

Winmostar tutorial
LAMMPS
Polymer modeling
V7.021

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2017/7/6

Contents

Configure

- I. Register a monomer
- II. Define a polymer
- III. Build a simulation cell
- IV. Execute simulations
 1. Equilibration
 2. Annealing calculation

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.
- The polymerization degree (the length of chain) , and rate of temperature reduction (and/or incalescence) also affect the simulation results.
- For the purpose of this tutorial, we will not show complete equilibration steps for polymers.

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.

2. Installation Guides for Solvers

For Windows

[Cygwin_wm Installation Guide](#) ※Gromacs/Amber Window Build Package(Cygwin)

(For Experts)Gromacs/Amber Build with Cygwin ※we recommend you to use the precompiled package

[GAMESS Installation Guide](#)

[NWChem Installation Guide](#) ※Window Build Package

(For Experts)NWChem Build with MinGW ※we recommend you to use the precompiled package.

[LAMMPS Installation Guide](#)

Installation guide for LAMMPS on Windows

Feb. 6, 2017

1. Getting LAMMPS

① Access to <http://rpm.lammps.org/windows.html>

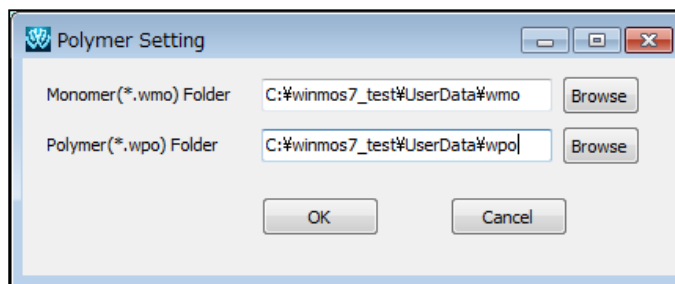
Visit [\[32-bit Windows download area\]](#) or [\[64-bit Windows download area\]](#).

LAMMPS-ICMS Windows Installer Repository

This repository is hosting pre-compiled Windows installers of the LAMMPS molecular dynamics simulation software package. The binaries are built semi-automatically with MinGW64 Linux to Windows cross compilers using up-to-date snapshots of the LAMMPS-ICMS repository hosted at the [Institute for Computational Molecular Science](#) at Temple University. The LAMMPS binaries contain all optional packages included in the source distribution except GPU (because it is not GPU compatible). GPU-CUDA (CUDA does not support cross compilation), KOKOS and USER-INTL (do not support cross-compilation with GCC), USER-EXTL (requires external binary libraries) (requires to bundle a full Python runtime), USER-CMAKE (only useful when linking to a 3rd software), USER-OPENCL (requires external library), USER-OPENCL (requires to bundle a full Python runtime), USER-CMAKE (only useful when linking to a 3rd software), USER-OPENCL (requires external library), USER-OPENCL (requires to bundle a full Python runtime), USER-CMAKE (only useful when linking to a 3rd software), USER-OPENCL (requires external library), USER-OPENCL (requires to bundle a full Python runtime).

Some Notes on GPU Support
These Windows binaries include (experimentally on Windows) GPU acceleration via the GPU package. This is achieved through compiling the GPU package in OpenCL mode and linking to an OpenCL (v2.2) compatible ICD loader. This means the executables do not contain any vendor provided code and should be compatible with GPUs from both AMD and NVIDIA. The GPU package has been compiled for mixed precision computation and is currently somewhat tuned for Nvidia (Fermi generation) GPUs. It does not yet work with OpenCL drivers for GPUs (like those included in the Intel and AMD OpenCL ICDs).

- Configuration of polymer tool
Click **MD | Polymer | Setting**. Set folders for monomer files (extension **.wmo**) and polymer files (extension **.wpo**) as need.



I. Register a monomer

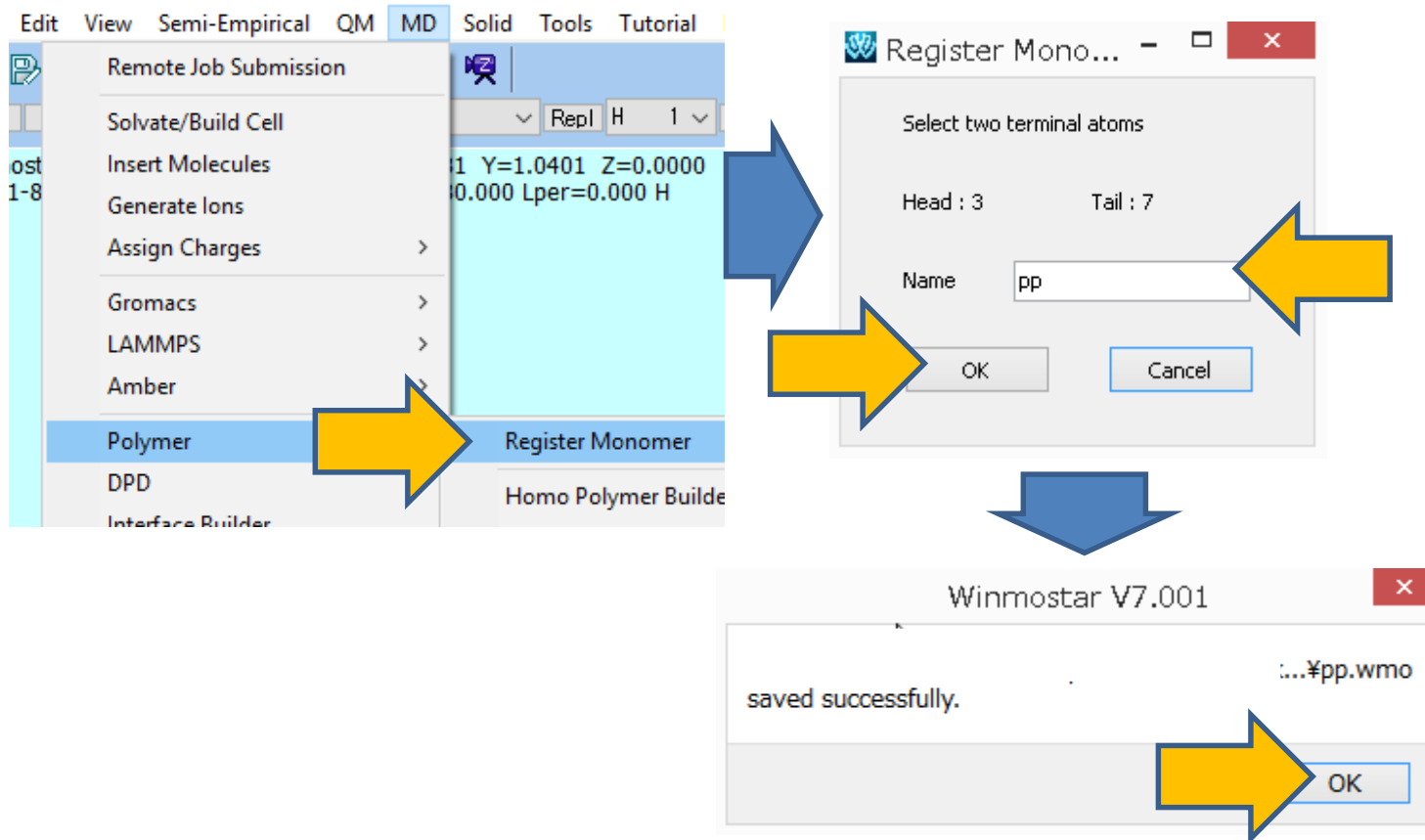
This tutorial will describe how to model a polypropylene.

1. Model a monomer of polypropylene (propane, C_3H_8) on the main window.
2. Click **MD | Assign Charges | By Acptype | Execute**.
3. Uncheck **User Charge** to hide charge information.
4. Click two hydrogens to be the end points of the monomer.



I. Register a monomer

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



II. Define a polymer

1. Click **MD | Polymer | Homo Polymer Builder**.
2. Set **Polymer Name** to **pp15**, **Polymerization Degree** to **15**, Select **pp** in **Monomer List**
3. Click **Build**.
4. Click **Close**.

The image illustrates the process of defining a polymer in the software. It shows the 'MD' menu with 'Homo Polymer Builder' selected. The 'Homo Polymer Builder' dialog box is open, showing the following settings:

- Polymer Name:** pp15
- Polymerization Degree:** 15
- Monomer List:** pp
- Tacticity:** Isotactic (selected)
- Head/Tail Configuration:** Head to Tail (selected)
- Racemo Ratio:** 0

The 'Build' button is highlighted with a yellow arrow. A 'Winmostar V7.001' dialog box is shown below, indicating that the file '..¥pp15.wpo' was saved successfully, and the 'OK' button is highlighted with a yellow arrow.

III. Build a simulation cell

1. Click **MD | Polymer | Polymer Cell Builder**.
2. Set **Polymers Available** to **pp15**, **Number** to **30**, and click **>> Add >>**.
3. Click **Build**. Save as **pp15_30.mol2**.

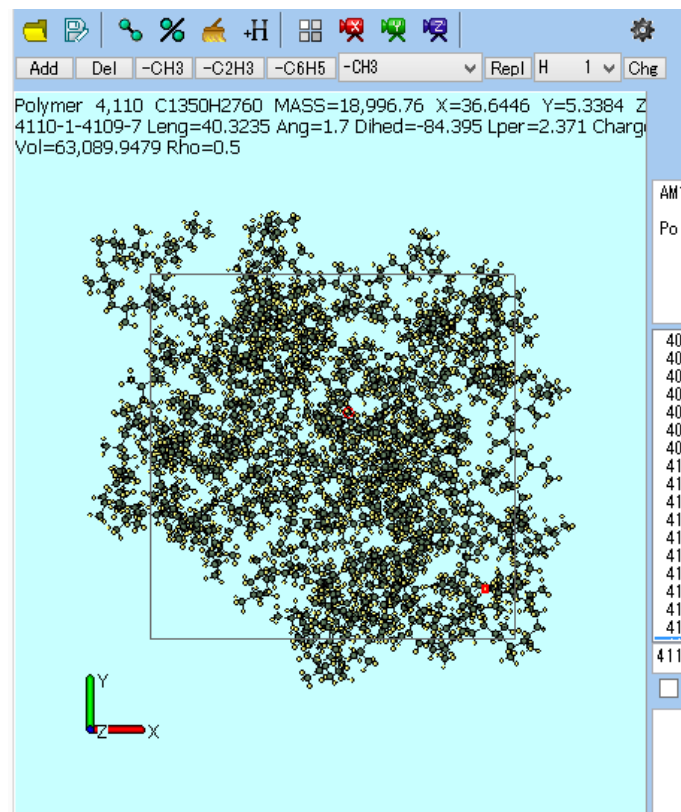
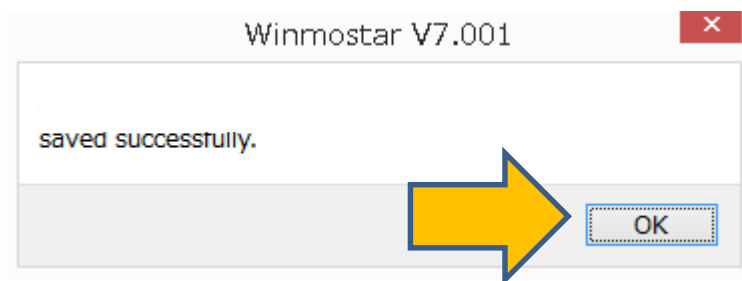
The screenshot illustrates the software interface for building a simulation cell. The 'MD' menu is open, and the 'Polymer Cell Builder' option is selected. The 'Polymer Cell Builder' dialog box is shown with the following configuration:

- Box Configuration:**
 - Density [g/cm³]: 0.5
 - X-Axis Length [Å]: 39.8095
 - Y-Axis Length [Å]: 39.8095
 - Z-Axis Length [Å]: 39.8095
 - Cubic Cell
- Periodic Boundary Condition:**
 - X
 - Y
 - Z
- Polymers Available:**
 - pp15 (selected)
- Polymers Used:**

Name	Number
pp15	30
- Number:** 30
- Buttons:** >> Add >>, << Delete <<, Display, Delete, Build, Close

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**.



IV. Execute simulations

1. Equilibration (*NPT*, high pressure)

1. Click **MD | LAMMPS | Keywords Setup**.
2. On **Basic** tab, uncheck **Generate Velocity**, set **Ensemble** to **npt**, **Pressure** to **200**, then click **OK**.
3. Click **MD | LAMMPS | Start LAMMPS**.

LAMMPS Setup

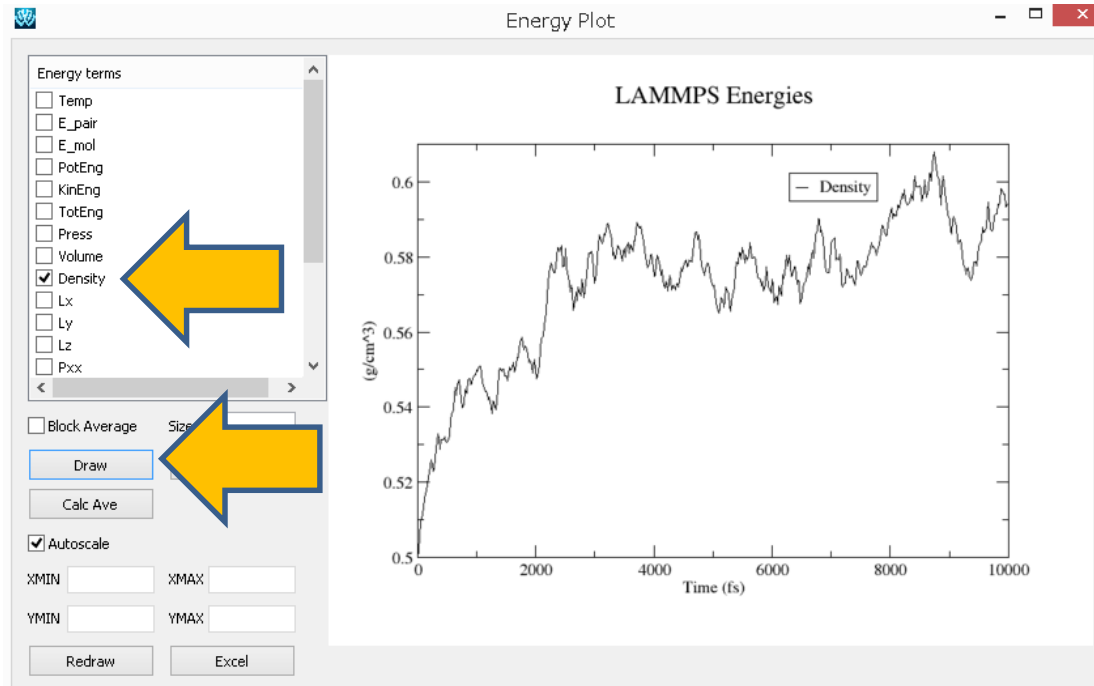
Basic | Advance | Output | Interaction | Non-equilibrium (1) | Non-equilibrium (2) | Options | Force Field

<input checked="" type="checkbox"/> Extending Simulation	Time Step [fs]	2.0	<input type="checkbox"/> Generate Velocity
Units: real	# of Time Steps	5000	Pressure Control: iso
Atom Style: full	Ensemble	npt	
Pair Style: lj/cut/coul/cut	Temperature [K]	550	
Potential File	Pressure [atm]	200	

IV. Execute simulations

1. Equilibration (*NPT*, high pressure)

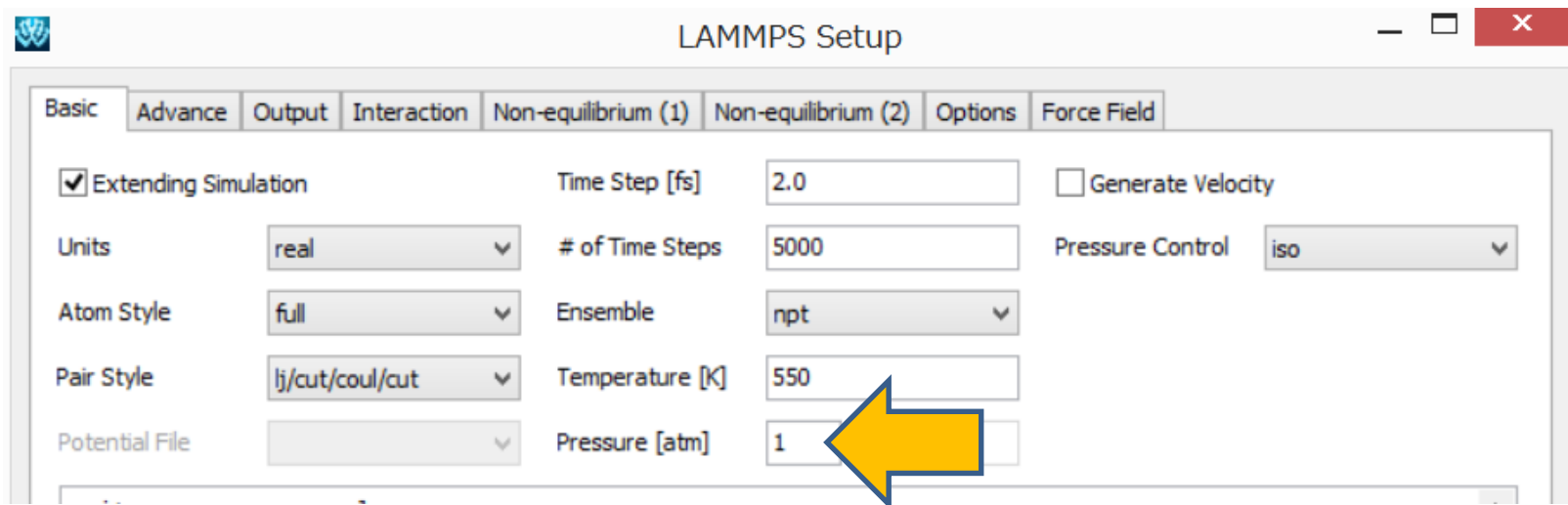
1. Click **MD | LAMMPS | Energy plot**. Open the default file.
2. On **Energy terms**, check **Density**, then click **Draw**.
3. The graph will show convergence of density values to a constant (although the convergence may be difficult to see with the given conditions, it serves the purpose of this tutorial).



IV. Execute simulations

1. Equilibration (*NPT*, low pressure)

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

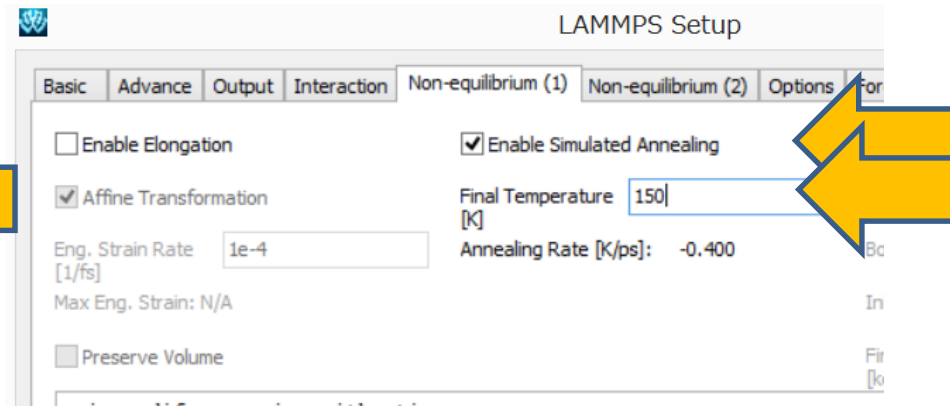
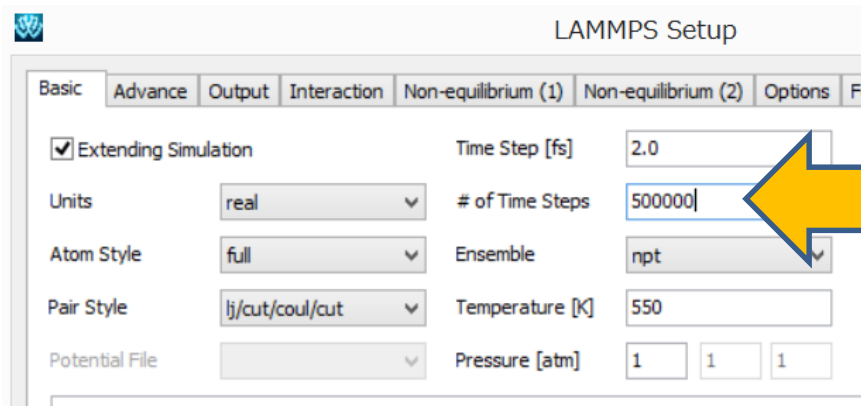


IV. Execute simulations

2. Annealing calculation

Next, use simulated annealing in order to calculate glass-transition temperature.

1. Click **MD | LAMMPS | Keywords Setup.**
2. On **Basic** tab, set **# of Time Steps** to **500000**
(set smaller value if you want to reduce calculation time.)
3. On **Non-equilibrium** tab, check **Enable Simulated Annealing**,
Set **Final Temperature** to **150**, then click **OK.**
4. Click **MD | LAMMPS | Start LAMMPS.**



IV. Execute simulations

2. Annealing calculation

1. Click **MD | LAMMPS | Energy plot**. Then open the file selected by default.
2. On **Energy Terms**, check **Temp** and **Density**, and click **Draw**.
3. Click **Excel**.

In the exported CSV file, plot column B on the X-axis and Column C on the Y-axis to get a Temperature-Specific Volume curve.

Estimations of glass transition temperatures can be found on inflection points (at around 280 – 300K) on this curve for a given distribution fitting.

