winmostar tutorial

LAMMPS
Kremer-Grest Model

V11.6.5

26 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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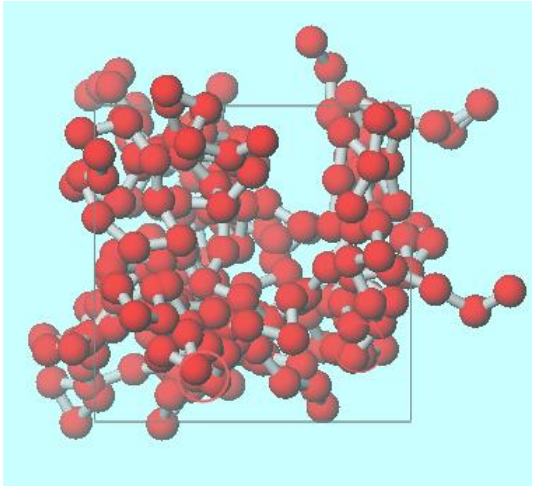
Overview

- This tutorial requires Winmostar V11 Professional Elite edition.
- This tutorial outlines the procedure for calculations using the Kremer-Grest model for polymer melts.

Reference: K. Kremer and G. S. Grest, J. Chem. Phys, 92, 5057, (1990).



Note :

- This guide is designed for quick operational verification with short chain lengths. To explore polymer characteristics more fully, such as entanglement, consider setting longer chain lengths (100 or more).
- Please note that the functionalities discussed in this book are not available in the Professional Economy or Student editions.

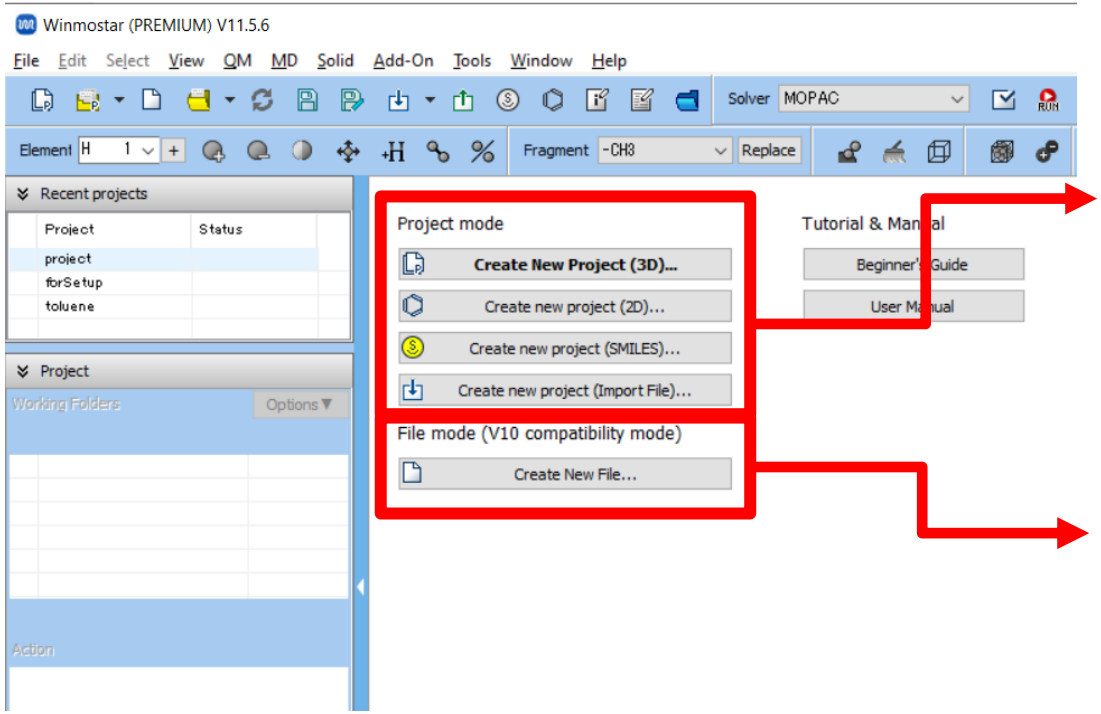
Preference of Operating Environment

- 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.

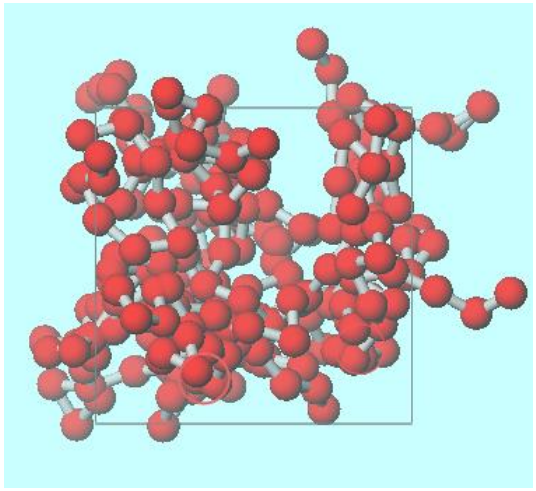
File Mode

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 'kgmd_lammps' 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. Enter '10' in **Enter Value** and click **OK**.
E. Click **Add** next to **Monomers Used**.
F. Enter '25' in **Enter Value** and click **OK**.
G. Click **Build**, enter '0.85' in **Enter Value**, and click **OK** to generate a randomly arranged polymer structure in Main Window.



B. Execution of Calculate (Equilibration)

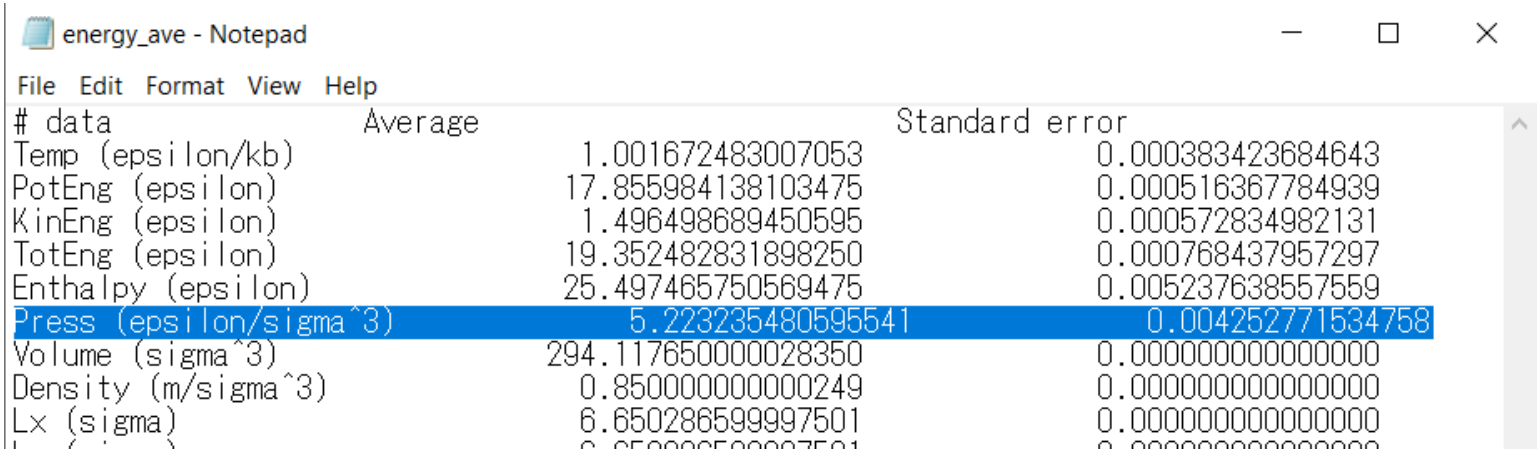
A. Select 'LAMMPS' from **Solver** and click  **(Workflow Setup)**.
B. If prompted with 'Some Molecules do not have charges. Do you want to assign charges now?', click **No**.
C. Check **Use parameters defined in external parameter file (for inorganic system, ReaxFF or DPD)** and click **Next**.
D. Check **Simulate using Kremer-Grest model** and click **OK**.
E. If 'Assigned force field parameters' appears, click **OK**.
F. Change **Preset** to 'Fluid/Amorphous/Crystal NVT Equilibration'.
G. Change **Temperature** for **2nd job** to '1'.
H. Change **Precision** for **1st job** and **2nd job** to 'High'.
I. Click **OK**, then set as appropriate in Job Setting window before clicking **Run**.

B. Execution of Calculate (Main Calculations)

A. Once **the status** of **the work folders** work1_LMP_MIN and work2_LMP_NVE has changed to **END** or **END(-)**, and then 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 'Fluid/Amorphous/Crystal NVT Production'.
E. Change **Temperature** to '1', **Simulation Time** to '7200', and **Precision** to 'High'.
F. Click **OK**, then set as appropriate in Job Setting window before clicking **Run**.

C. Result Analysis

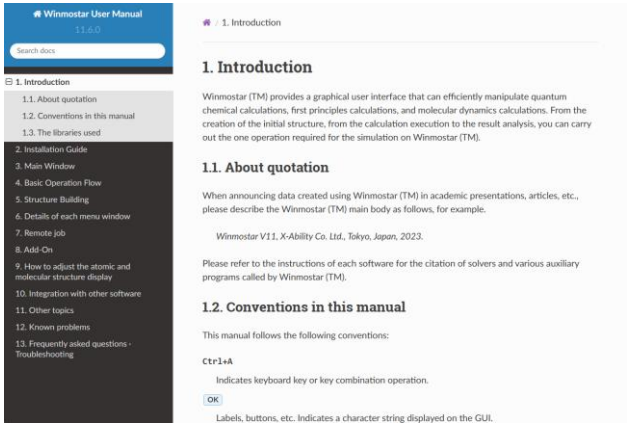
A. Once **the status** of **the work folder** work3_LMP_NVE changes to **END**or **END(-)**, click on work3_LMP_NVE and then click **Energy Plot** in **Action**.
B. Click **Calc Ave**, leave **First Frame** as the default value and click **OK**.
C. Check the pressure values displayed on the line for **Press**.



# data	Average	Standard error
Temp (epsilon/kb)	1.001672483007053	0.000383423684643
PotEng (epsilon)	17.855984138103475	0.000516367784939
KinEng (epsilon)	1.496498689450595	0.000572834982131
TotEng (epsilon)	19.352482831898250	0.000768437957297
Enthalpy (epsilon)	25.497465750569475	0.005237638557559
Press (epsilon/sigma^3)	5.223235480595541	0.00425277153475 8
Volume (sigma^3)	294.117650000028350	0.000000000000000
Density (m/sigma^3)	0.850000000000249	0.000000000000000
Lx (sigma)	6.650286599997501	0.000000000000000

Finally

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



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Scenes from Winmostar Training Session

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