winmostar tutorial

LAMMPS Dissipative Particle Dynamics (DPD)

V11.6.5

19 April 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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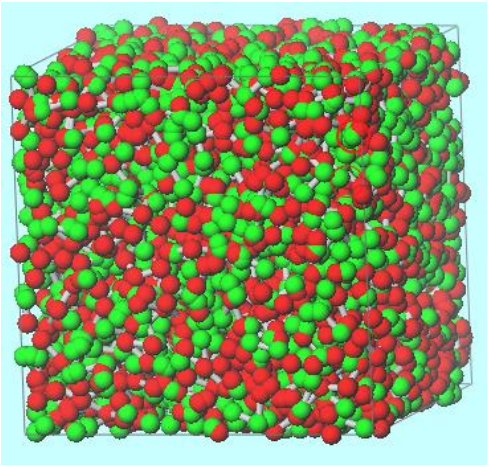
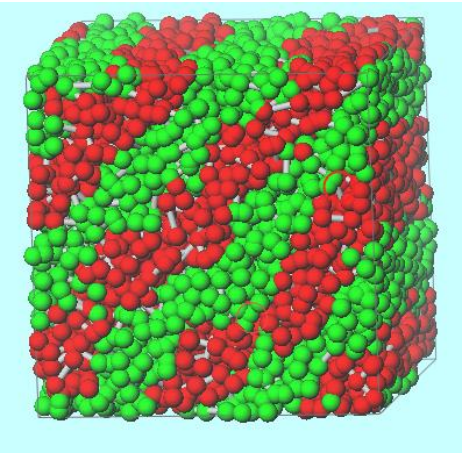
Overview

- Predicting the Phase Separation Structure of Diblock Copolymers Using DPD Method
- This tutorial demonstrates the procedure for predicting the phase separation structure of diblock copolymers using the Dissipative Particle Dynamics (DPD) method. As a quantitative evaluation method of the structure, the scattering function is calculated here.

Reference: R. D. Groot and T. J. Madden, J. Chem. Phys, 108, 20, (1998), 8713.



Initial Structure



Resulting Structure

※ Methods for mapping to full-atom MD structures are presented at the end of this document.

※ For methods on calculating DPD parameters, please refer to the Gromacs tutorial.

Note:

- The functionalities introduced in this book are not available in the Professional Economy Edition or the Student Edition.

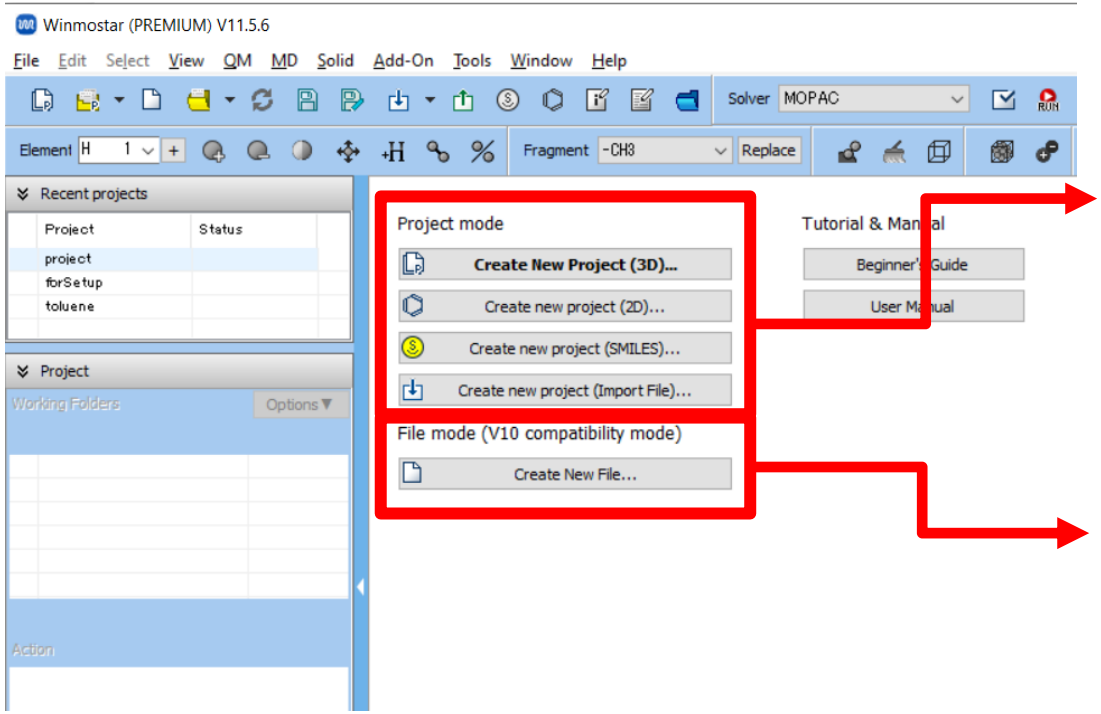
Preference of Operating Environment

- 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.

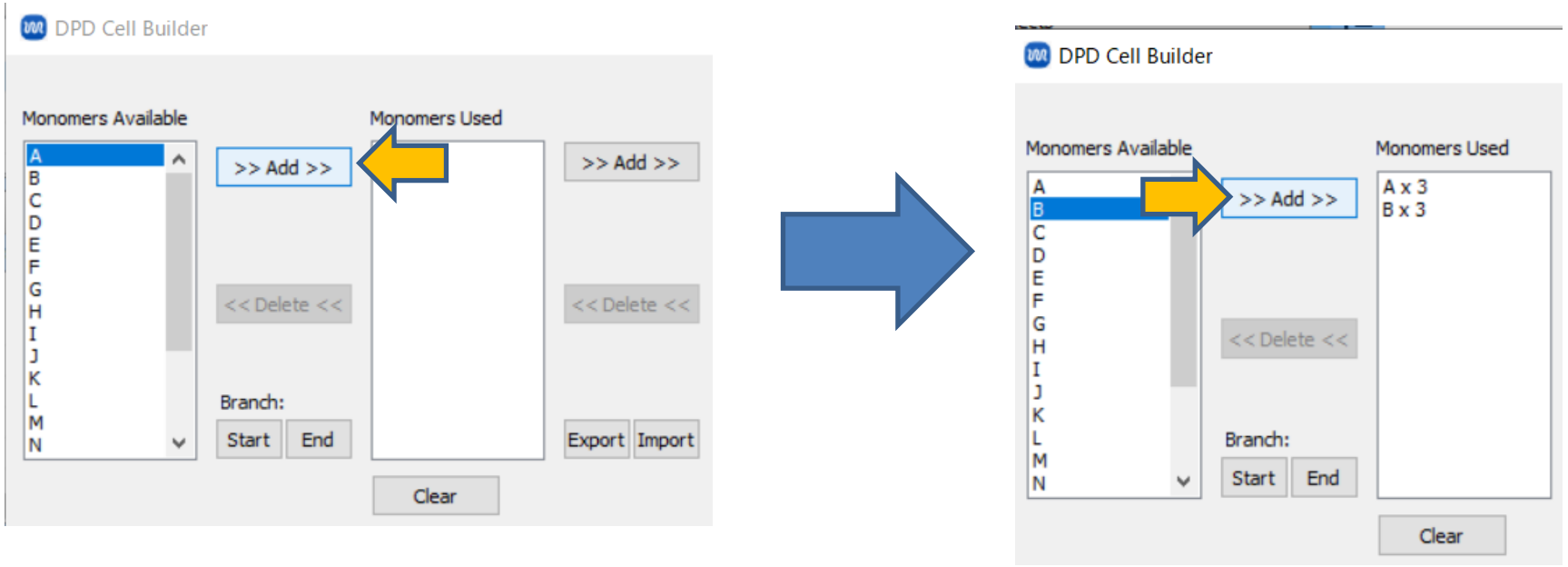
File Mode

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

A. Modeling of the System

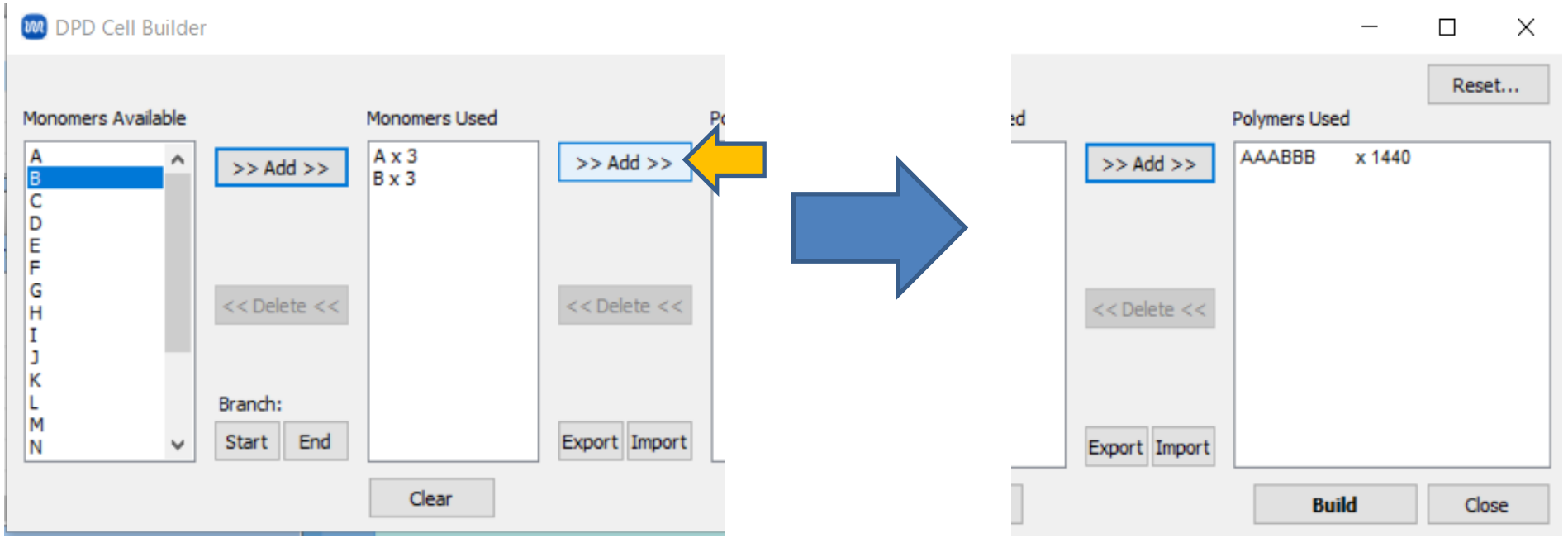
For basic operations, please refer to LAMMPS Basics tutorial.

A. Click **File | New Project**, enter 'dpd' as Project name, and click **Save**.
B. Click **MD | LAMMPS | Dissipative Particle Dynamics | DPD Cell Builder**.
C. Select **A** from **Monomers Available** and click **Add**.
D. In **Enter Value** dialog, type '3' and click **OK**.
E. Similarly, select **B**, click **Add**, and in **Enter Value** dialog, type '3' and click **OK**.



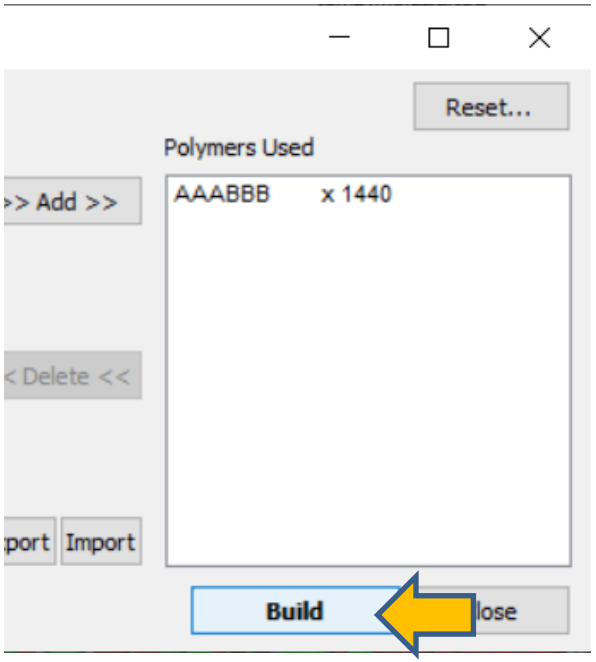
A. Modeling of the System

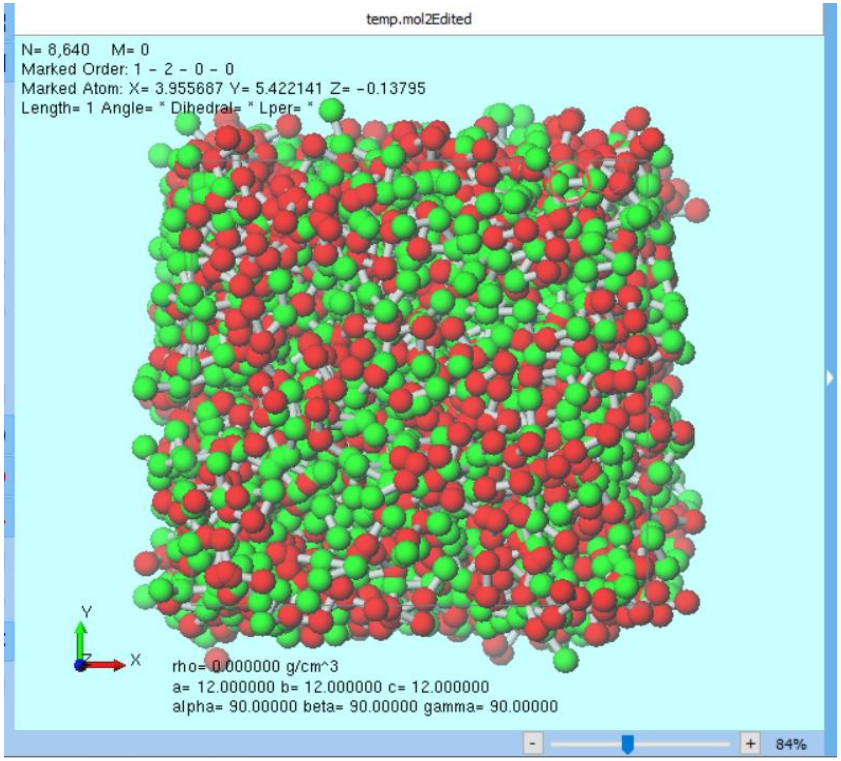
A. Click **Add** on the right side of **Monomers Used**.
B. In **Enter Value** dialog, type '1440' and click **OK**.



A. Modeling of the System

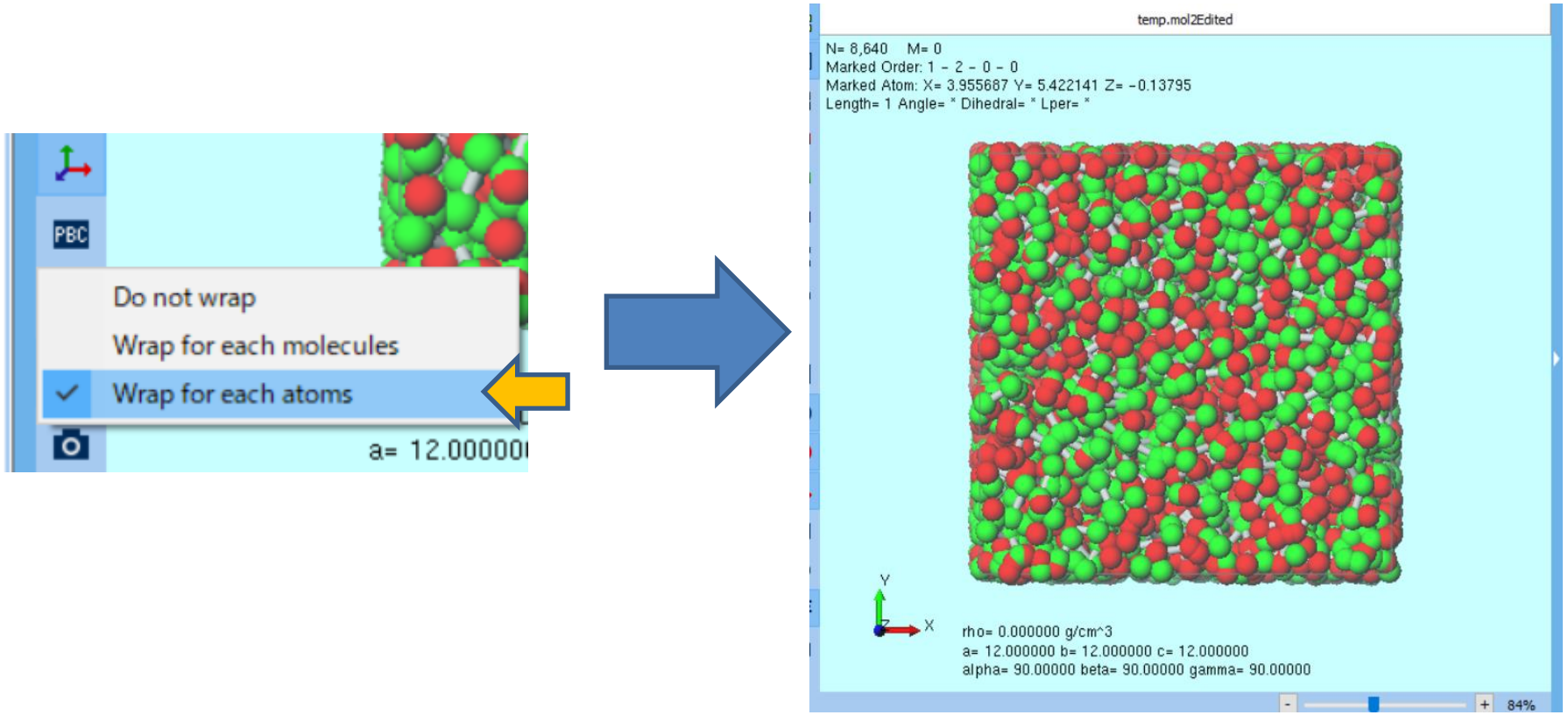
A. Click **Build** and enter '5.0' in **Enter Value**, then click **OK**. This action will generate a structure in the main window where diblock polymers (composed of A-A-A-B-B-B sequence) are randomly arranged.





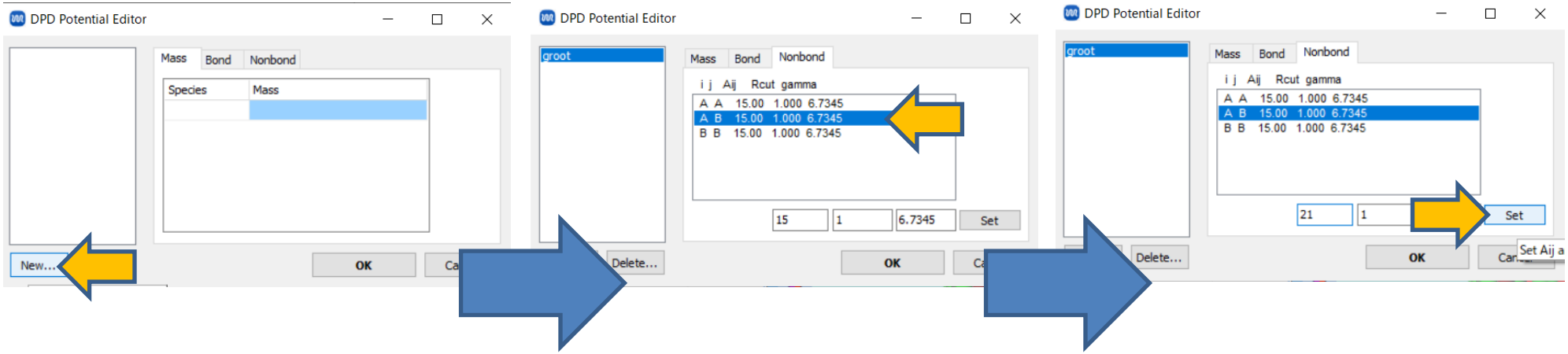
A. Modeling of the System

A. Click PBC **Wrap Around Cell Boundary | Wrap for each atoms**, to visually organize the distribution of particles A and B.



A. Modeling of the System

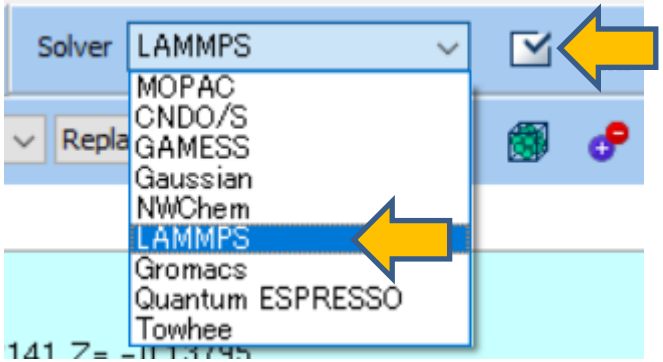
A. Click **MD | LAMMPS | Dissipative Particle Dynamics | DPD Potential Editor**.
B. Click **New**, enter the name 'groot' in **Enter name**, and click **OK**.
C. Click **Nonbond** tab, and select the line 'A B 15.00 1.000'.
D. Change the value in the textbox below from '15' to '21', and click **Set**. (Both **Aij** and **Rcut** are dimensionless units).
E. Click **OK** to close **DPD Potential Editor**.



There are several methods for determining **Aij** for any monomer, one of which is introduced in [Winmostar tutorial Gromacs Solubility/χ/DPD parameter].

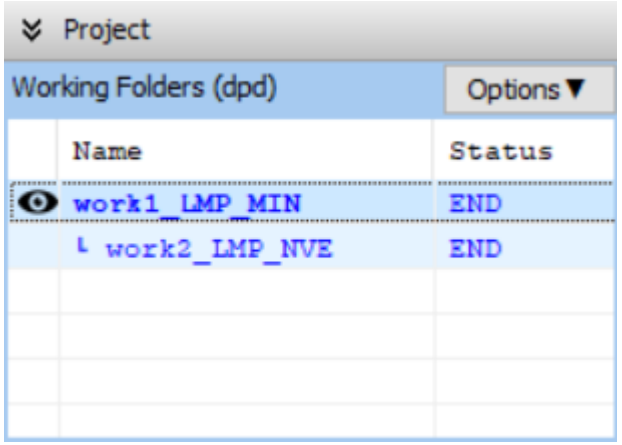
B. Execution of Calculate (Equilibration)

A. Select 'LAMMPS' from Solver and click **(Workflow Setup)**.
B. If asked 'Some molecules do not have changes. Do you want to assign charges now?', click **No**.
C. Check **Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)** and click **Next**.
D. Check **Simulate using Dissipative Particle Dynamics** and select 'groot' from **Potential file**, then click **OK**.
E. If 'Assigned force field parameters' appears, click **OK**.
F. Change **Preset** to 'DPD NVT Equilibration'.
G. If you want to speed up the computation by reducing accuracy, change **Precision** of **1st job** and **2nd job** to 'Low'.
H. Click **OK**, then set up **Job Setting** as needed and click **Run**.



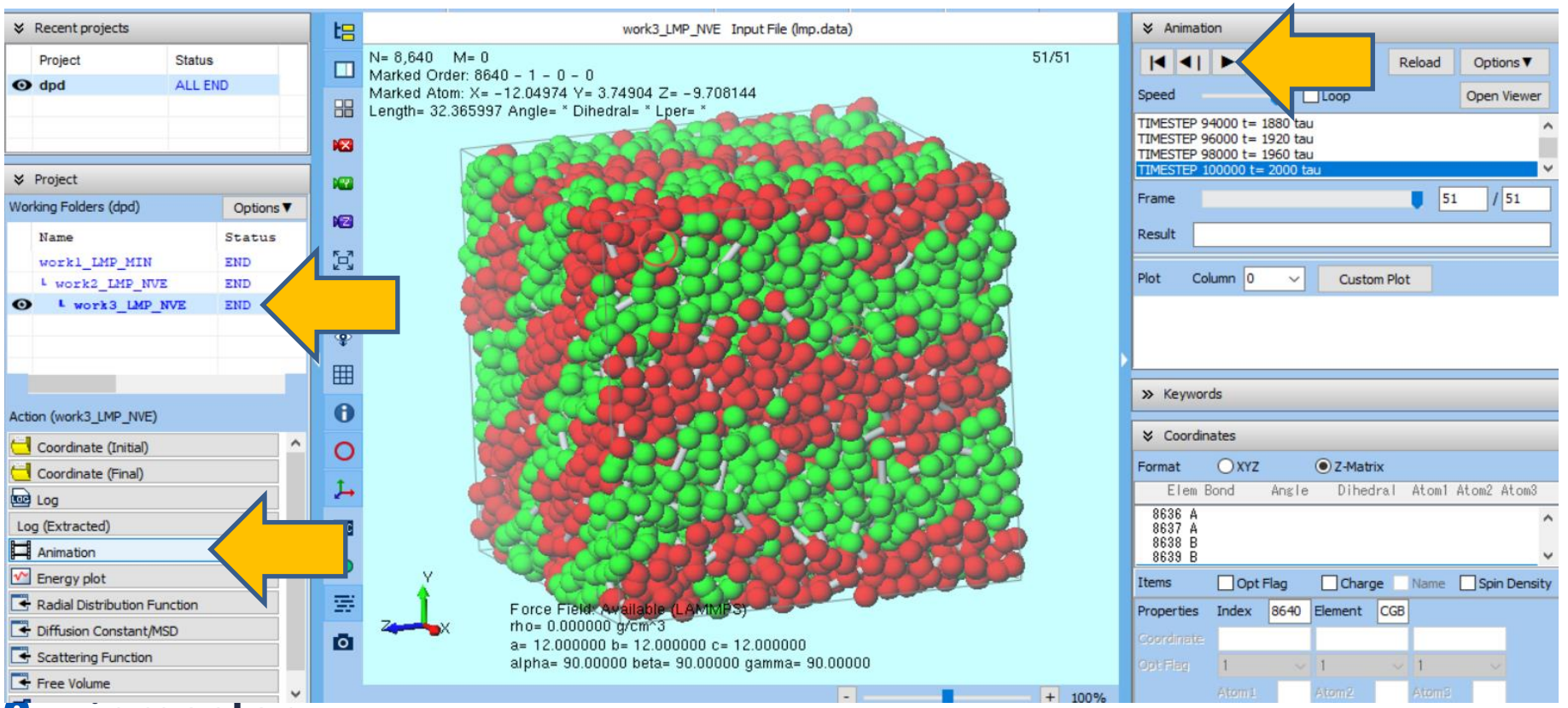
B. Execution of Calculate (Main Calculation)

A. Once **the status** of **the work folders** work1_LMP_MIN and work2_LMP_NVE changes to **END** or **END(-)**, click **(Workflow Setup)**.
B. If prompted with 'Do you want to continue from previous run?', click **Yes**.
C. Select work2_LMP_NVE and click **OK**.
D. Change **Preset** to 'DPD NVT Production'.
E. If you want to speed up the computation by reducing accuracy, change **Precision** of **1st job** to 'Low'.
F. Click **OK**, then set up **Job Setting** as needed and click **Run**.



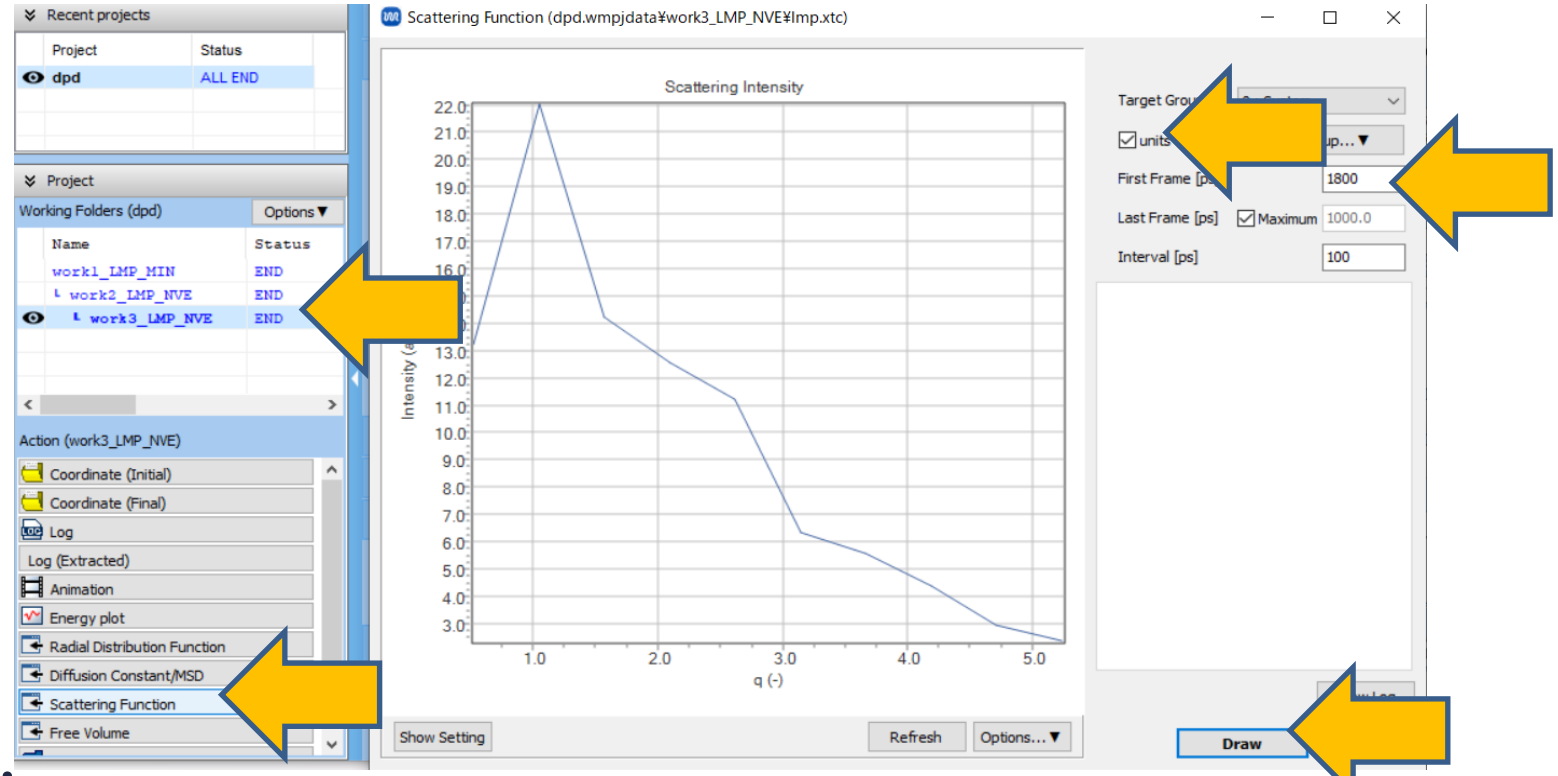
C. Result Analysis

A. Once **the status** of work3_LMP_NVE folder changes to **END** or **END(-)**, click work3_LMP_NVE and then click **Animation** in **Action**.
B. In Animation Panel, click ▶ **(Play/pause)** button to visualize the trajectory and observe how it converges to a lamellar phase.



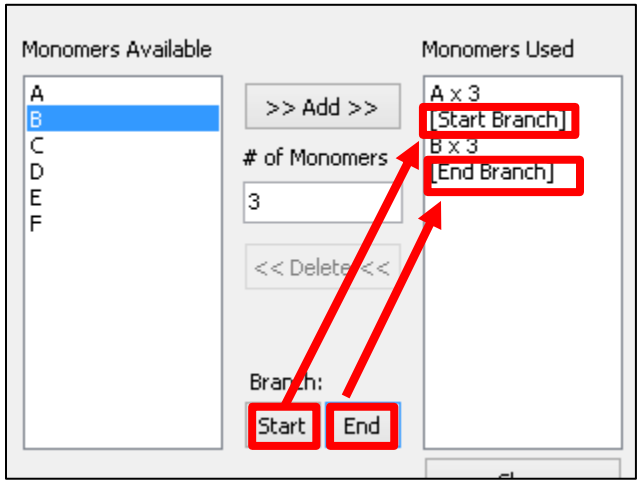
C. Result Analysis

A. Click **Scattering Function** in Action.
B. Check the box for **units = lj**, enter **1800** in **First Frame**, and click **Draw**. A peak can be observed near the repetition unit of the lamellar structure, with a wavenumber q approximately 1, and a corresponding length l around 6.42 (l = 2π/q).



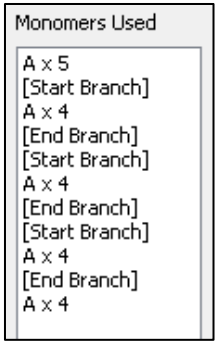
Supplement 1: Creating Branches

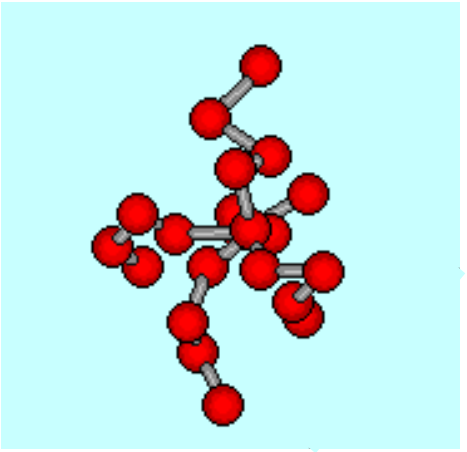
Branches can be introduced into molecules using **Start** and **End**.



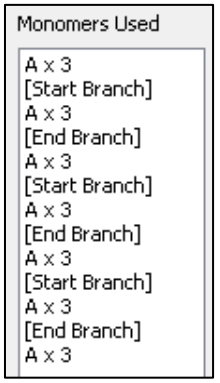
Start: Generates a branch from the particle immediately preceding it.
End: Ends the branch initiated by **Start**.

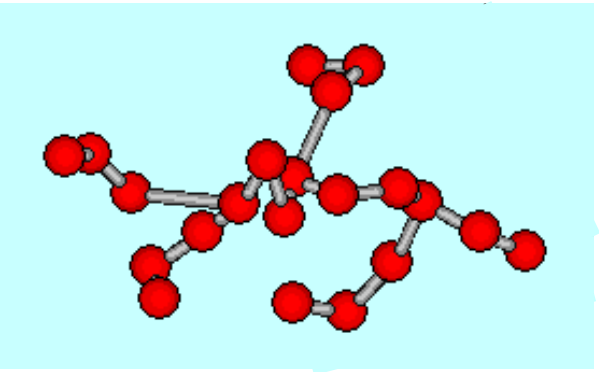
Example: Star-shaped Polymer





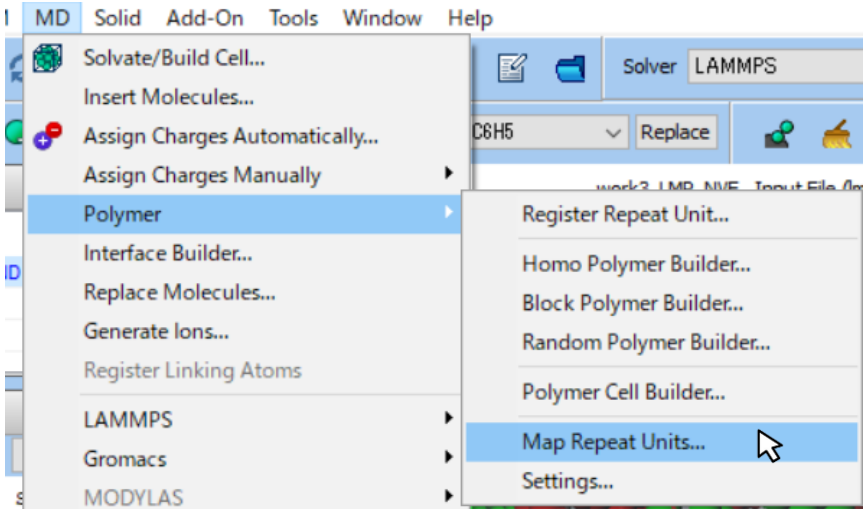
Comb Polymer

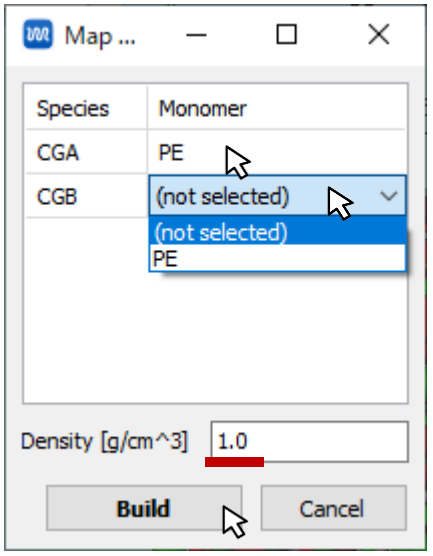




Supplement 2: Conversion to Classical MD Coordinates

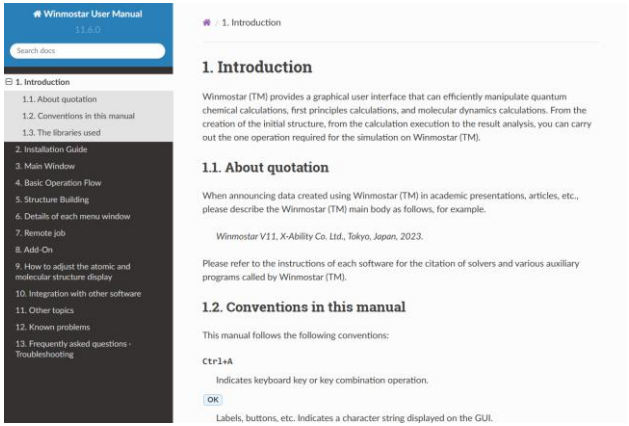
To obtain classical (all-atom) MD coordinates from particle configurations acquired with DPD:
Select **MD | Polymer | Map Repeat Units**.
In **Monomer** field, specify which monomer to assign to each particle, set **Density**, and then click **Build**.
Monomers must be registered under **MD | Polymer | Register Repeat Unit**.
(For more details, refer to 'Winmostar™ LAMMPS Tutorial on Glass Transition Temperature (Polymer)').
Note that the more particles there are, the longer the conversion process will take.





Finally

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



Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending Winmostar Introductory Training Session, Winmostar Basic Training Session, or Individual Training Session. (See page 2 for details.)
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