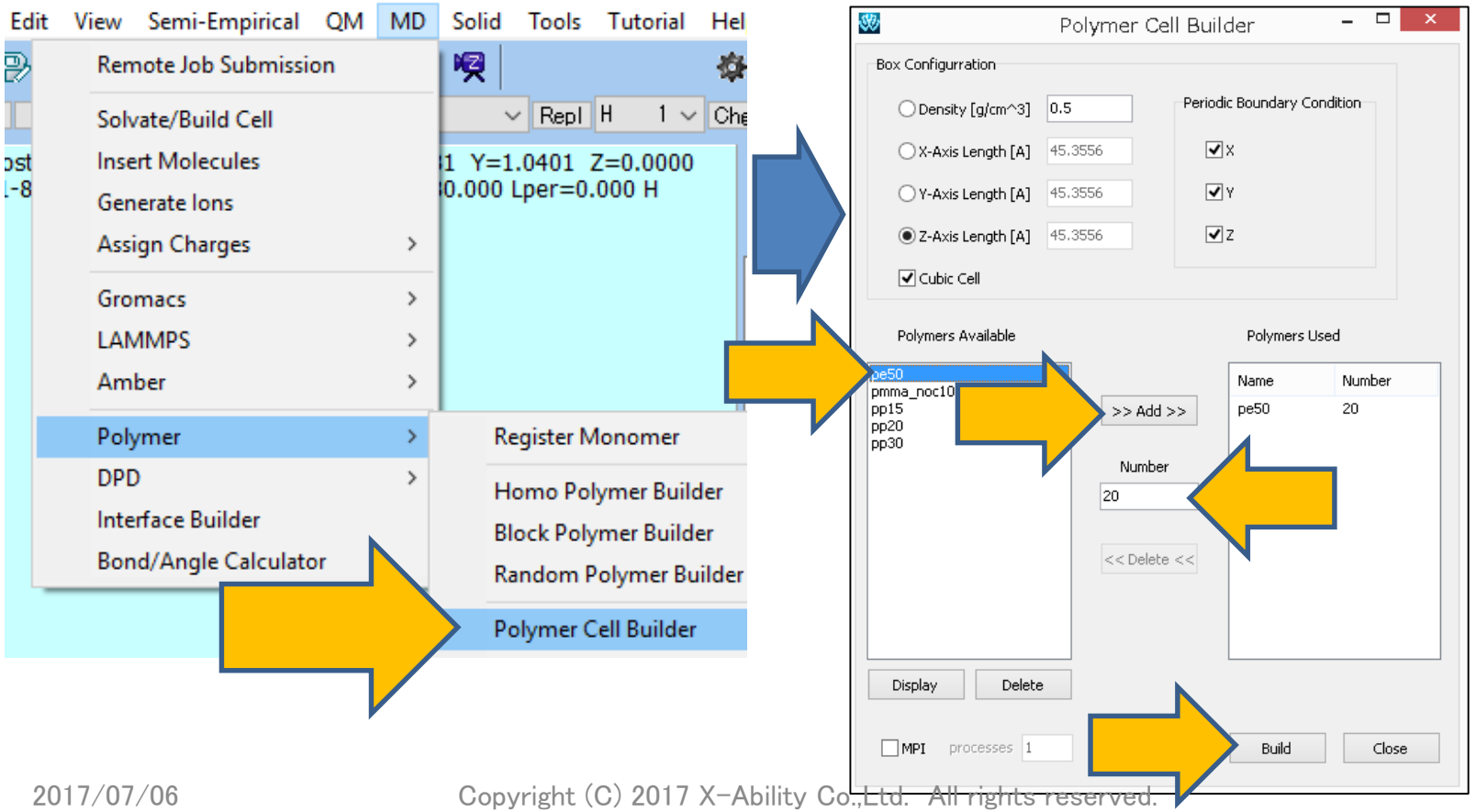
1. Click **MD** | **Polymer** | **Homo Polymer Builder**.
2. Set **Polymer Name** to **pe50**, **Polymerization Degree** to **50**, Select **pe** in **Monomer List**.
3. Click **Build**.
4. Click **Close**.



X-Ability
クロスアビリティ

III. Build Cell

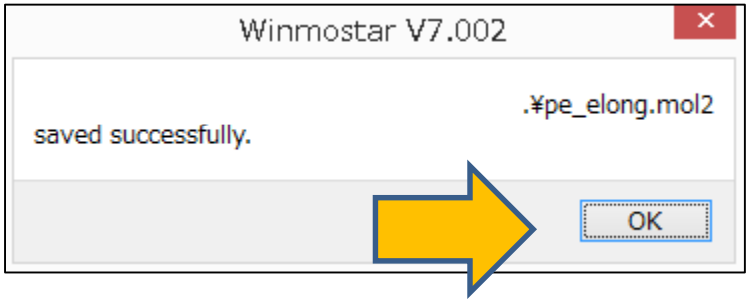
1. Click **MD** | **Polymer** | **Polymer Cell Builder**.
2. Set **Polymers Available** to **pe50**, **Number** to **20**, and click **>> Add >>**.
3. Click **Build**. Save as **pe_elong.mol2**.

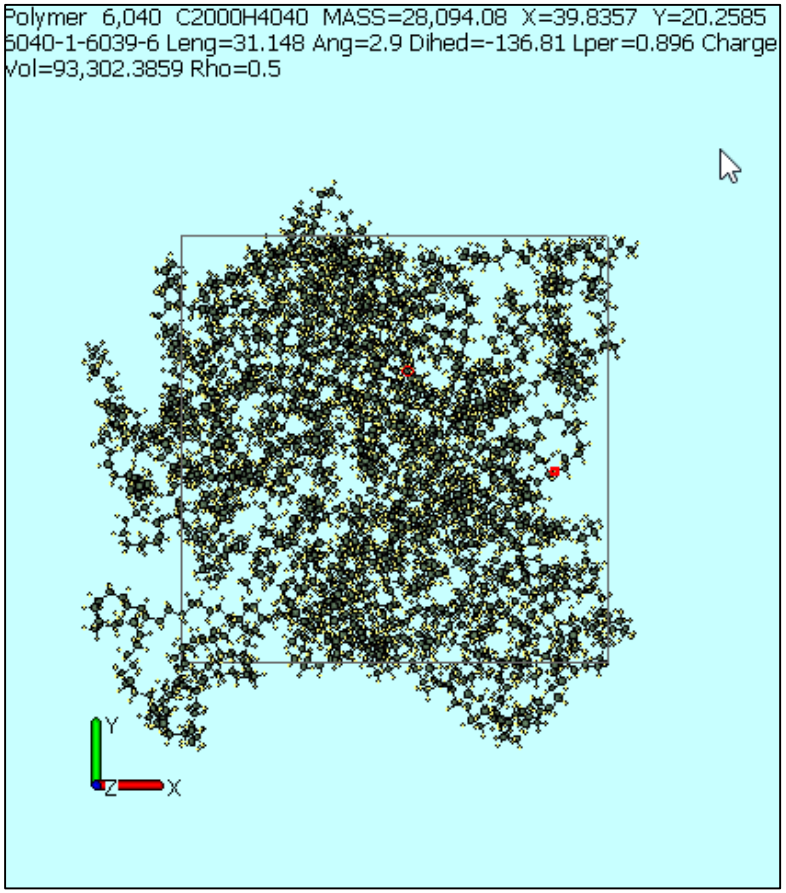


X-Ability
クロスアビリティ

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**.



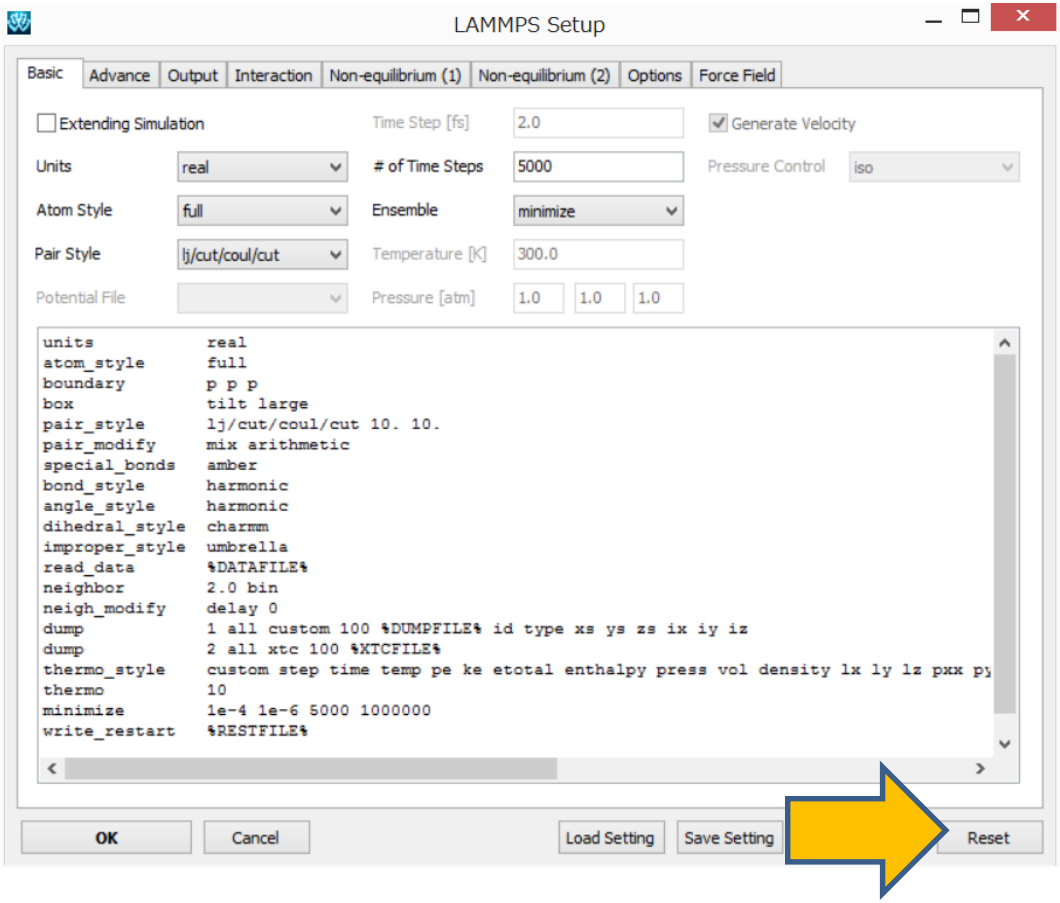


X-Ability
クロスアビリティ

IV. Execute simulations

1. Equilibration

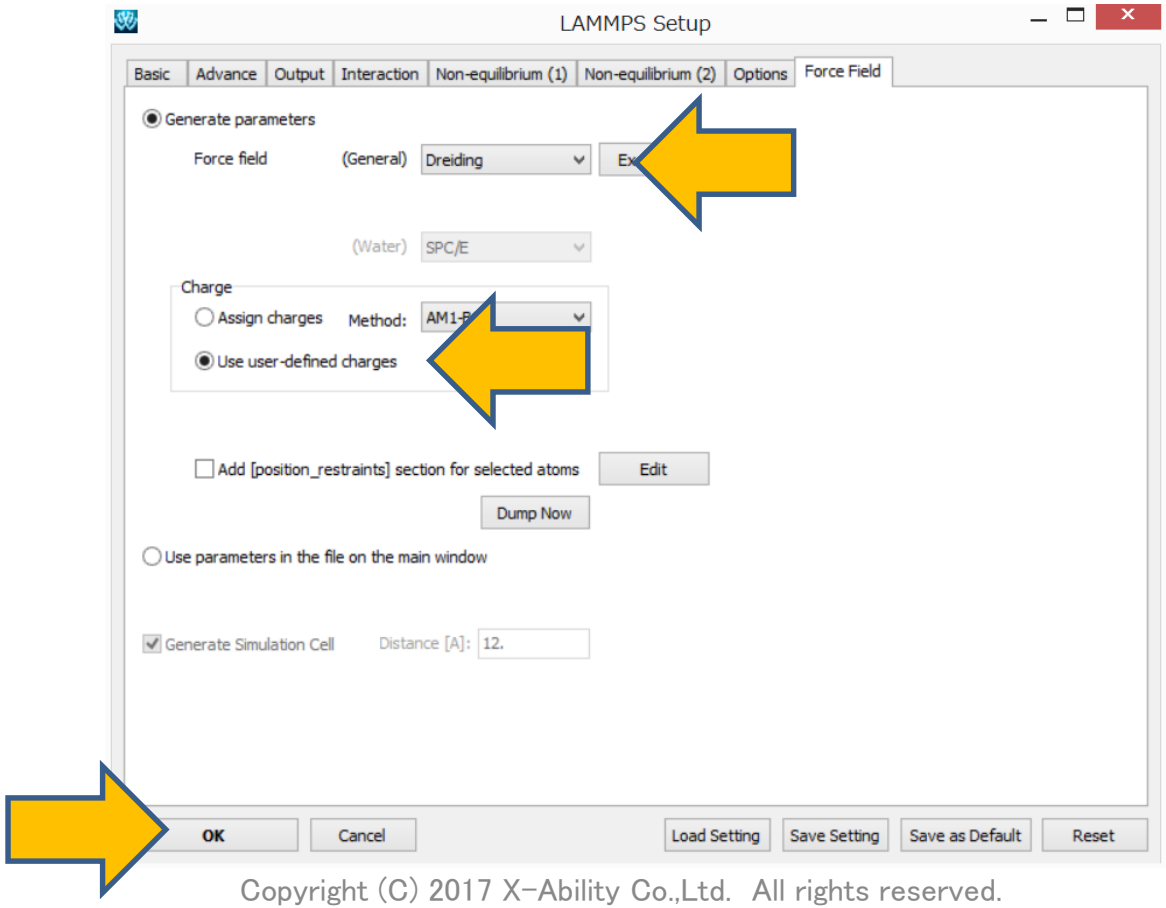
1. Click **MD** | **LAMMPS** | **Keywords Setup**.
2. Click **Reset**.



X-Ability
クロスアビリティ

IV. Execute simulations
1. Equilibration

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

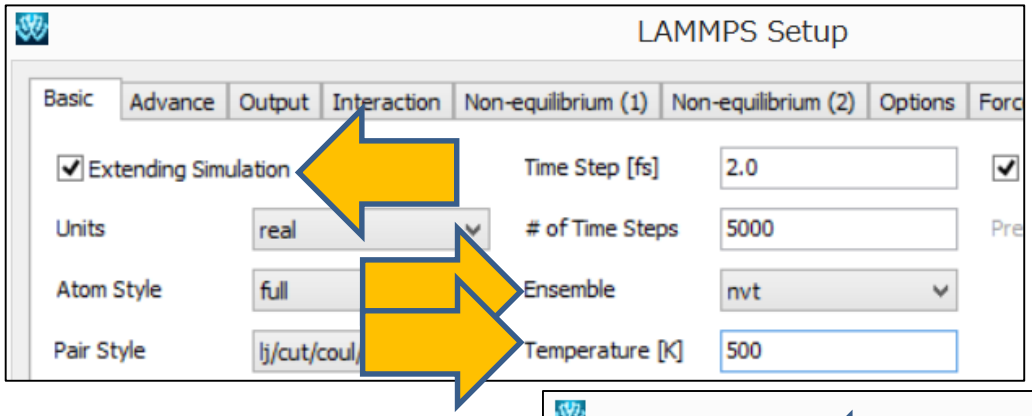


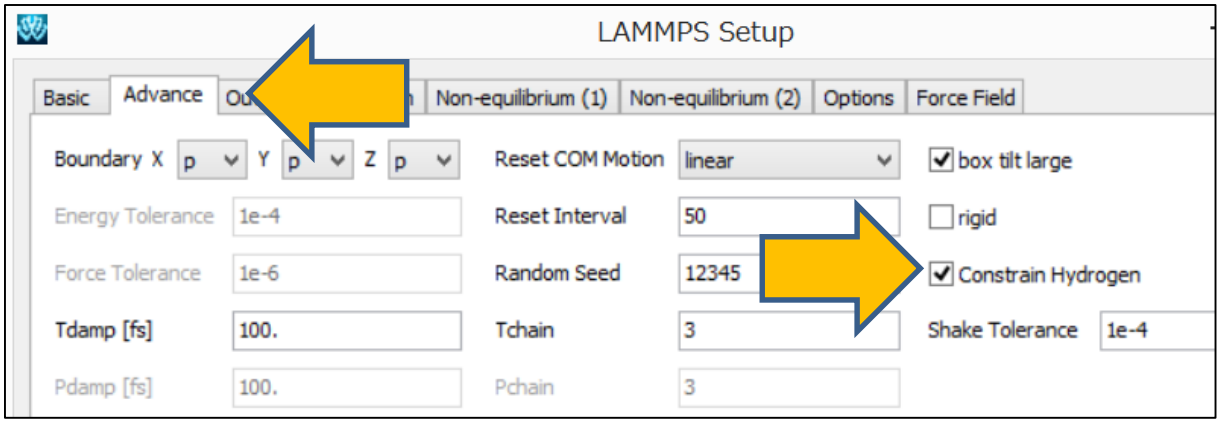
X-Ability
クロスアビリティ

IV. Execute simulations

1. Equilibration

1. Click **MD** | **LAMMPS** | **Keywords Setup**.
2. Check **Extending Simulation**, Set **Ensemble** to **nvt, Temperature** to **500**. In **Advance** tab, check **Constrain Hydrogen**. Click **OK**.
3. Click **MD** | **LAMMPS** | **Start LAMMPS**.

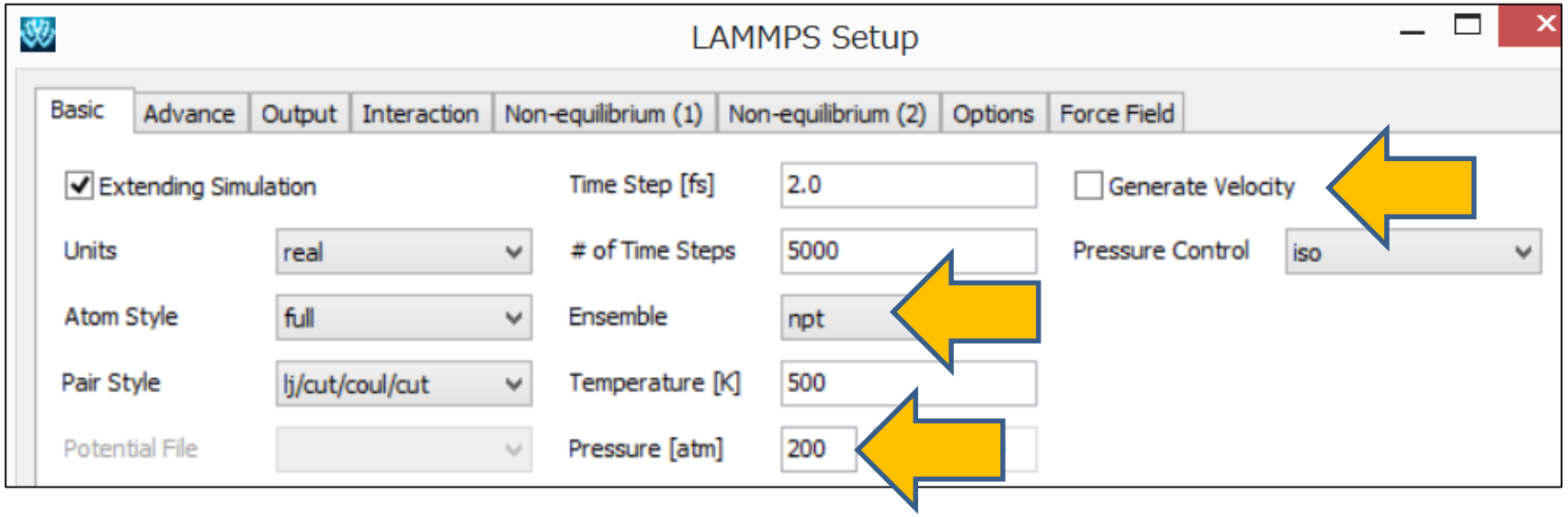




X-Ability
クロスアビリティ

IV. Execute simulations
1. Equilibration

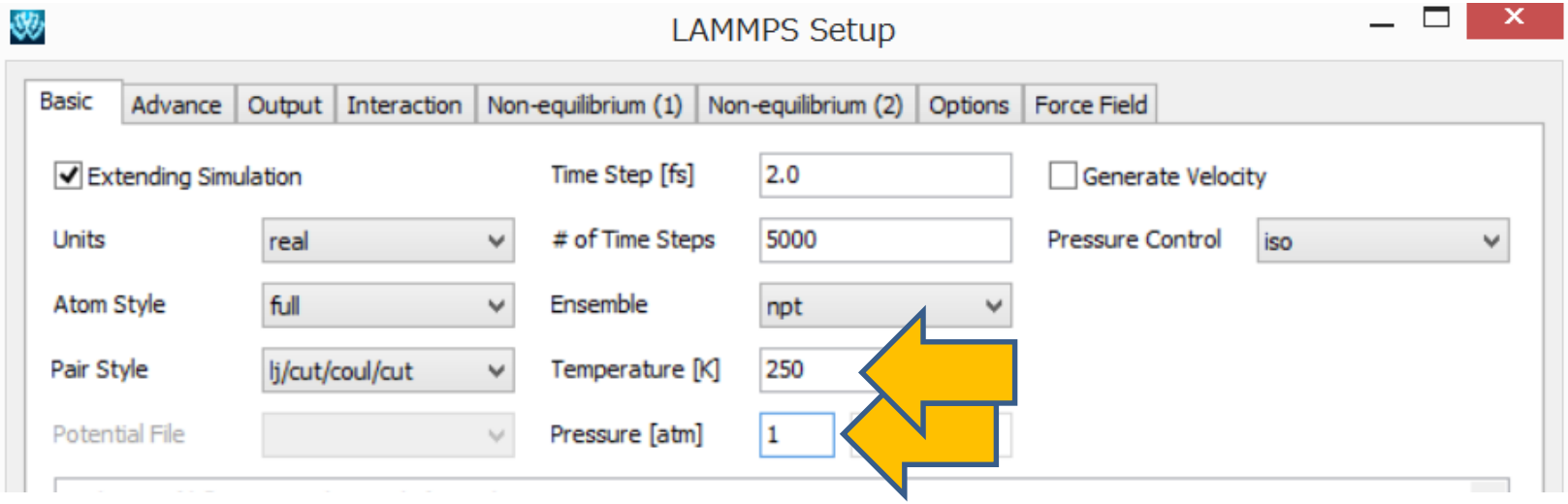
1. Click **MD** | **LAMMPS** | **Keywords Setup**.
2. Uncheck **Generate Velocity** in the **Basic** tab,
   Set **Ensemble** to **npt**, **Pressure** to **200**, then click **OK**.
3. Click **MD** | **LAMMPS** | **Start LAMMPS**.



X-Ability
クロスアビリティ

IV. Execute simulations
1. Equilibration

1. Click **MD** | **LAMMPS** | **Keywords Setup.**
2. In **Basic** tab, set **Temperature** to **250**, **Pressure** to **1,** then click **OK**.
3. Click **MD** | **LAMMPS** | **Start LAMMPS**.

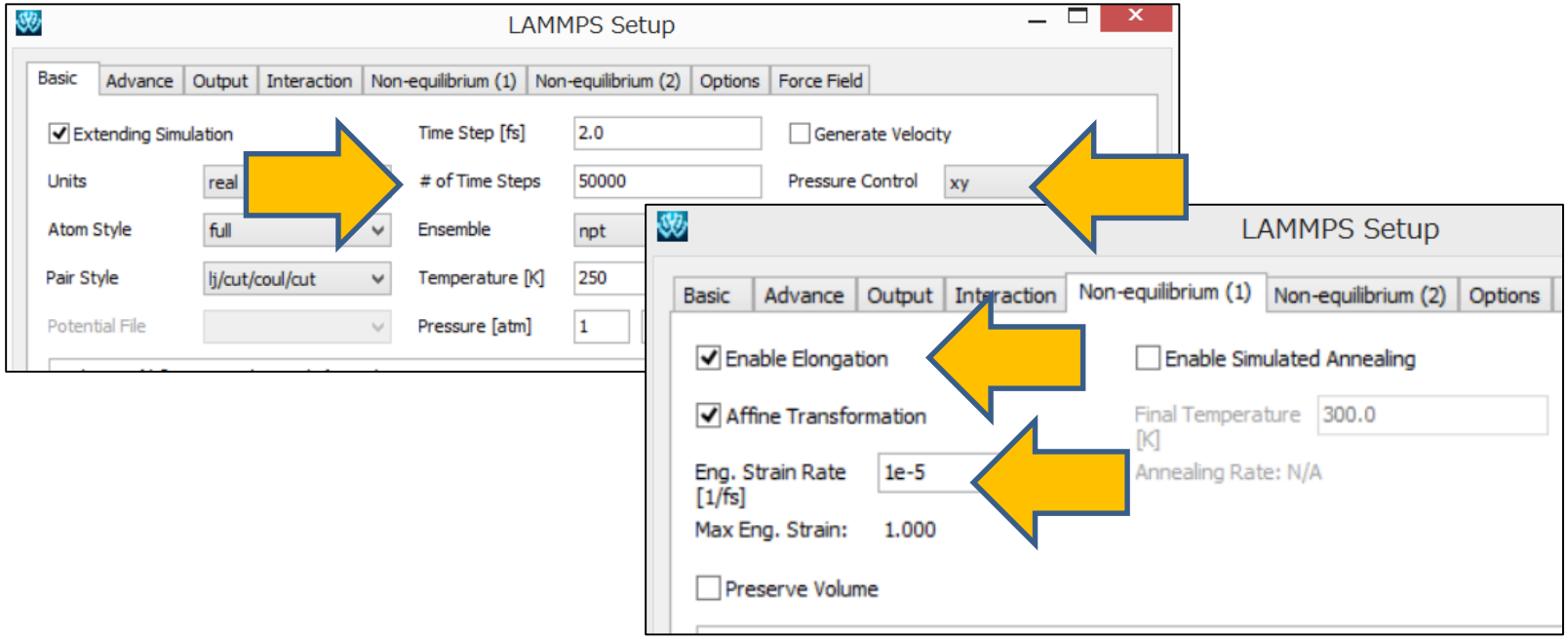


X-Ability
クロスアビリティ

IV. Execute simulations
2. Elongation

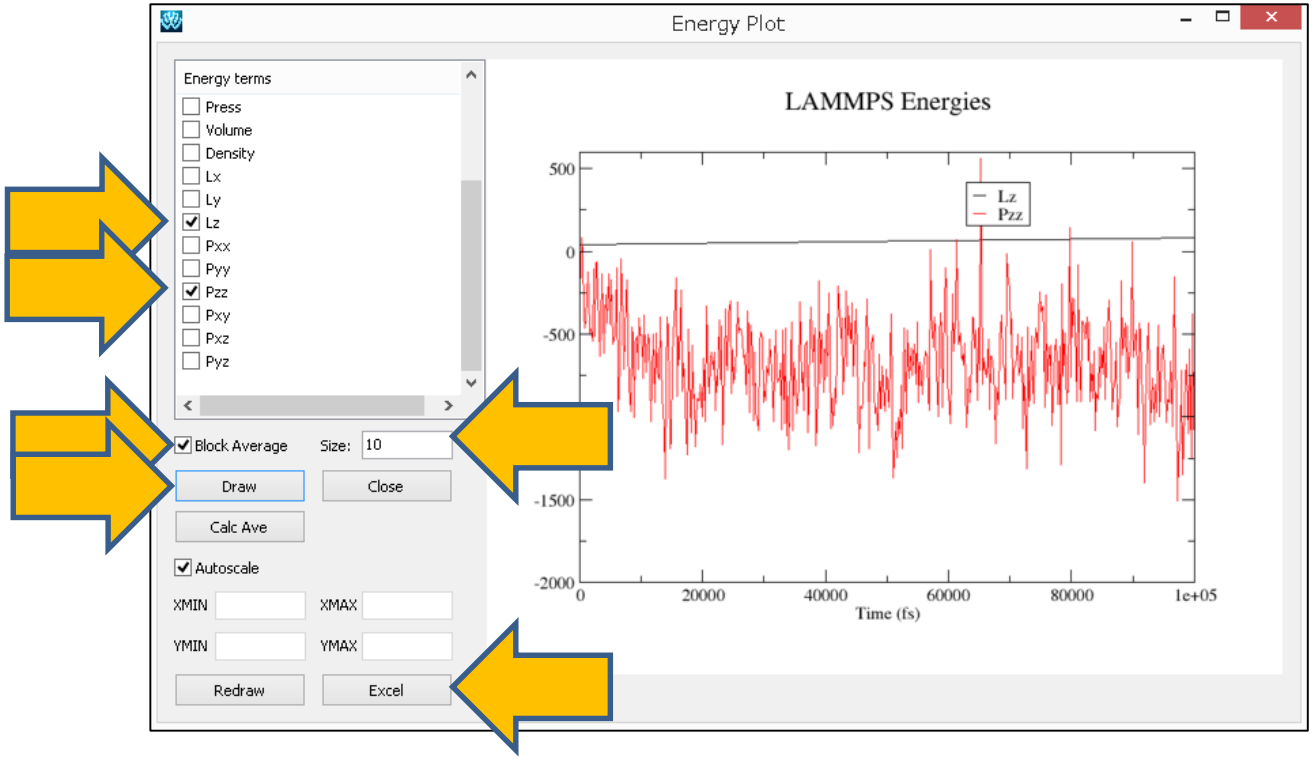
Next, calculate elongation to produce strain and stress curve.

1. Click **MD | LAMMPS | Keywords Setup.**
2. On Basic tab, set # **of Time Steps** to **50000, Pressure Control** to **xy**,
3. On **Non-equilibrium (1)** tab, check **Enable Elongation**, set **Eng,** set **Strain Rate** to **1e-5**, then click **OK.**
4. Click **MD** | **LAMMPS** | **Start LAMMPS**



IV. Execute simulations
2. Elongation

1. Click **MD** | **LAMMPS** | **Energy Plot**. Open the file by default.
2. Check **Lz**（System size of z direction）and **Pzz** (Pressure of z direction）in **Energy terms**. Check **Block Average, set Size** to **10**.
3. Click **Draw**, then Click **Excel.**



X-Ability
クロスアビリティ

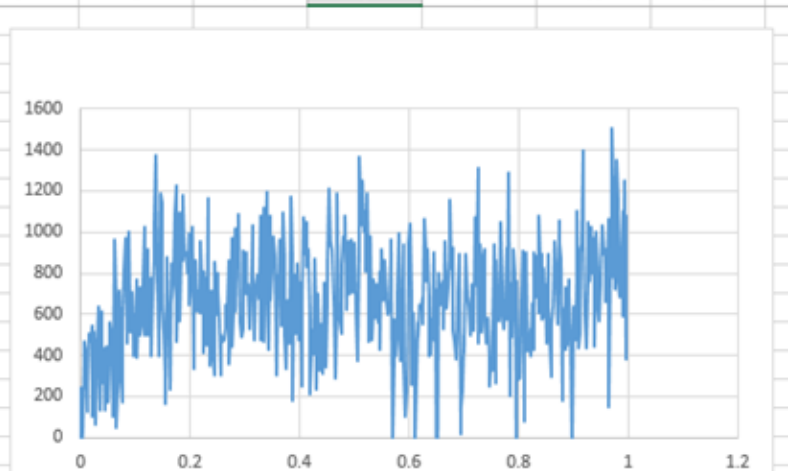
IV. Execute simulations
2. Elongation

Columns **A**, **B**, and **C** contains MD time steps, **Lz**（System size of z direction）and **Pzz** (Pressure of z direction）respectively. Columns **D** and **E** contain strain and stress respectively, and can be calculated as described below.

To calculate column **D**: Normalize the first value of **Lz** in column **B** (**41.07478**) and subtract 1.
To calculate column **E**: Multiply -1 to **Pzz** values in column **C**.

The graph manifests stress-strain curve by taking values from column **D** for the X-axis and column **E** for the Y-axis. (Graph shown is plotted with a lower limit of 0 in the Y-axis)

	A	B	C	D	E
1	90	41.07478	−242.805	0	242.8052
2	290	41.15685	80.80134	0.001998	−80.8013
3	490	41.23893	−20.9201	0.003996	20.92012
4	690	41.32101	−387.214	0.005995	387.2144
5	890	41.40308	−463.817	0.007993	463.8168
6	1090	41.48516	−411.668	0.009991	411.6679
7	1290	41.56723	−121.9	0.011989	121.8999
8	1490	41.64931	−266.743	0.013987	266.7427
9	1690	41.73138	−501.391	0.015986	501.3914
10	1890	41.81346	−467.279	0.017984	467.2794
11	2090	41.89554	−542.803	0.019982	542.8025
12	2290	41.97761	−104.616	0.02198	104.6157
13	2490	42.05969	−510.723	0.023978	510.7234
14	2690	42.14176	−76.4638	0.025977	76.4638
15	2890	42.22384	−62.1454	0.027975	62.14539
16	3090	42.30591	−457.98	0.029973	457.9798
17	3290	42.38799	−635.133	0.031971	635.1335
18	3490	42.47007	−451.749	0.033969	451.7491

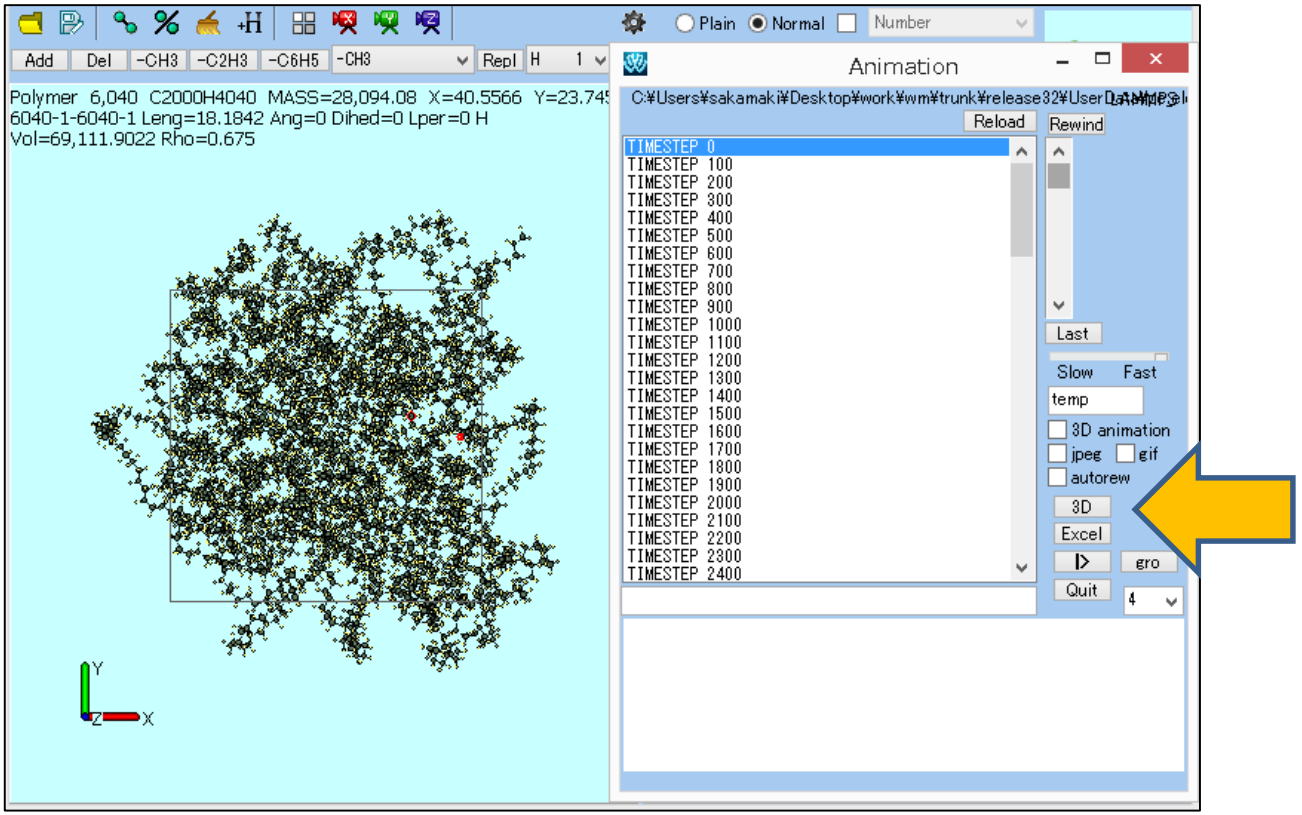


reference: Hossain, D., Tschopp, M.A., Ward, D.K., Bouvard, J.L., Wang, P., Horstemeyer, M.F., Polymer, 51 (2010) 6071−6083.

IV. Execute simulations

2. Elongation

1. Click **MD** | **LAMMPS** | **Import Trajectory** in the main window.
2. Open the files selected by default.
3. Click **3D** in **Animation** window.



X-Ability
クロスアビリティ

IV. Execute simulations
2. Elongation

1. Click **View** | **Preferences** on the **Winmostar 3D**.
2. Check **Rainbow** in **Preferences window**.
3. Click **|>** (Play) button to check the polymers are elongating.