winmostar tutorial

LAMMPS/Gromacs Calculation of Glass Transition Temperature (Polymer, Scan Calculation)

V11.6.5

16 February 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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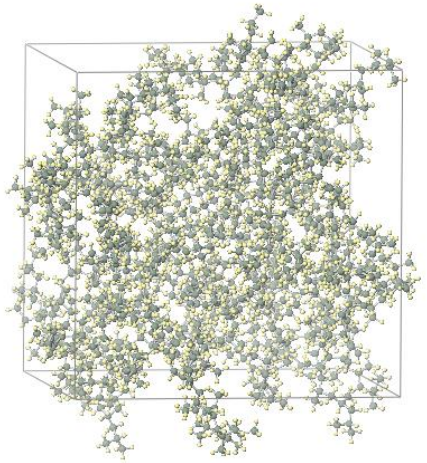
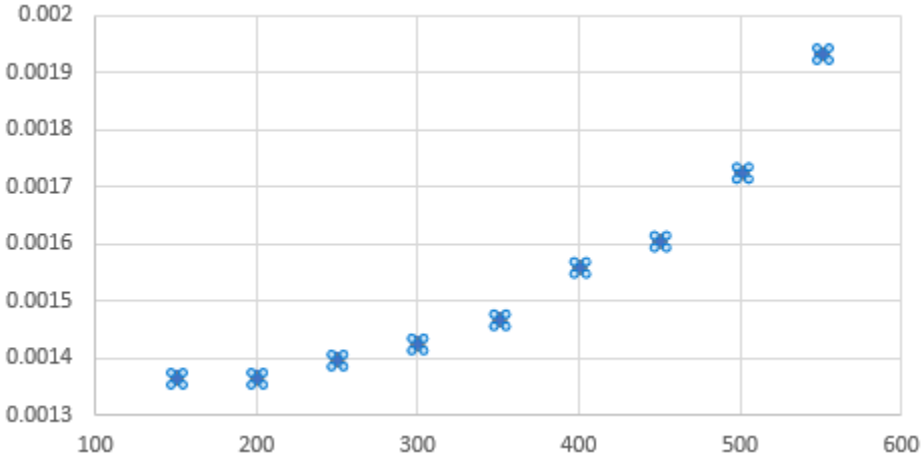
Overview

- This tutorial requires Winmostar V11 Professional Elite edition.
- The calculation of a polypropylene melt is performed at various temperatures to determine the glass transition temperature.



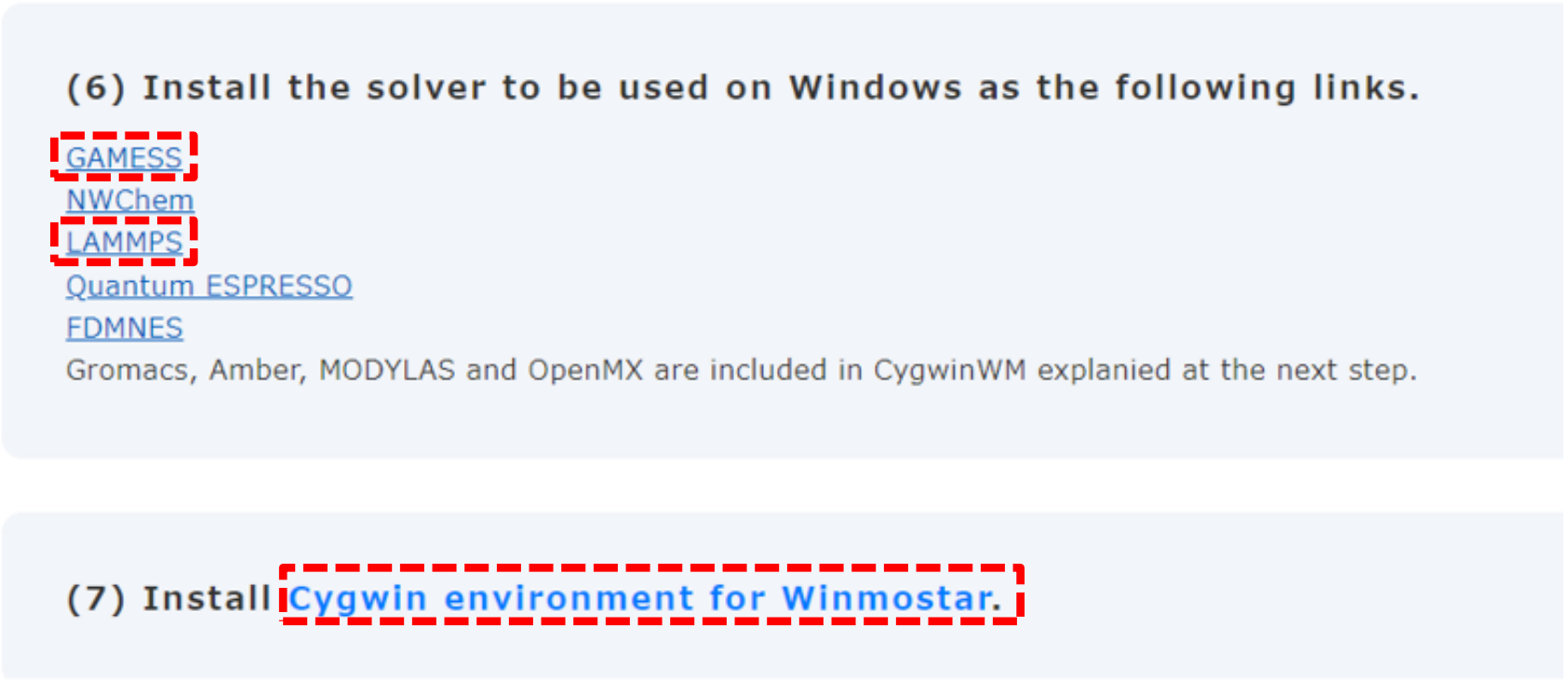


Points to note:

- The number of steps required for equilibration varies depending on the type of molecules and their initial density.
- The calculation method for interactions, force fields, and methods for calculating charges also affects the results.
- The degree of polymerization (chain length) influences the results.
- Due to the tutorial nature of this document, calculations are executed with a shorter number of steps.

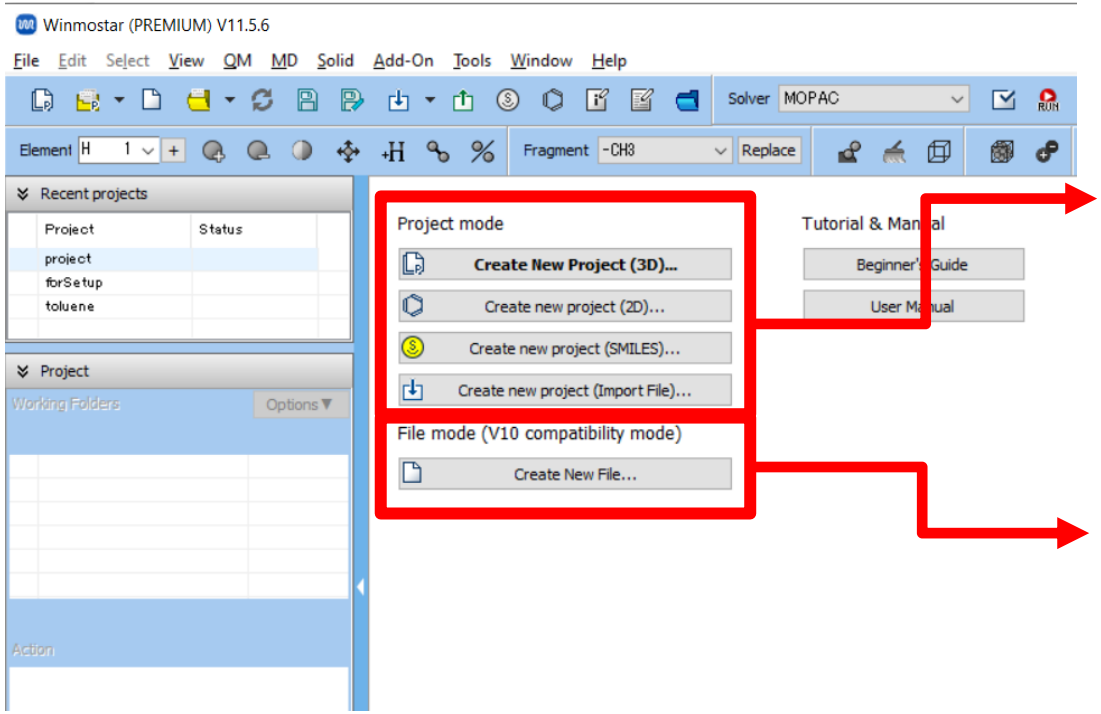
Preference of Operating Environment

- To use this feature, the setup of Cygwin and GAMESS is required. For using LAMMPS, the setup of LAMMPS is necessary.
- **https://winmostar.com/en/installation/** The installation method for GAMESS, LAMMPS and Cygwin on Windows.



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.

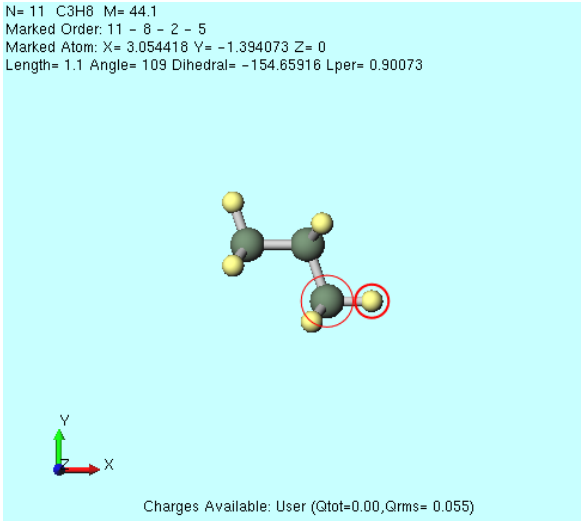
File Mode

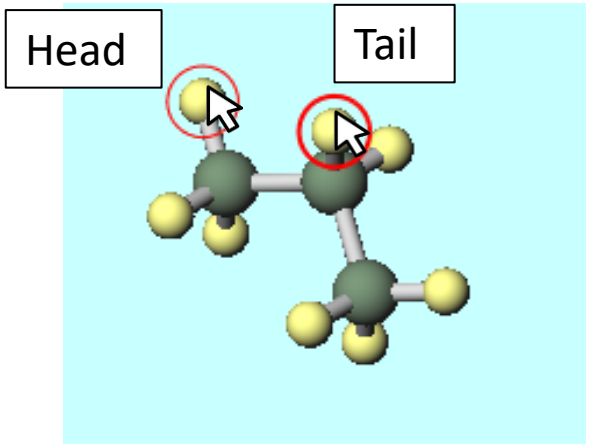
Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

A. Modeling of the System

Refer to LAMMPS Basics Tutorial or Gromacs Basics Tutorial for basic operation methods.

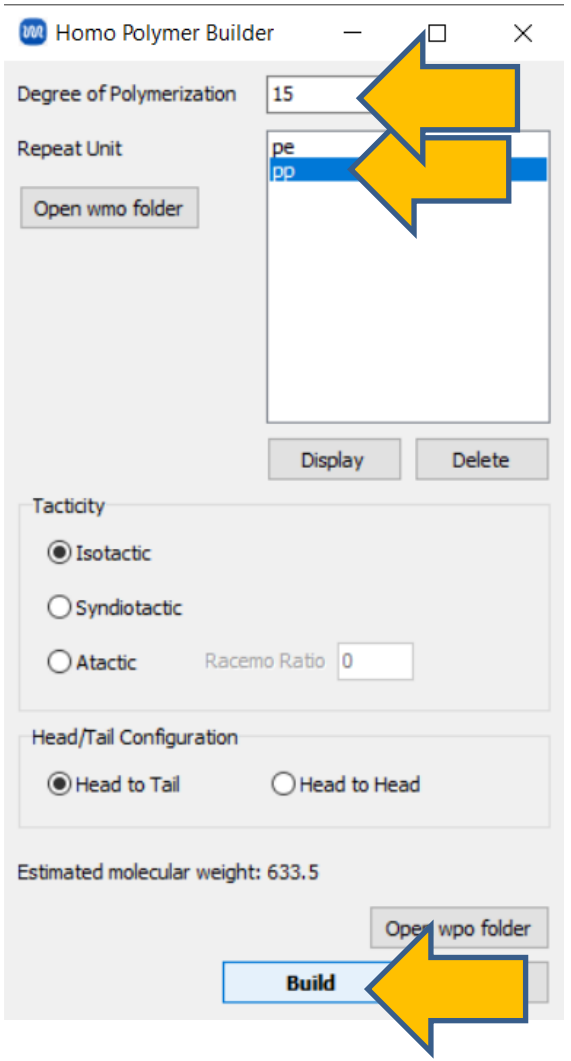
A. Click **File | New Project**, enter '`glasstemp_scan`' in **Project name**, and click **Save**.
B. Click **Replace** three times to create the repeating unit of polypropylene (propane, C_3H_8).
C. Click **Assign Charges Automatically** and then click **OK**.
D. If the message 'Successfully assigned charges' appears, click **OK**.
E. Continue by clicking on the two locations (Head and Tail) where it will bond with the neighboring repeating unit upon polymerization.





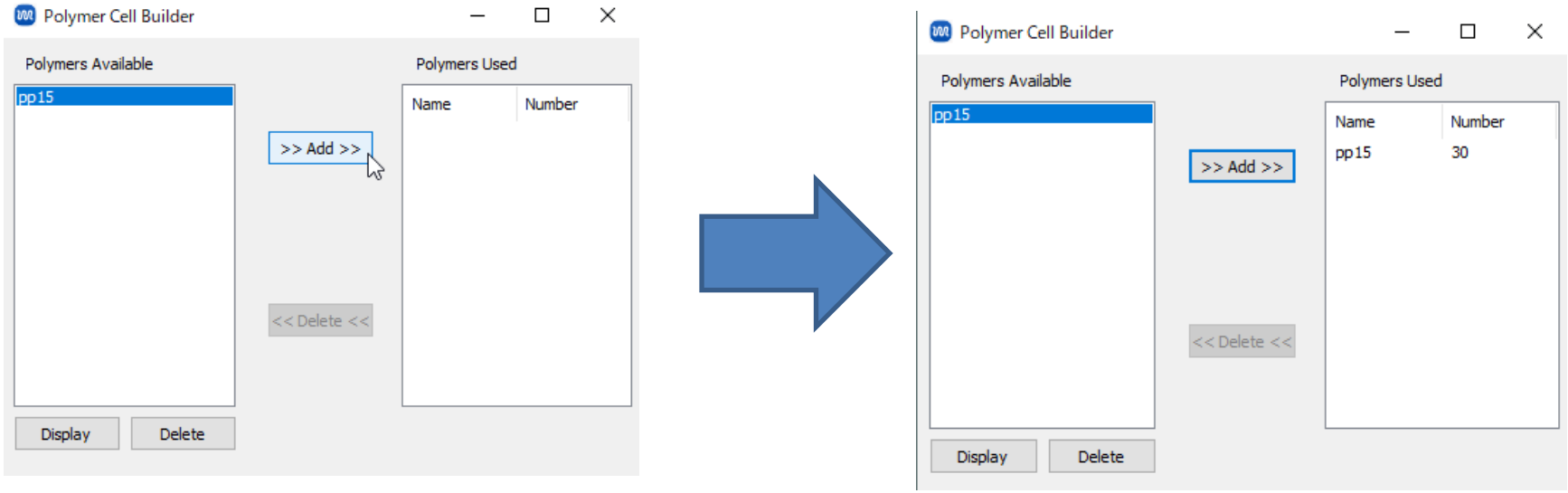
A. Modeling of the System

A. Click **MD | Polymer | Register Repeat Unit** and then click **OK**.
B. Enter 'pp' in **Repeat Unit Name** and click **OK**.
C. If you see the message '...pp.wmo saved successfully.' click **OK**.
D. Click **MD | Polymer | Homo Polymer Builder** and set it up as follows:
   - Change **Degree of Polymerization** to '15'.
   - Select 'pp' for **Repeat Unit**.
E. Click **Build**, enter 'pp15' in **Enter polymer name**, and click **OK**.
F. If you see the message '...pp15.wpo saved successfully.' click **OK**.
G. Click **Close** to exit **Homo Polymer Builder** window.



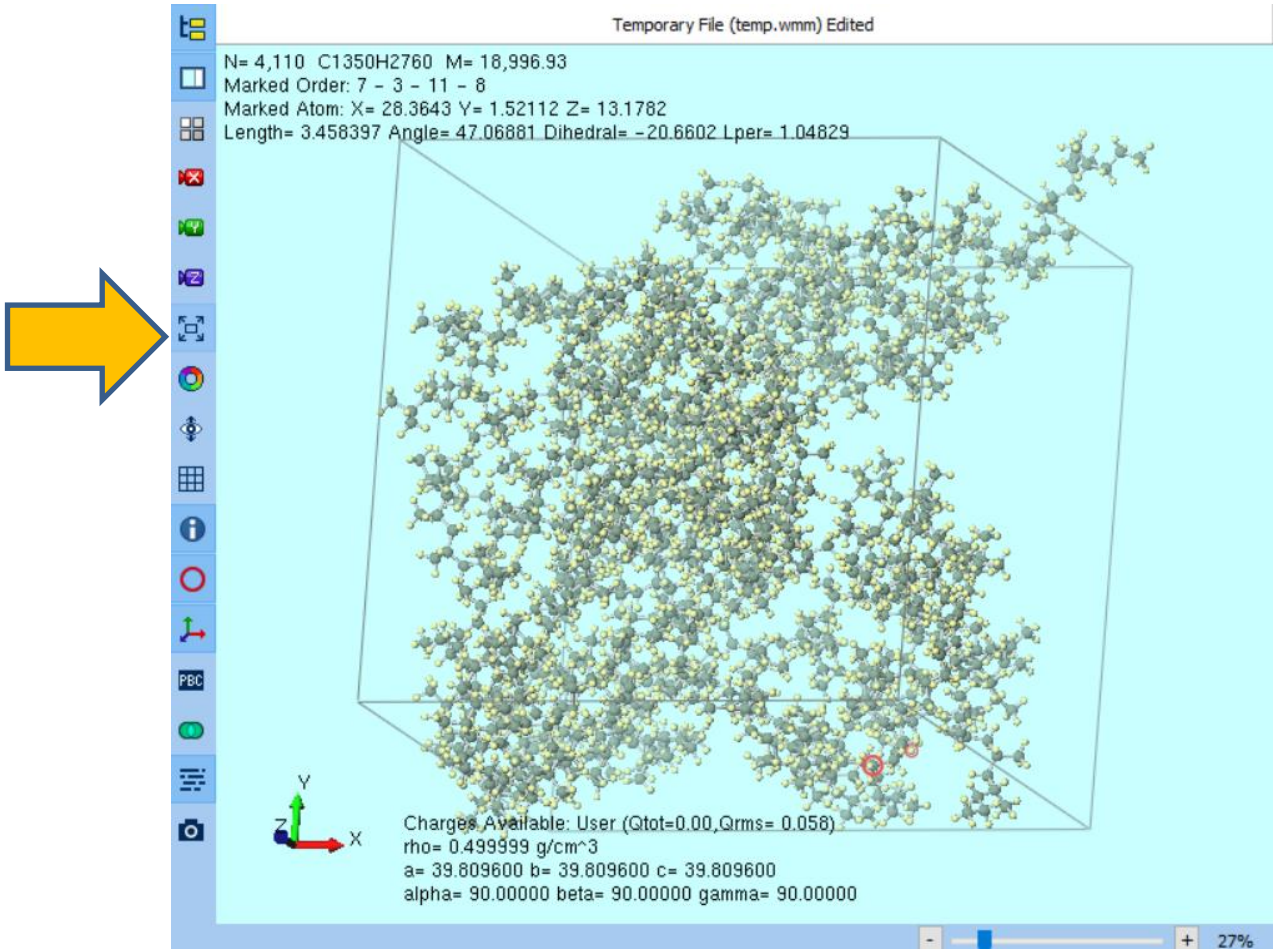
A. Modeling of the System

A. Click **MD | Polymer | Polymer Cell Builder**.
B. Select **pp15** from **Polymers Available** and click **Add**.
C. Enter '30' in **Enter Value** field and click **OK**.
D. Verify that 'pp15 30' appears in **Polymers Used**, then click **Build**.
E. A black window will appear, and after a few seconds of processing to build the polymer, the message 'Successfully generated polymer system.' will appear. Click **OK**.
F. Click **Close** to exit **Polymer Cell Builder** window.



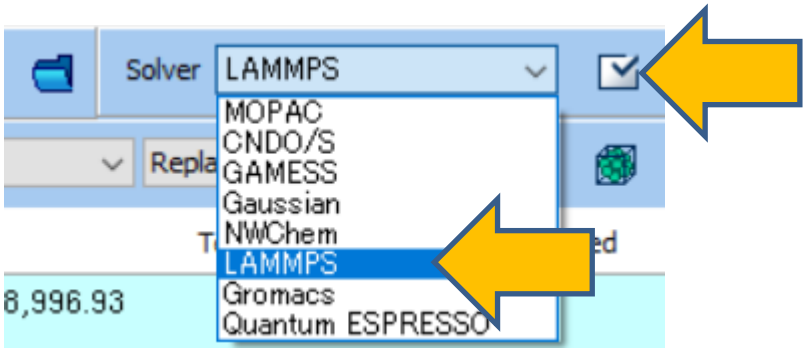
A. Modeling of the System

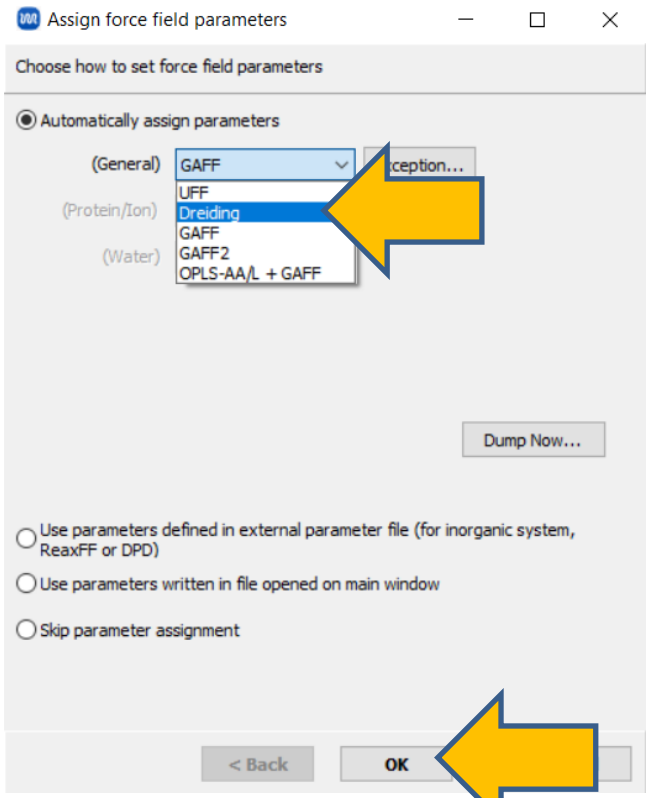
A. Click **Fit to Window** to view the entire system.



B. Execution of Calculation

A. Select 'LAMMPS' or 'Gromacs' as **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, once the message 'Assigned force field parameters' appears, click **OK**.

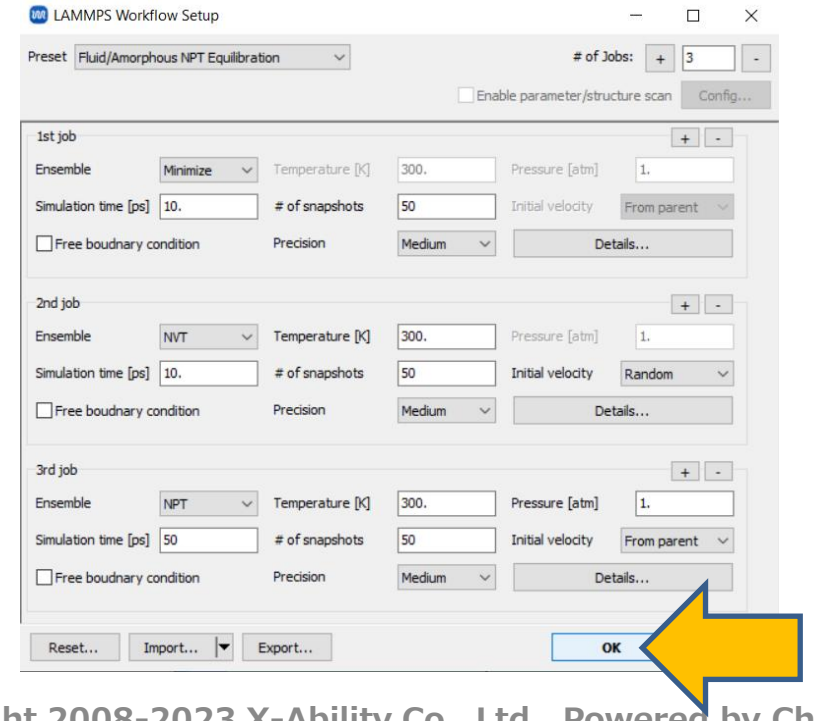




B. Execution of Calculation

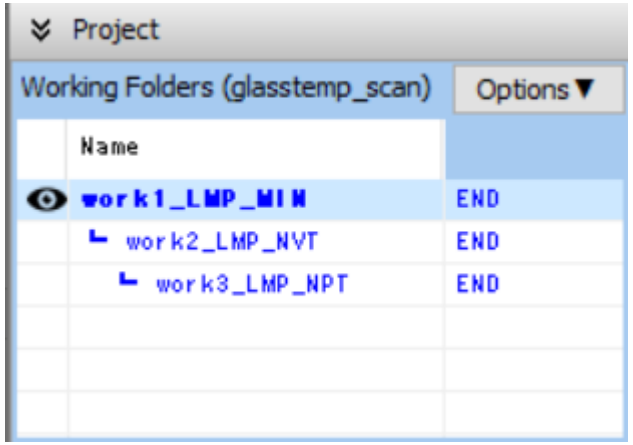
A. If you wish to reduce computational accuracy to finish calculations faster, change **Precision** to 'Low' for **1st job**, **2nd job**, and **3rd job**, and modify **Simulation time** for **3rd job** to '10'.
   - Choosing **Preset** like 12-Step Compression or 21-Step Compression-Decompression will help stabilize the equilibration calculations.

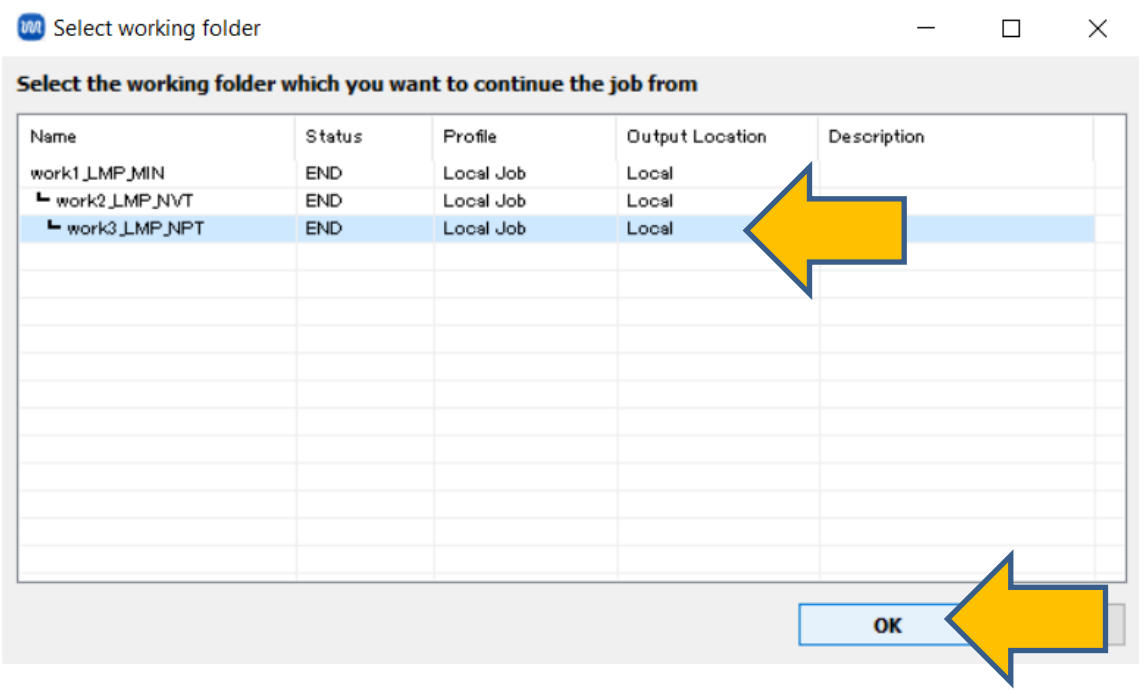
B. Click **OK**, then in **Job Setting** window, make the necessary adjustments and click **Run**.



B. Execution of Calculation

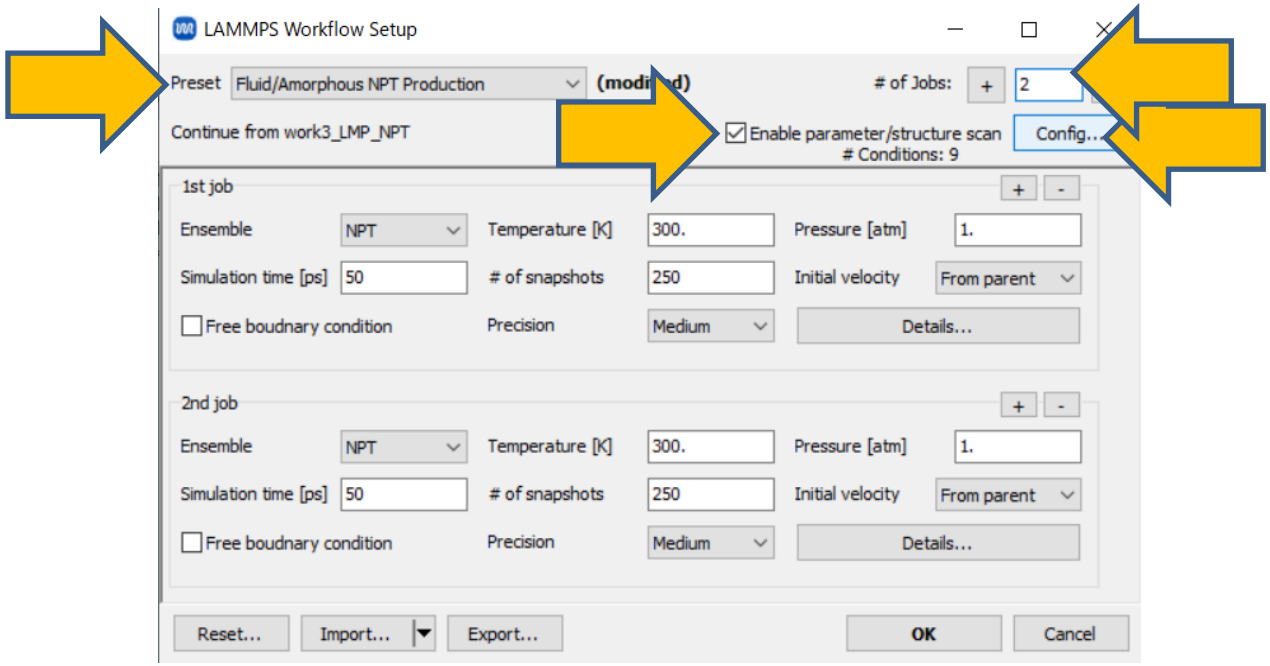
A. Once **the status** of all working folders from work1 to work3 has changed to **END** or **END(-)**, click **(Workflow Setup)** again.
B. If prompted with 'Do you want to continue from previous run?', click **Yes**.
C. Select work3 and click **OK**.





B. Execution of Calculation

A. Change **Preset** to 'Fluid/Amorphous NPT Production.'
B. Click **+** once under **# of Jobs** to add a job. Adjust **Simulation time** as needed.
    - Increasing **Simulation time** smooths out the resulting graph.
C. To reduce computational precision for quicker results, set **Precision** to 'Low' and **Simulation time** to '10' for both **1st job** and **2nd job**.
D. Check **Enable parameters/structure scan** and click **Config**.

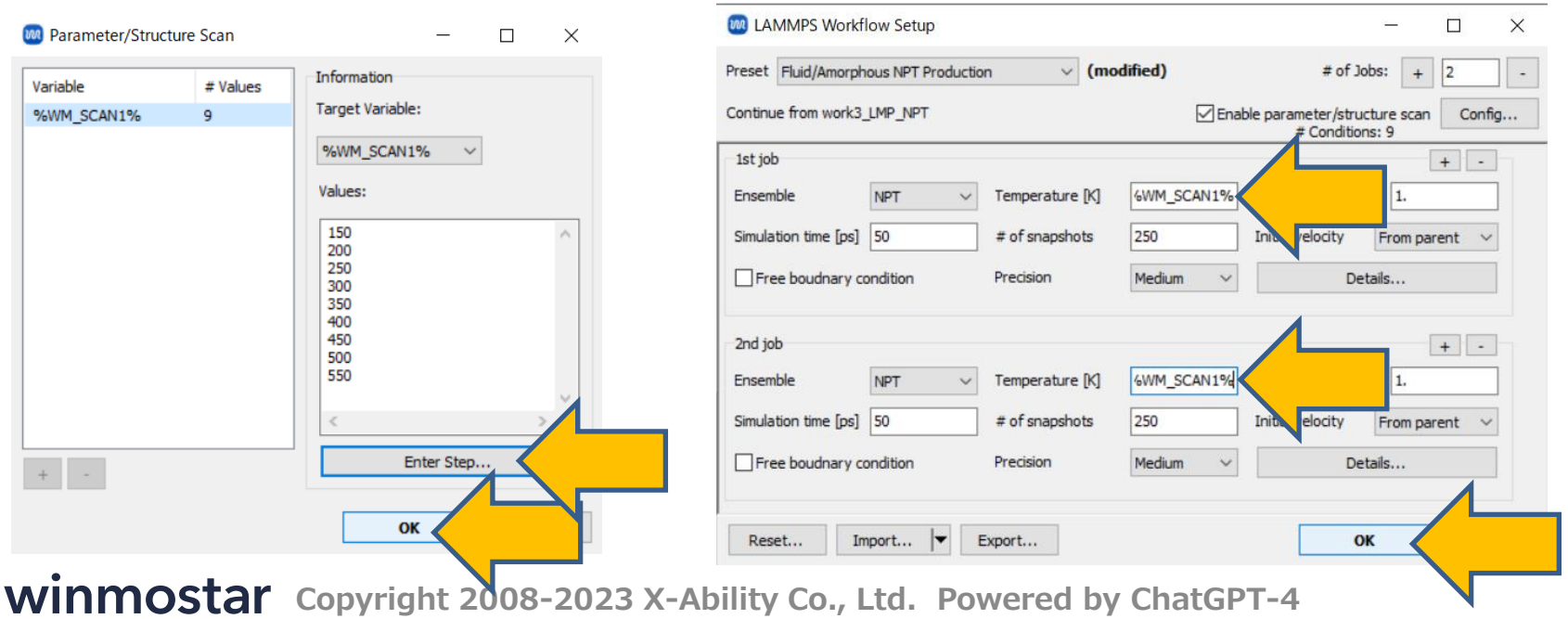


B. Execution of Calculation

A. Click **Enter Step...**, set **Minimum value** to '150', **Interval** to '50', and **Number of steps** to '9'.
   - Ensure the range of **Values** covers the anticipated glass transition temperature. A smaller **Interval** stabilizes the final fitting.

B. Click **OK** in **Parameter/Structure Scan** window.

C. In **Workflow Setup** window, input '`%WM_SCAN1%`' for **Temperature** of **1st job** and **2nd job**, then click **OK**. In **Job Setting** window, make the necessary adjustments and click **Run**.



C. Analysis of Results

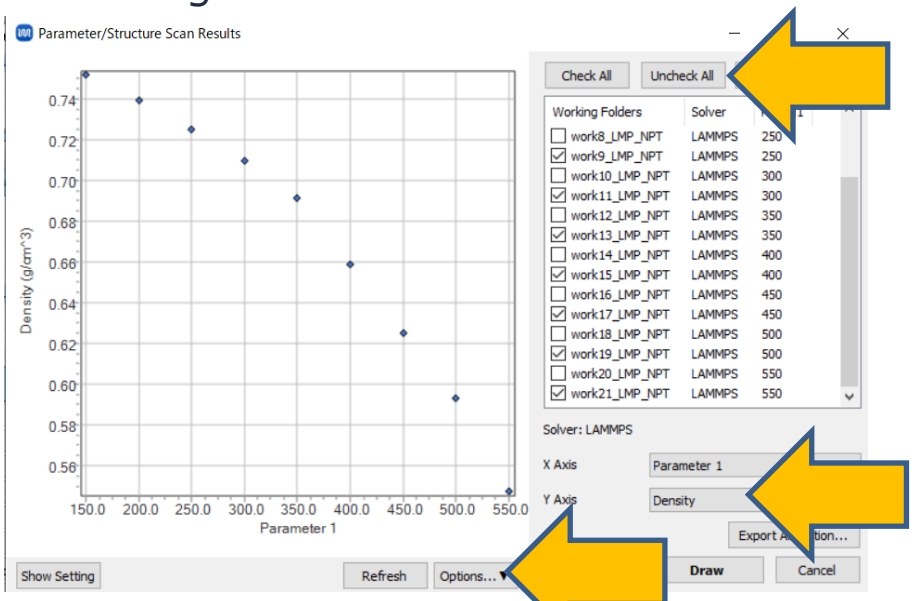
A. Once **the status** of work folders from work4 to work21 changes to **END** or **END(-)**, click on **File | Project | Parameters/Structure Scan Result**.

B. Click **Uncheck All**, then check the boxes for work5, 7, 9, 11, 13, 15, 17, 19, 21. Change **Y Axis** to 'Density' and click **Draw**.

C. After the process completes and the graph appears, click on **Options | Export csv & Open Excel**.

 - Note that units differ between LAMMPS (g/cm^3) and Gromacs (kg/m^3).

D. Click Save inSave As dialog.



C. Analysis of Results

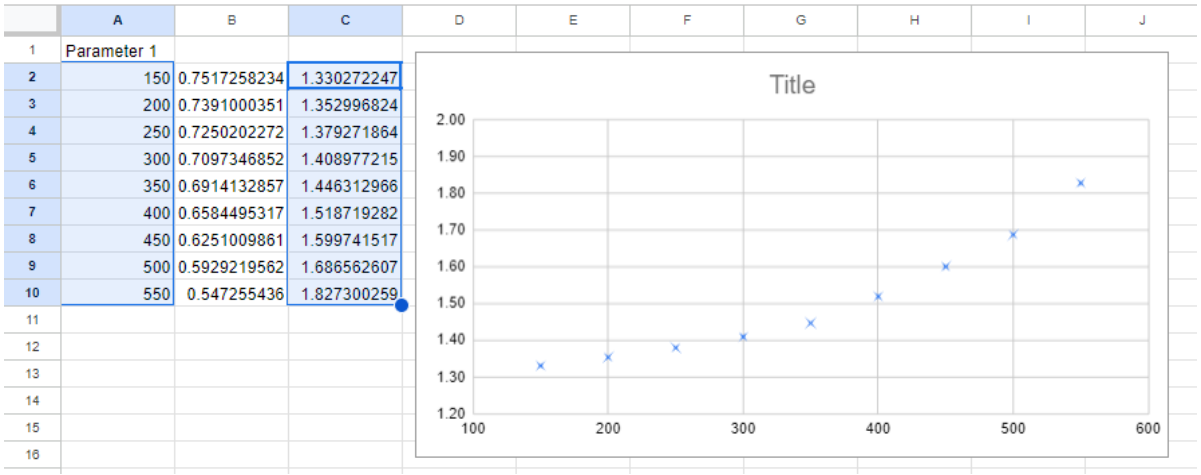
A. Plot the first column of the output csv file on the x-axis and the reciprocal of the second column on the y-axis (temperature-specific volume curve). The temperature at the inflection point of this curve is an estimated value of the glass transition temperature.

※ Fit the high-temperature side and the low-temperature side with linear functions respectively, and use their intersection as the inflection point.

※ The inflection point may become less visible if calculations are done with reduced accuracy.

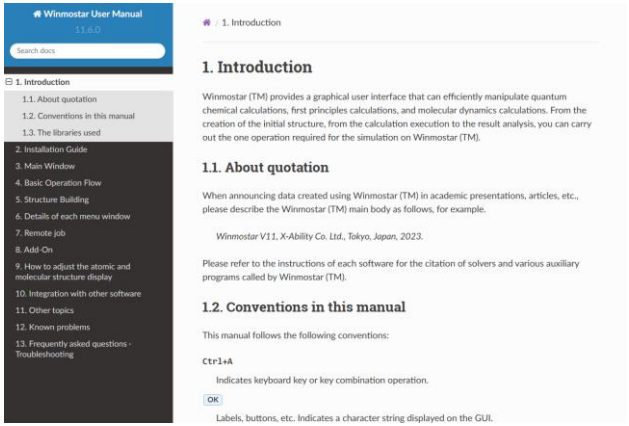
※ Reproducibility improves with a larger number of molecules and longer computation times than those used in this tutorial.

※ Instead of running independent MD simulations at each temperature as in this tutorial, a temperature scanning method can also be used.



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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