winmostar tutorial

LAMMPS Calculation of Glass Transition Temperature (Polymer, Cooling Calculation)

V11.6.5

18 March 2024 X-Ability Co., Ltd.

About This Manual

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session:We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - Individual Training Session:You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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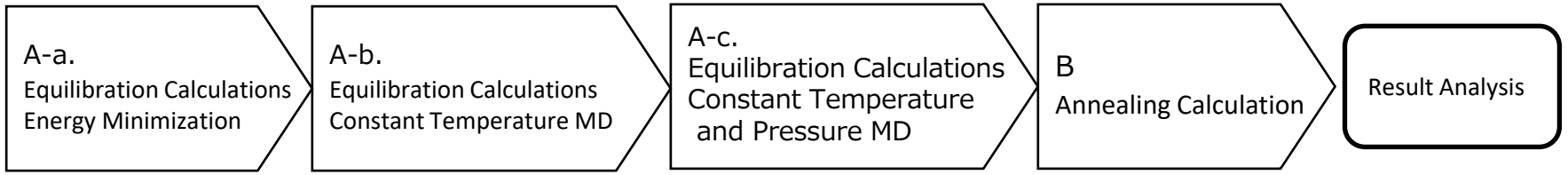
Overview

- The glass transition temperature is calculated from the cooling process of the polypropylene melt. The process flow is shown below.



Note:

- The number of steps required for equilibration may vary depending on the type of molecule and its initial density.
- The method of interaction calculation, force field, and method of charge calculation can affect the results.
- The degree of polymerization (chain length) and the rate of cooling (heating) also affect the results.
- Due to the tutorial nature, here we do not perform calculations with a sufficient number of steps for equilibration of the polymer system.

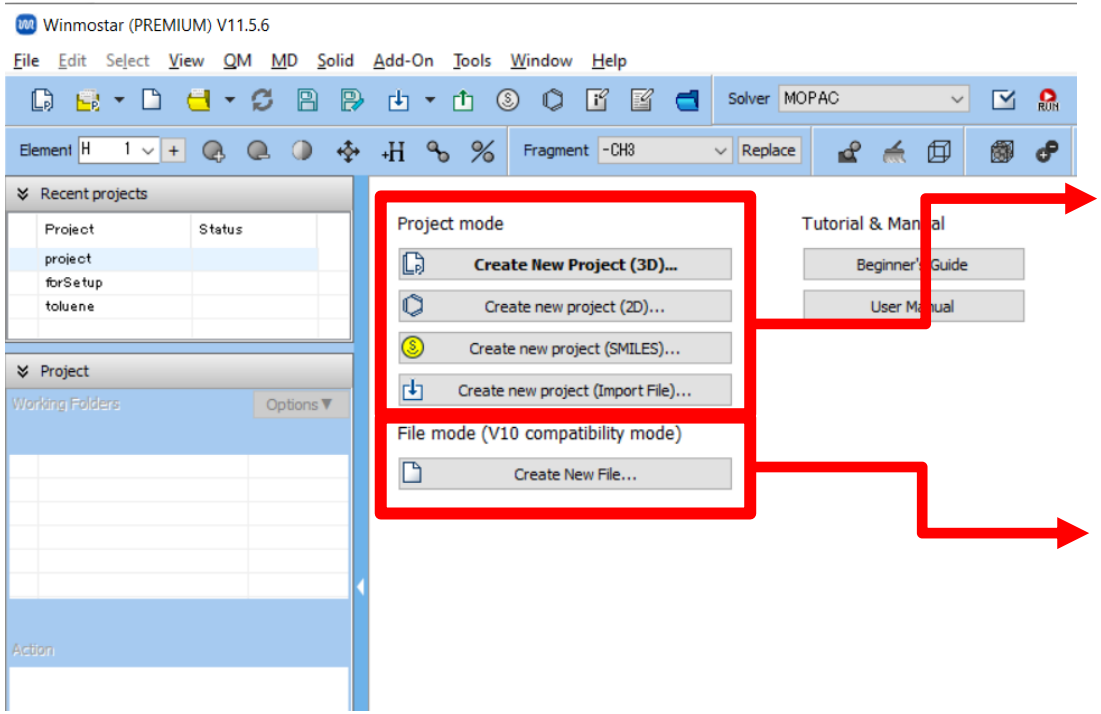
Preference of Operating Environment

- If you are using Winmostar V11.5.0 or later and are on a 64-bit environment, please install and configure CygwinWM version 2023/04/05 or later.
  - The CygwinWM version 2023/04/05 and later includes the recommended version of 64-bit LAMMPS.

- If the above does not apply to you, or if you wish to use a version of LAMMPS other than the recommended version, you will need to separately install and configure the Windows version of LAMMPS.

Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.
For operations in File Mode, please refer to tutorial for version 10.



Project Mode New Features in V11

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

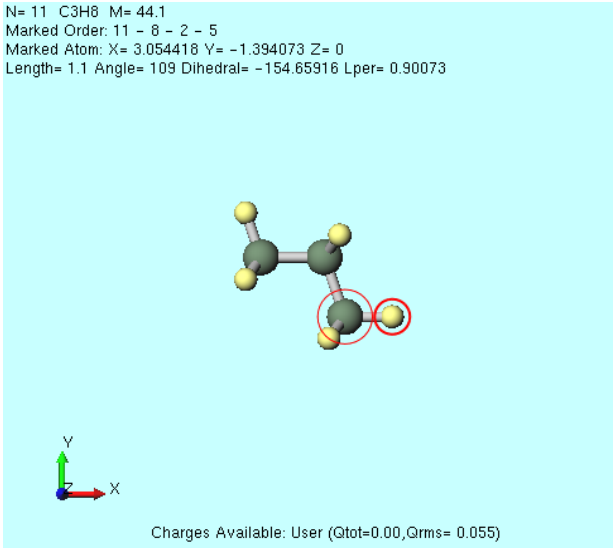
File Mode

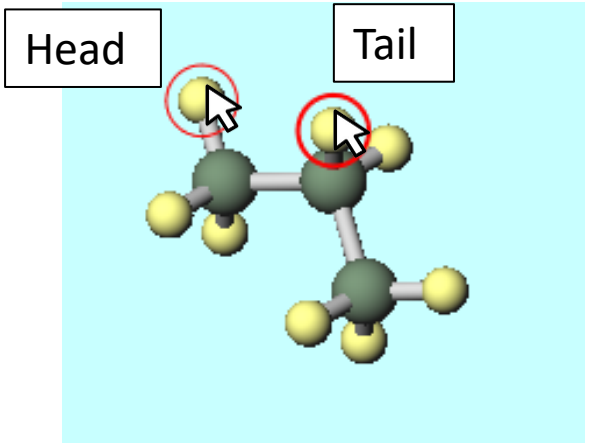
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System

For basic operations, please refer to LAMMPS Basics tutorial.

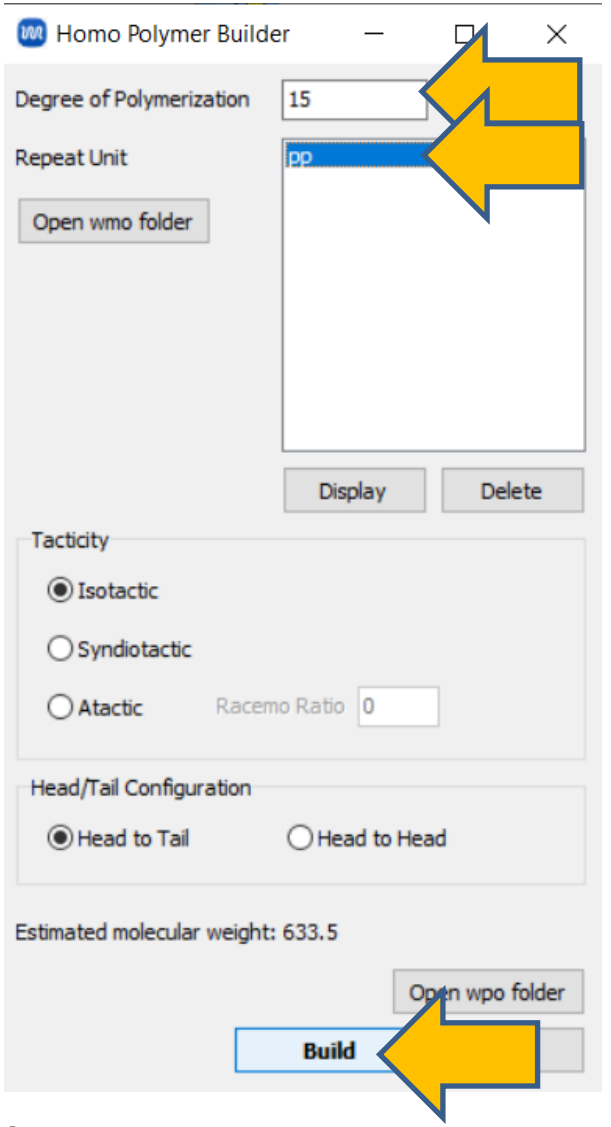
A. Click **File | New Project**, enter '`glasstemp`' in **Project name**, and click **Save**.
B. Click **Replace** three times to create the repeating unit of polypropylene (propane, C_3H_8).
C. Click **Assign Charges Automatically** and then click **OK**.
D. When 'Successfully assigned charges' is displayed, click **OK**.
E. Continue by clicking on two points (Head and Tail) that will bond with the adjacent repeating unit when polymerized.





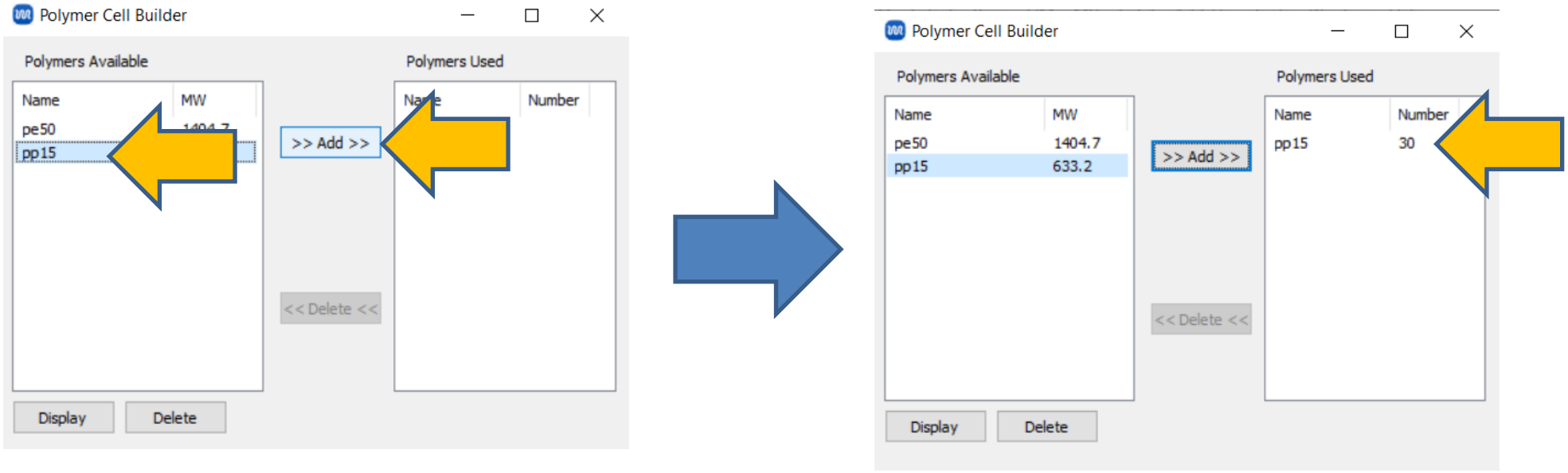
A. Modeling of the System

A. Click **MD | Polymer | Register Repeat Unit** and then click **OK**.
B. Enter 'pp' as **Repeat unit name** and click **OK**.
C. When '…pp.wmo saved successfully.' is displayed, click **OK**.
D. Click **MD | Polymer | Homo Polymer Builder** and set as follows:
   - Change **Degree of Polymerization** to '15'.
   - Select 'pp' as **Repeat Unit**.
E. Click **Build** and enter 'pp15' as **Enter polymer name** and click **OK**.
F. When '…pp15.wpo saved successfully.' is displayed, click **OK**.
G. Click **Close** to close **Homo Polymer Builder** window.



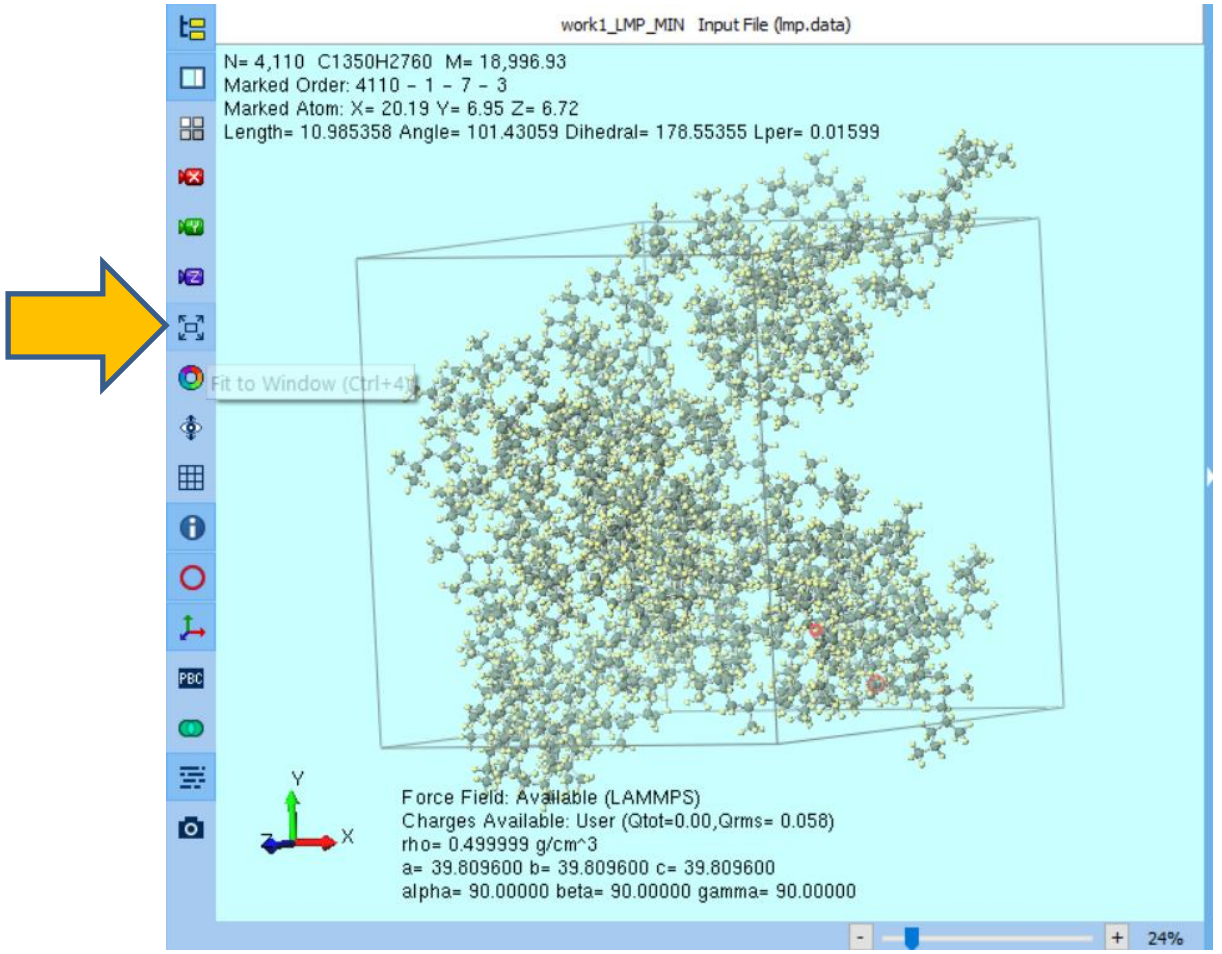
A. Modeling of the System

A. Click **MD | Polymer | Polymer Cell Builder**.
B. Select **pp15** from **Polymers Available** and click **Add**.
C. Enter '30' in **Enter Value** and click **OK**.
D. Ensure 'pp15 30' is displayed under **Polymers Used** and click **Build**.
E. A black window appears, and the polymer building process runs for several seconds. Once 'Successfully generated polymer system.' is displayed, click **OK**.
F. Click **Close** to close **Polymer Cell Builder** window.



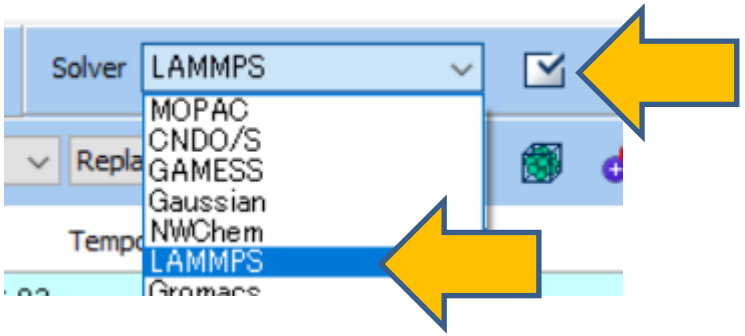
A. Modeling of the System

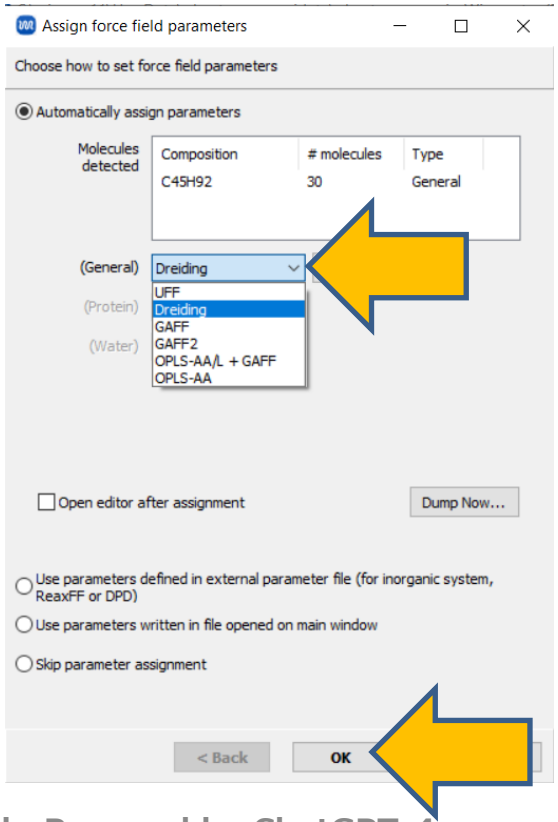
A. Click  **Fit to Window** to review the entire system.



B. Execution of Calculation

A. Select 'LAMMPS' from **Solver** and click **(Workflow Setup)**.
B. Change **Automatically assign parameters (General)** to **Dreiding** and click **OK** at the bottom right.
C. After a few seconds of processing, if 'Assigned force field parameters' is displayed, click **OK**.



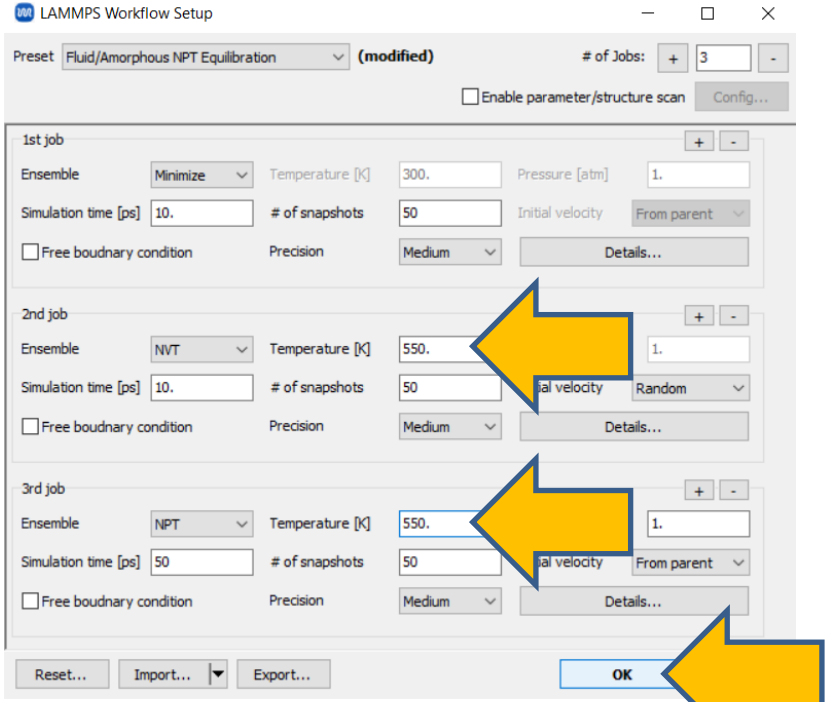


B. Execution of Calculation

A. In **LAMMPS Workflow Setup** window, make the following changes:
   A. Change **Temperature** of **2nd job** to '550'.
   B. Change **Temperature** of **3rd job** to '550'.

B. If you want to decrease the computation accuracy to finish the calculation faster, change **Precision** of **1st job**, **2nd job**, and **3rd job** all to 'Low'.

C. Click **OK**, then adjust settings as appropriate in **Job Setting** window before clicking **Run**.

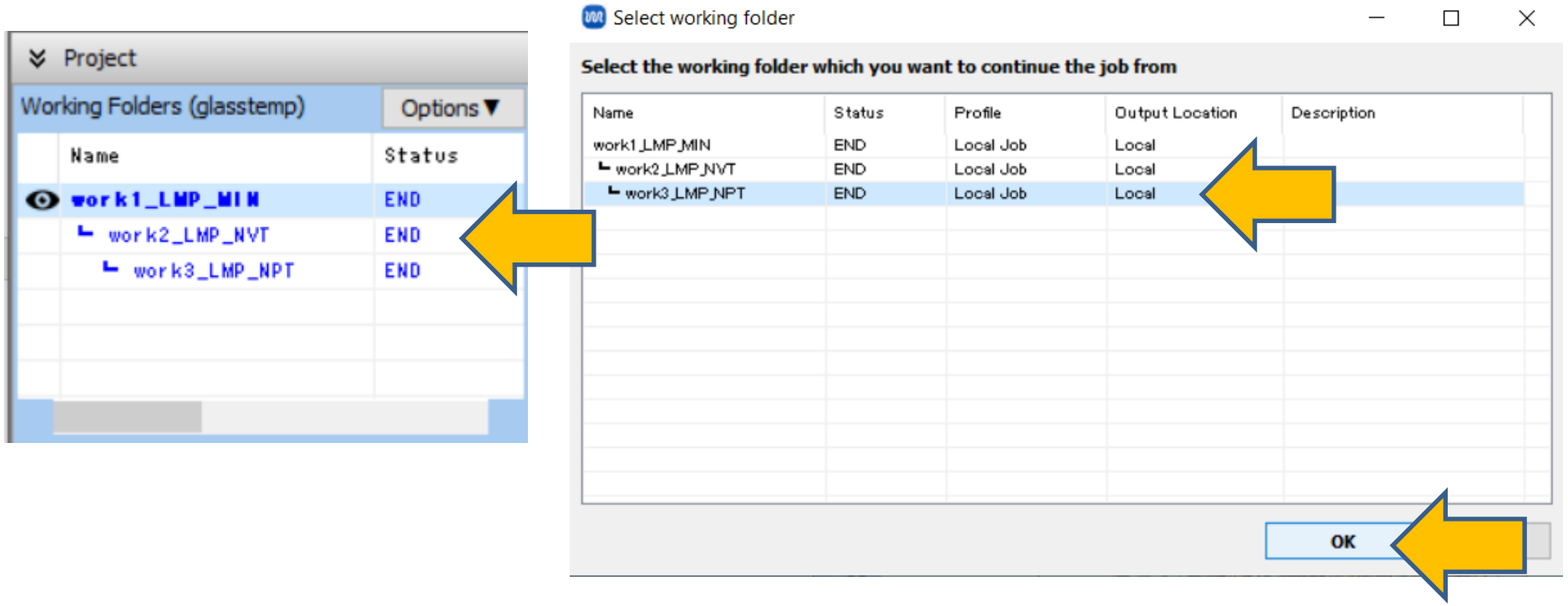


B. Execution of Calculation

A. Once **the status** of work folders from work1_LMP_MIN to work3_LMP_NPT changes to **END** or **END(-)**, click again **(Workflow Setup)**.

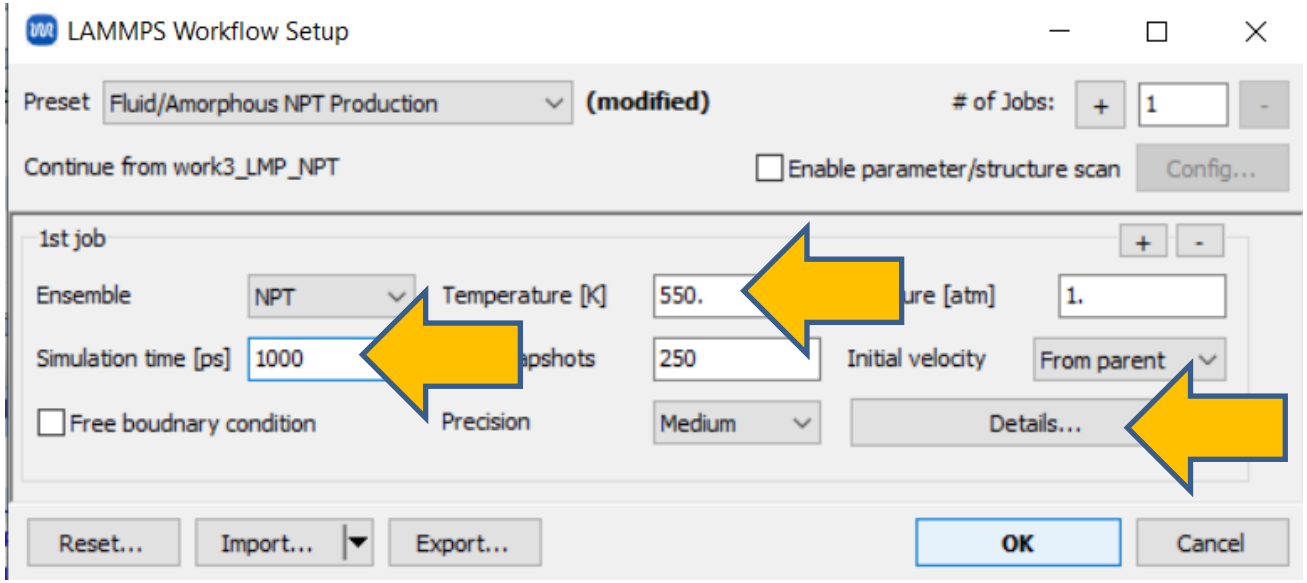
B. If prompted 'Do you want to continue from previous run?', click **Yes**.

C. Select work3_LMP_NPT and click **OK**.



B. Execution of Calculation

A. Change **Preset** to 'Fluid/Amorphous NPT Production'.
B. Modify the settings as follows:
    A. Change **Temperature** of **1st job** to '550'.
    B. Change **Simulation time** of **1st job** to '1000'.
C. If you want to reduce computational accuracy to finish the calculation faster, change **Precision** of **1st job** to 'Low', and **Simulation time** to '50'.
D. Click **Details…**.



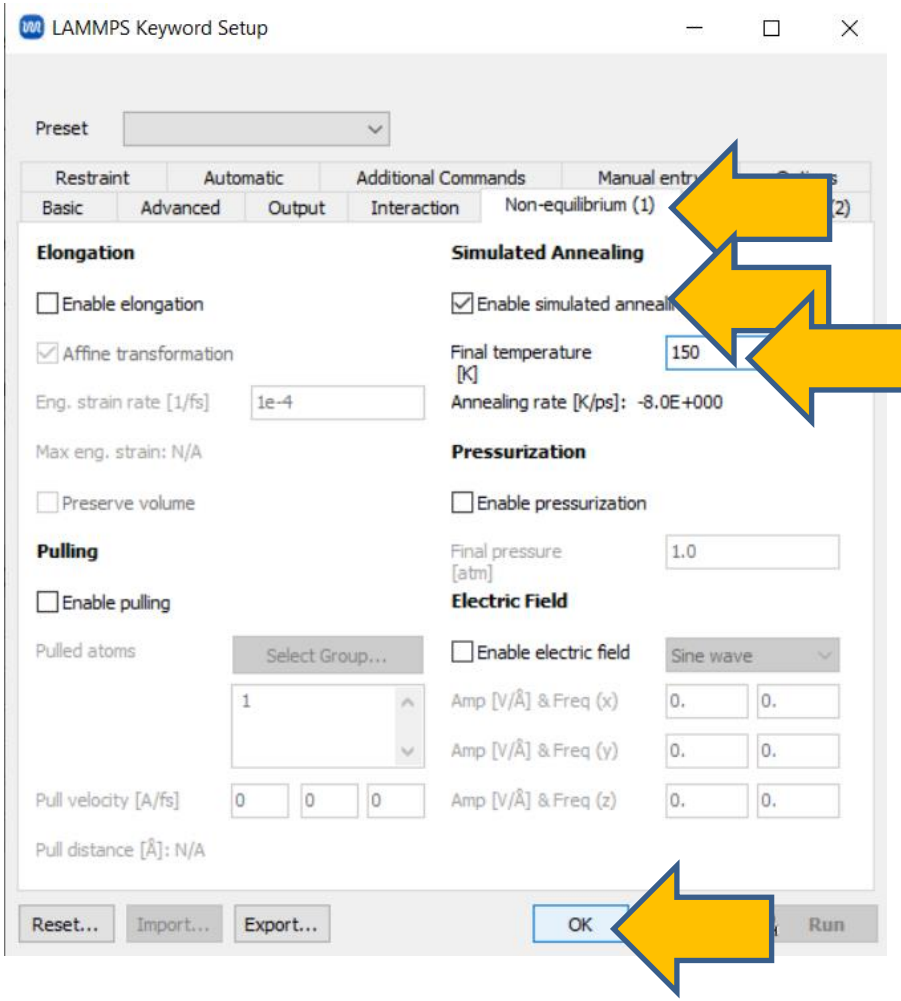
B. Execution of Calculation

A. In **LAMMPS Keyword Setup** window, navigate to **Non-equilibrium(1)** tab and make the following changes:
   A. Check **Enable simulated annealing**.
   B. Change **Final temperature** to '150'.

B. Click **OK** to close **LAMMPS Keyword Setup** window.

C. Click **OK** in **LAMMPS Workflow Setup** window.

D. In **Job Setting** window, make any necessary adjustments and then click **Run**.

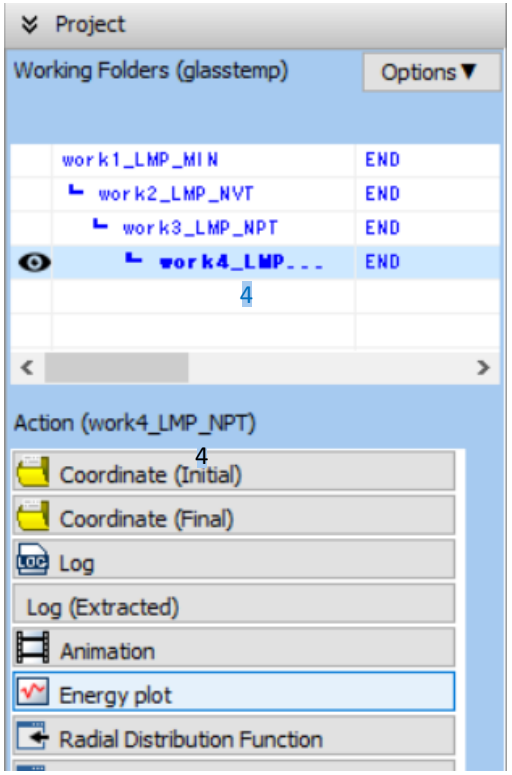


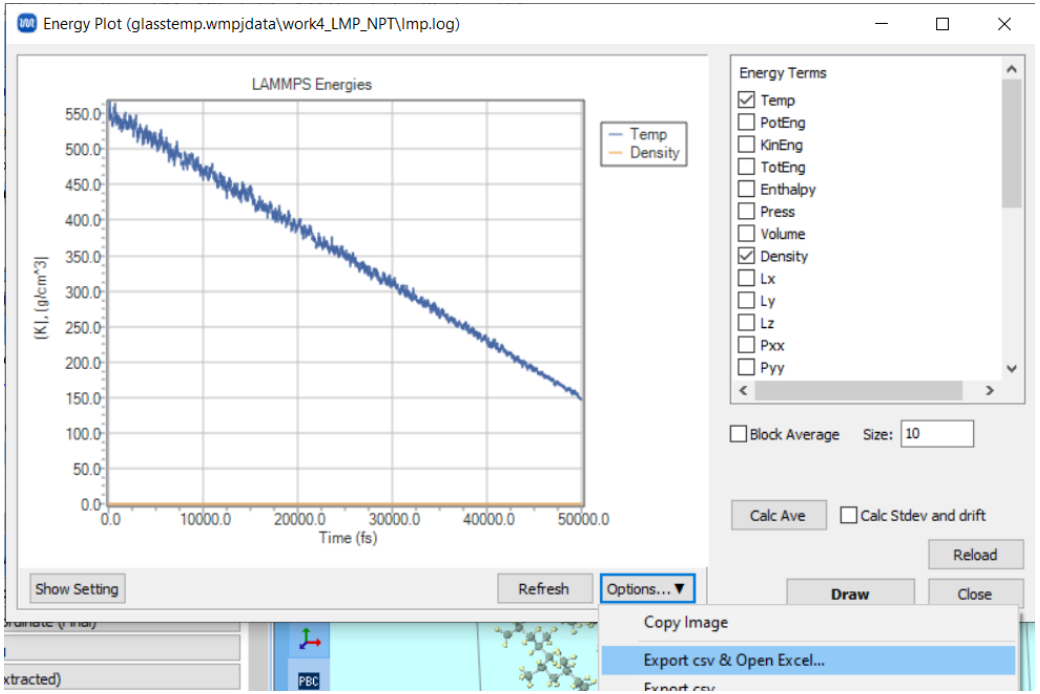
C. Analysis of Results

A. Once **the status** of work folder for work4_LMP_NPT changes to **END** or **END(-)**, click 'work4_LMP_NPT' and then click **Energy plot** in **Action**.

B. In **Energy Terms**, check **Temp** and **Density**, then click **Draw**, followed by clicking **Options | Export csv & Open Excel**.

C. Click **Save** in **Save as** dialogue.





C. Analysis of Results

A. Plot the second column of the exported csv file on the x-axis and the reciprocal of the third column on the y-axis (temperature-volume curve). The temperature at the inflection point of this curve is estimated as the glass transition temperature.

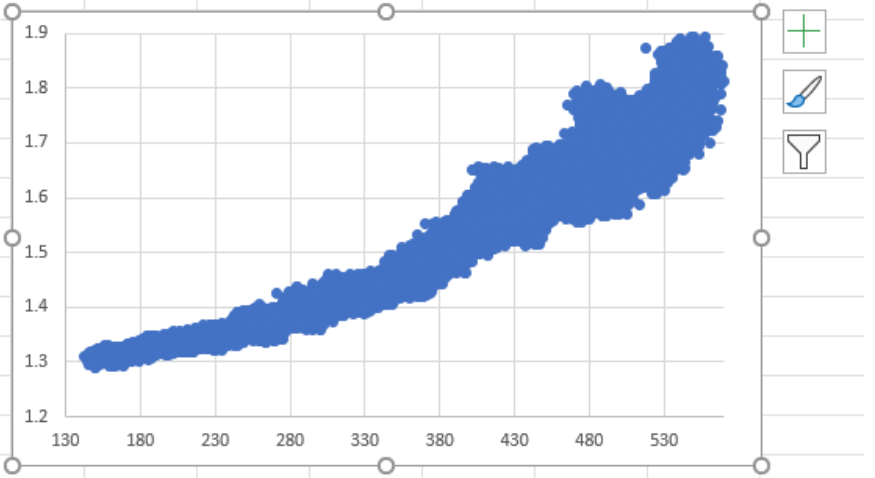
※ Fit each side of the high temperature and low temperature with a linear function and take their intersection as the inflection point.

※ If the calculation is done with reduced precision, the inflection point may become less visible.

※ Increasing the number of molecules and extending the calculation time beyond what is described in this book will improve reproducibility.

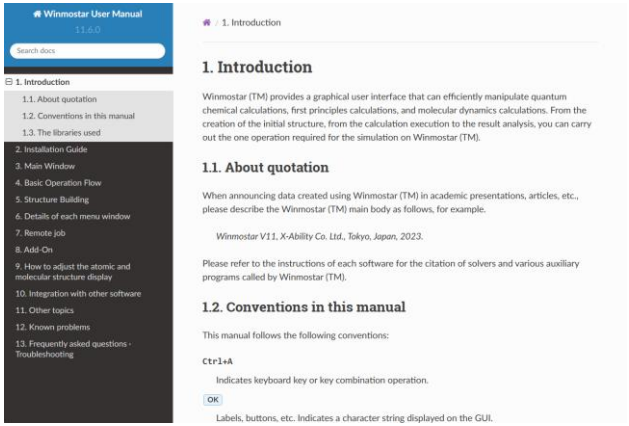
※ Instead of scanning temperatures as in this book, it is also possible to run MD independently at each temperature.

	A	B	C	D
1	0	545.1006	0.558961	1.789035
2	20	543.6751	0.556907	1.795631
3	40	533.0029	0.55619	1.797946
4	60	543.1331	0.558639	1.790065
5	80	546.2025	0.559273	1.788037
6	100	549.0053	0.557796	1.79277
7	120	552.4273	0.555233	1.801045
8	140	545.3665	0.555048	1.801647
9	160	543.451	0.553895	1.805397
10	180	549.2693	0.55492	1.802063
11	200	560.966	0.557006	1.795313
12	220	556.9979	0.553887	1.805422
13	240	567.8934	0.553399	1.807013



Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



Winmostar User Manual

Scenes from Winmostar Training Session

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