

Winmostar tutorial

LAMMPS

Dissipative Particle Dynamics (DPD)

V7.021

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Contents

Configure

- I. Build a simulation cell
- II. Potential setting
- III. LAMMPS setting
- IV. Execute simulations
- V. Analyze

Appendix 1: Insert branches

Appendix 2: Convert to coordinates of classical MD

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 Instllation Guide ※Gromacs Amber Window Build Package(Cygwin)
(For Experts)Gromacs/Amber Build with Cygwin ※we recommend you to use the precompiled p

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

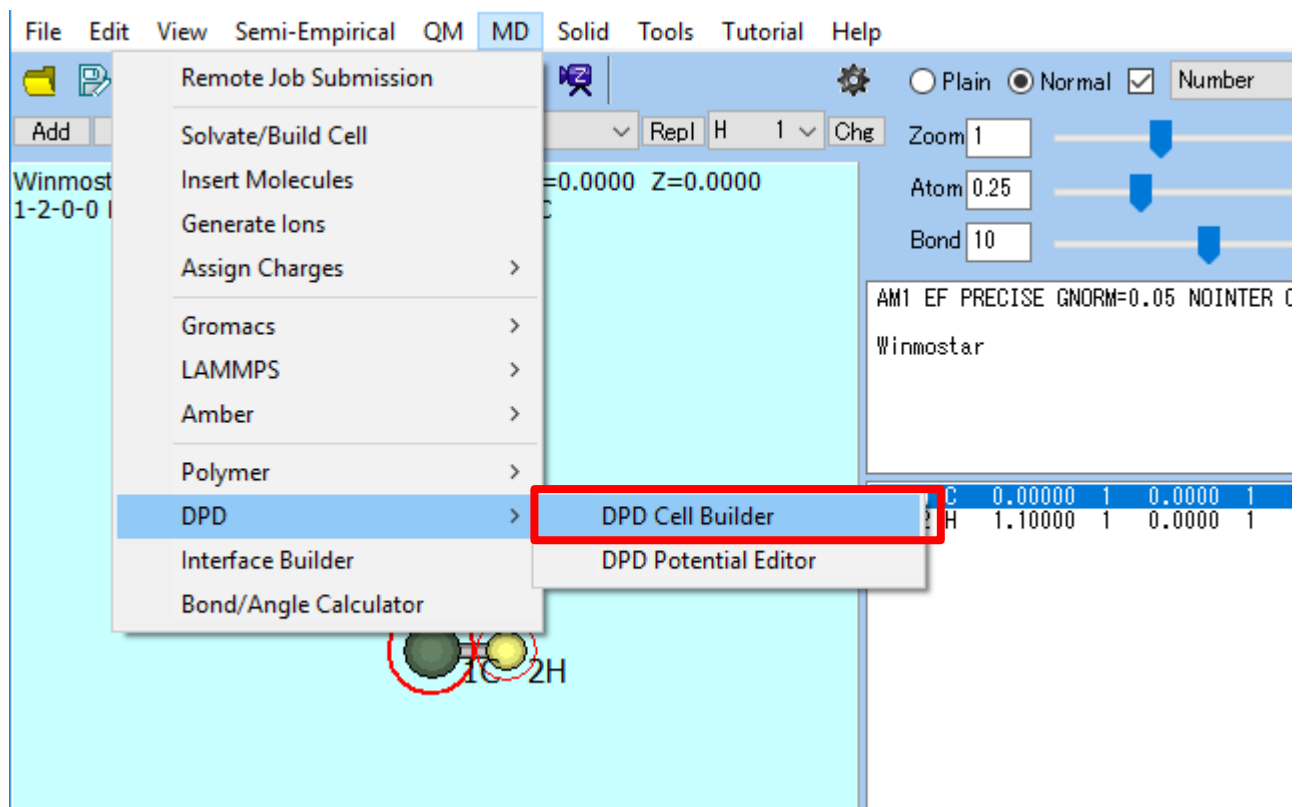
This repository is hosting pre-compiled windows installers of the LAMMPS molecular dynamics simulation software package. The binaries are built semi-automatically with MinGW64 Linux to Windows cross compilers using up-to-date versions of the LAMMPS-ICMS repository hosted at the [url for Computational Molecular Science](#) at Temple University. The LAMMPS binaries contain all optional packages included in the source distribution except [XCU](#) (license is not GPL compatible), [GROMACS](#) (includes does not support cross compilation), [KOMPACT](#), and [LIGANDS](#). (do not support cross-compilation with XCU, LIGANDS) (requires external library) [PSTools](#) (requires to bundle a full Python runtime), [LIGANDS](#) (only useful when linking to a GM software), [LIGANDS](#) (requires external library), [SEAL](#) (implemented in the LIGANDS package which is included). The [small](#) executable additionally does not contain the [LIGANDS](#) and [LIGANDS](#) packages, since those require API-0 functions, which are not available without linking to a real API library.

Some Notes on GPU Support

These Windows binaries include experimental on Windows GPU acceleration via the GPU package. This is achieved through compiling the GPU package in OpenCL mode and linking to an OpenCL 1.1 compatible ICD loader. This means the executables do not contain any vendor provider 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 SDKs.

I. Build a simulation cell

Click **MD | DPD | DPD Cell Builder**.



I. Build a simulation cell

1. Click **A** in **Monomers Available** box, set **# of Monomers** to **3**, then click **Add**.
2. Click **B**, set **# of Monomers** to **3**, then click **Add**.

The screenshot shows a software interface for building a simulation cell. It is divided into several sections:

- Monomers Available:** A list box containing letters A through F. Item B is highlighted in blue. This section is enclosed in a red rectangular box.
- Monomers Used:** A list box containing "A x 3" and "B x 3".
- Monomers Available Controls:** A ">> Add >>" button is highlighted with a red box. Below it, a "# of Monomers" label is followed by a text input field containing the number "3". This entire control area is also enclosed in a red rectangular box.
- Monomers Used Controls:** A "<< Delete <<" button is located below the Monomers Used list box.
- Monomers Used Controls:** A "Clear" button is located below the Monomers Used list box.
- Polymers:** A section on the right with a ">> Add >>" button, a "# of Polymers" label, and an empty text input field.
- Polymers:** A "Density" label is located below the Polymers section.

An orange callout box with a pointer to the "# of Monomers" input field contains the text: "Click **Add** on **# of Monomers**".

I. Build a simulation cell

Set # of Polymers to 1440. Click Add.

Monomers Available

A
B
C
D
E
F

>> Add >>

of Monomers

3

<< Delete <<

Monomers Used

A x 3
B x 3

>> Add >>

of Polymers

1440

<< Delete <<

Clear

Polymers Used

Density 5

Build

Close

I. Build a simulation cell

1. Set **Density** to **5** (this unit has no dimension) , and click **Build**.
2. Click **Close**.

The simulation cell will be displayed here.

DPD Cell Builder

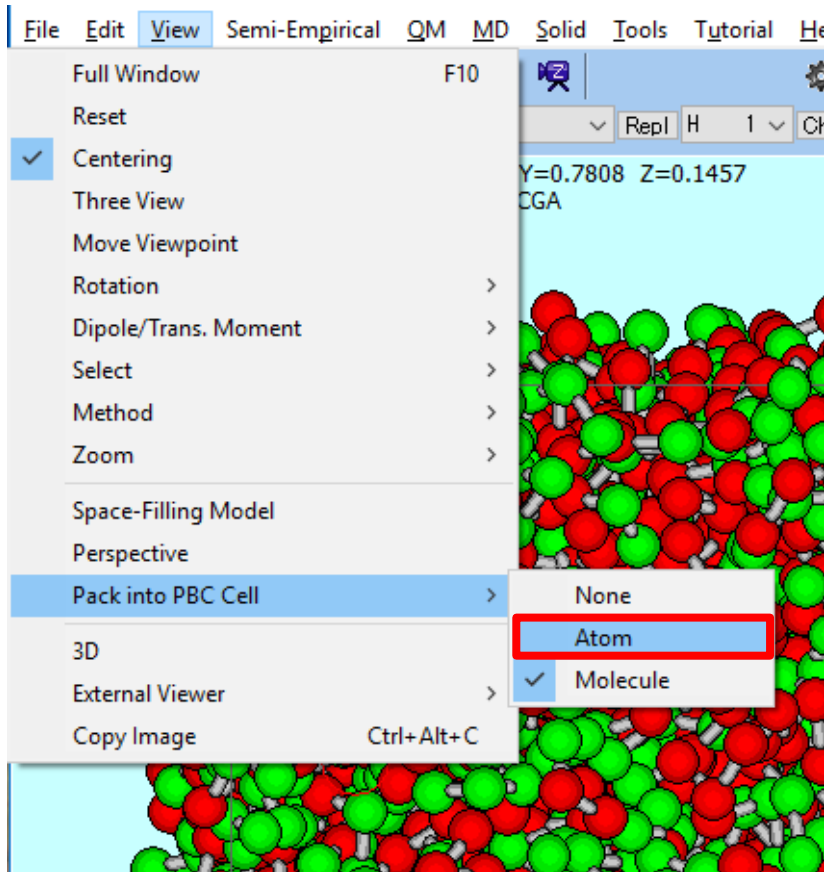
Monomers Available	Monomers Used	Polymers Used
A	A x 3	AAABBB x 1440
B	B x 3	
C		
D		
E		
F		

density 5

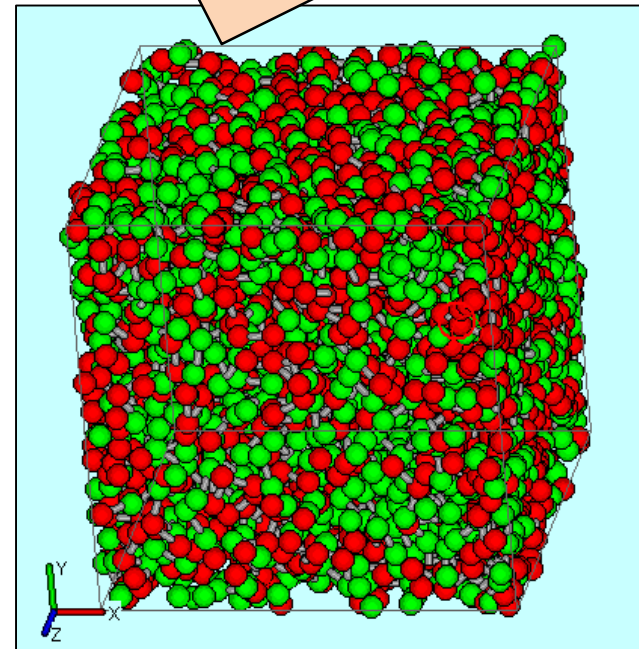
Build

I. Build a simulation cell

For the visualization, click **View | Pack into PBC cell | Atom**.

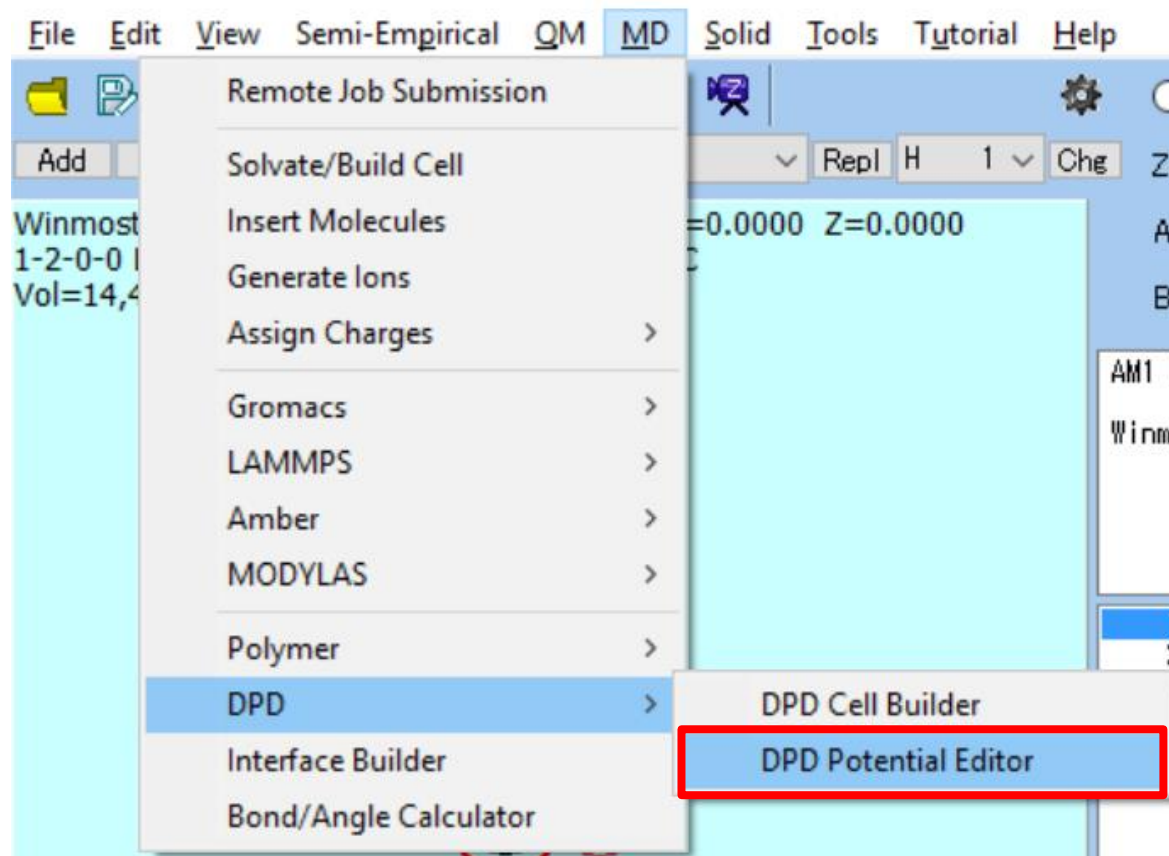


Particles crossing periodic boundaries are carried over to the other side.



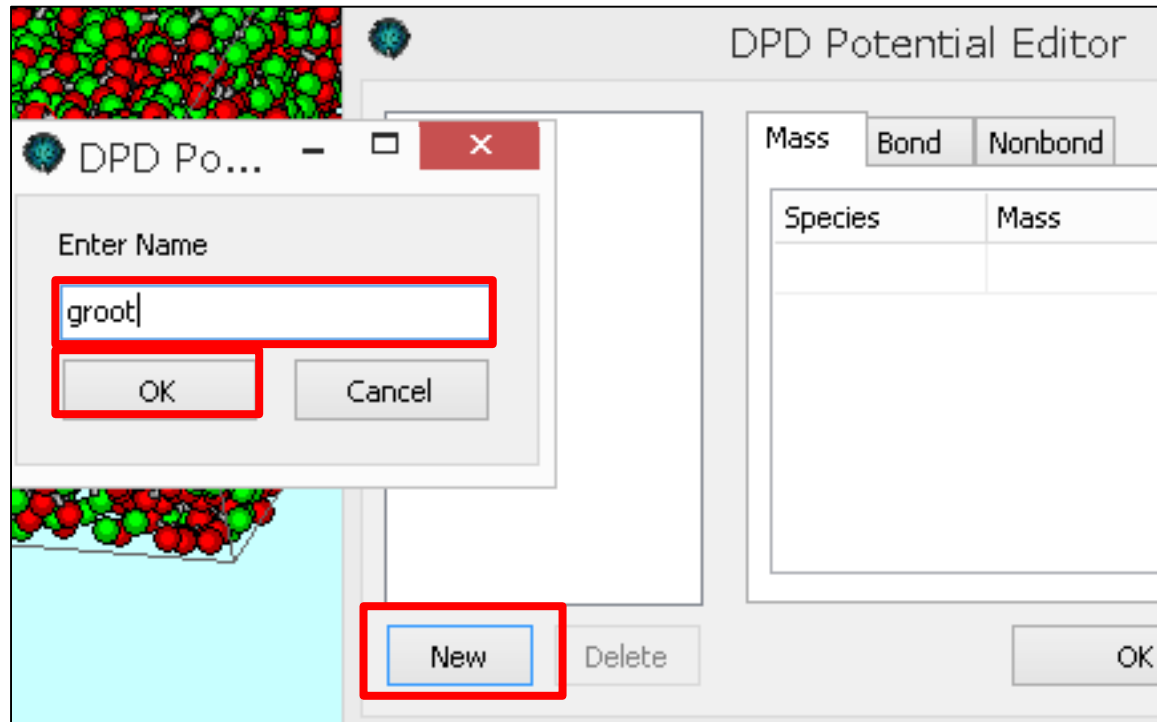
II. Potential setting

Click **MD | DPD | DPD potential editor.**



II. Potential setting

1. Click **New** to create a new potential file.
2. Set **Enter name** to **groot**, click **OK**.



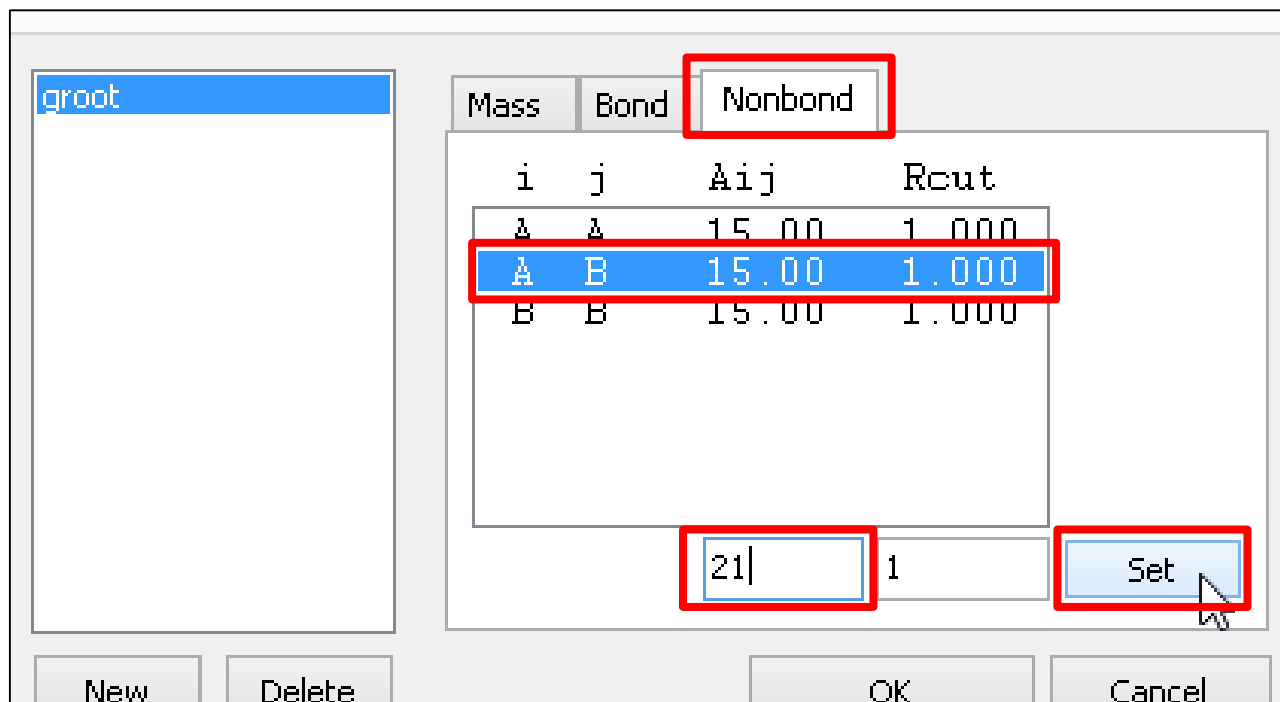
II. Potential setting

1. Click on **Nonbond** tab, click the row of **A B 15.00 1.00**.
2. Set the bottom textbox to 21, click **Set**.

(the unit of both A_{ij} and R_{cut} has no dimension.)

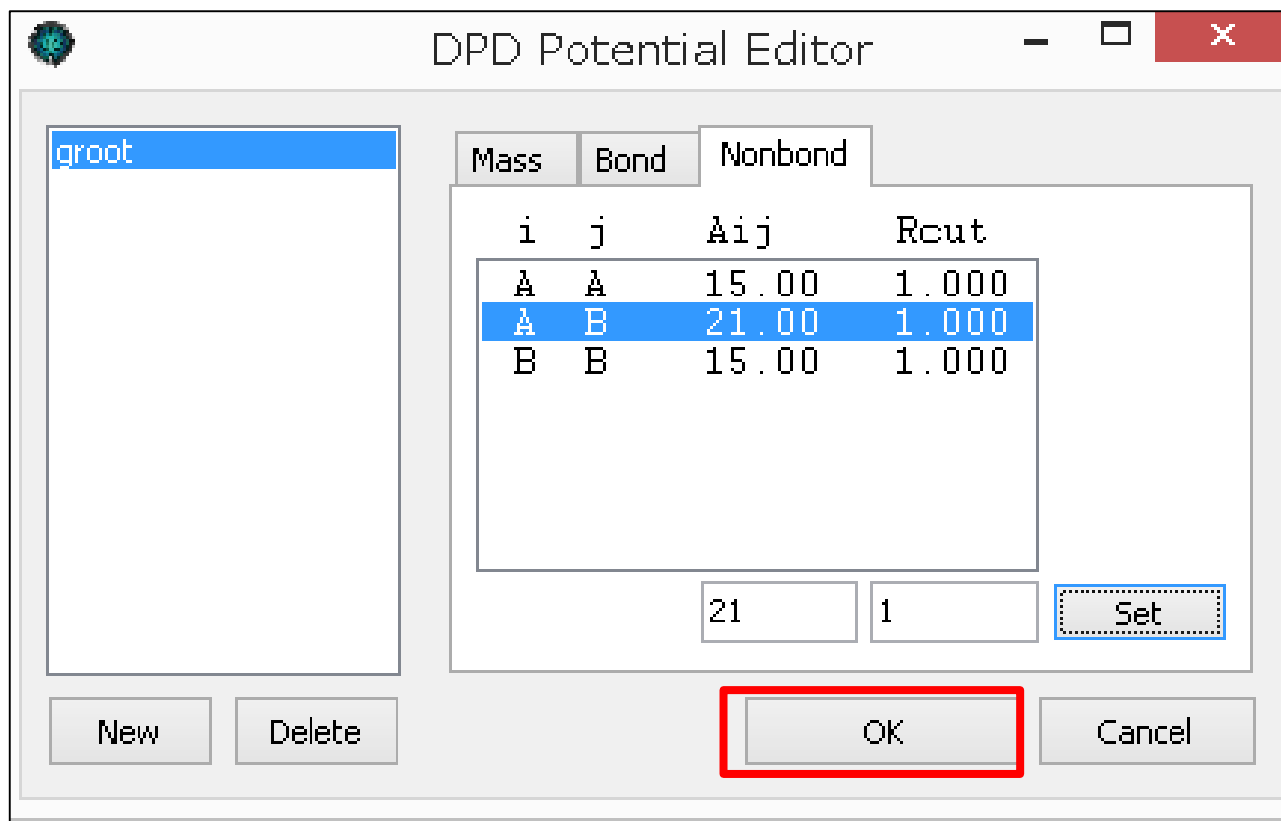
There are several ways to determine A_{ij} for any monomers.

For example, see Winmostar Gromacs tutorial “Solubility/ χ /DPD Parameters”



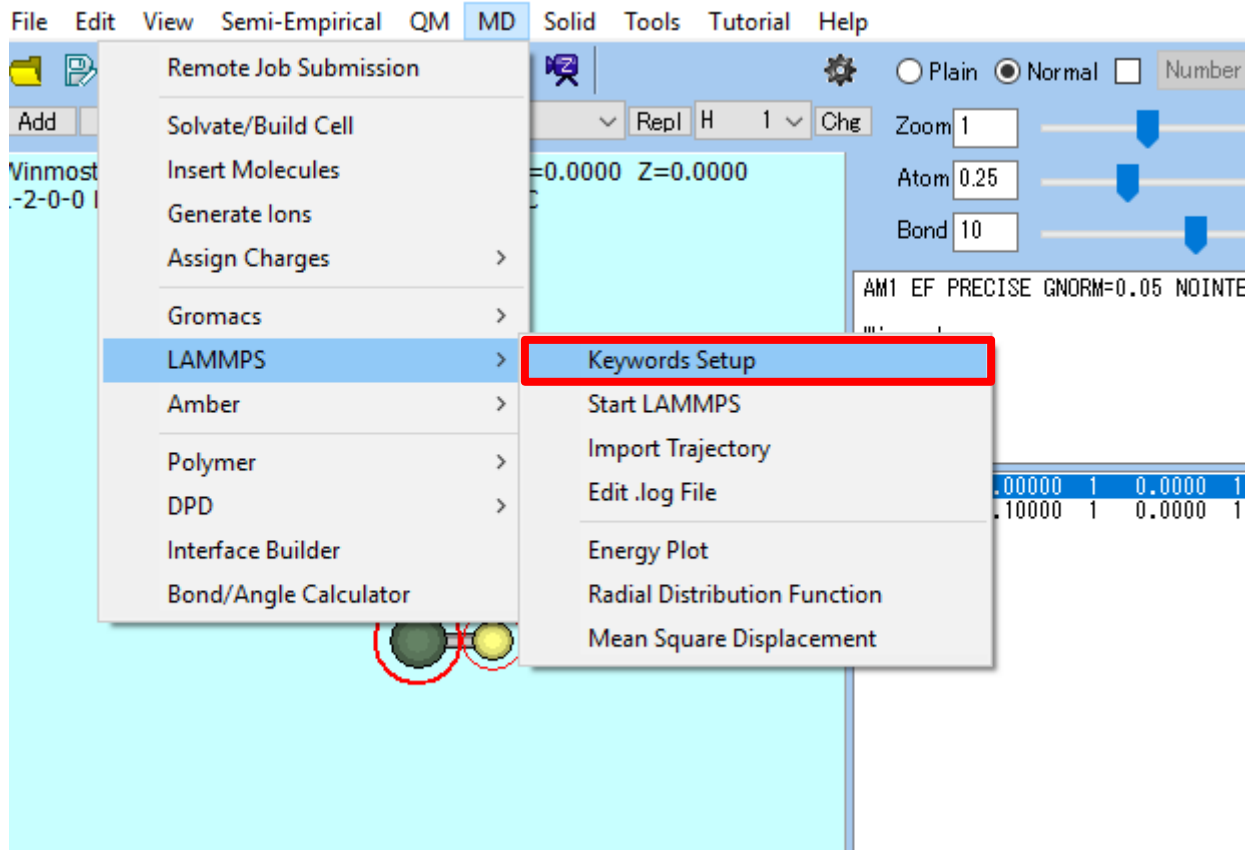
II. Potential setting

Click **OK** to Potential Editor.



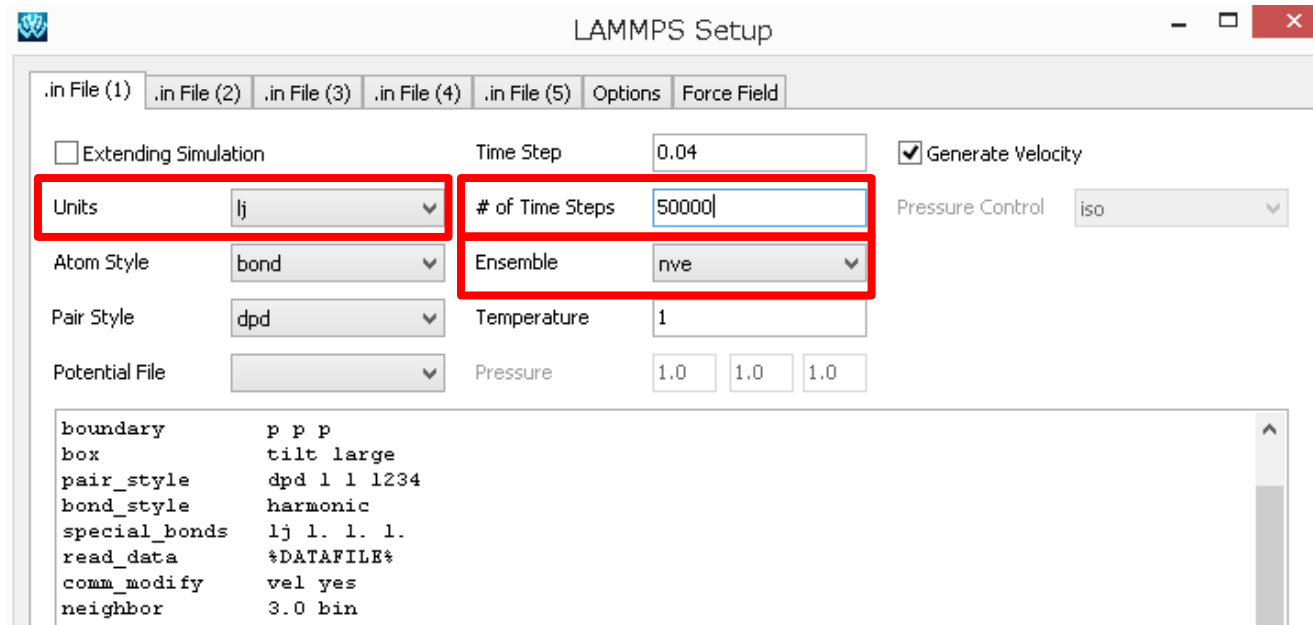
III. LAMMPS setting

Click **MD | LAMMPS | Keywords Setup.**



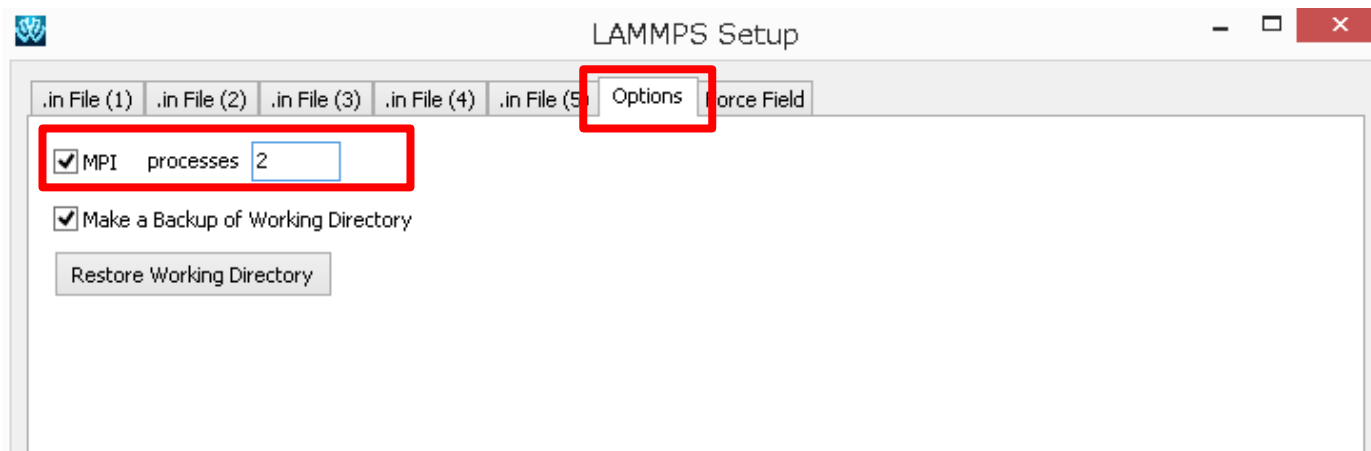
III. LAMMPS setting

1. Set **Units** to **LJ**, **Ensemble** to **nve**, **# of Time Steps** to **50,000**.
2. Click **OK**. (Temperature, pressure, and time parameters are dimensionless)



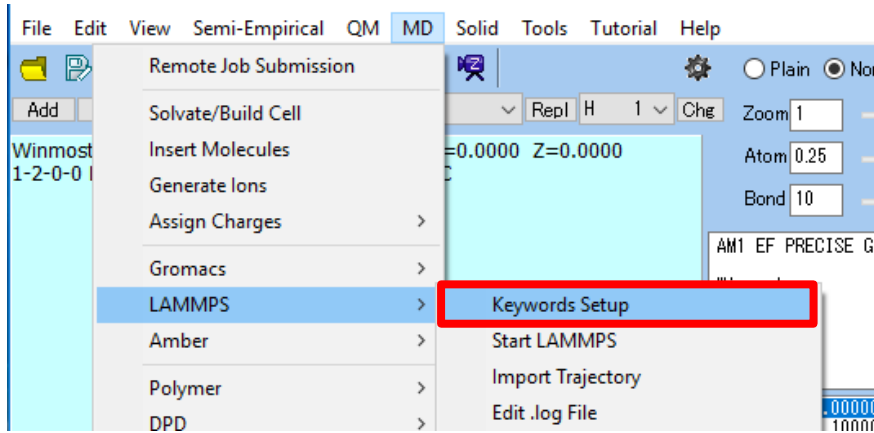
III. LAMMPS setting

Set MPI processes in the Option tab as needed.

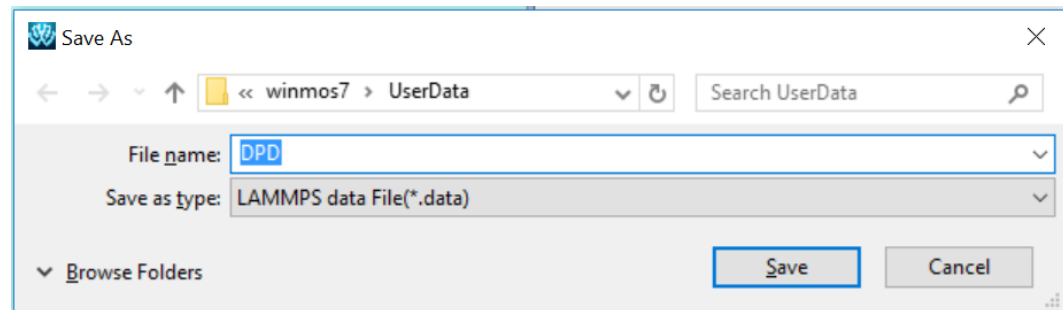


IV. Execute simulations

Click **MD | LAMMPS | Start LAMMPS**.



Set File Name to **DPD**. Click **Save**.



V. Analyze

Click **MD | LAMMPS | Import Trajectory**. Open the file by default.

The screenshot shows the X-Ability software interface. The 'MD' menu is open, and the 'LAMMPS' sub-menu is selected. The 'Import Trajectory' option is highlighted with a red box. The main window displays a 3D molecular model of a lamellar phase, consisting of red and green spheres arranged in a layered structure. A callout box points to the model with the text 'Lamellar phase appears due to microphase separation'. The right sidebar shows simulation parameters and a table of coordinates.

Atom 0.25
Bond 10

undo <-->
AM1 EF PRECISE GNORM=0.05 NOINT

Winmostar

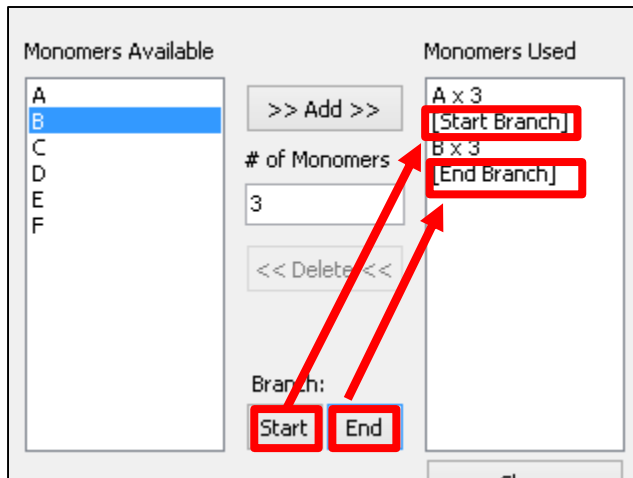
834	CG	0.27888	1	60.4903
835	CG	0.89821	1	118.0553
836	CG	0.88132	1	129.2125
837	CG	0.68401	1	127.3692
838	CG	0.81672	1	96.6628
839	CG	0.13273	1	38.8179
840	CG	0.88708	1	153.1635
841	CG	0.74628	1	59.1998
842	CG	0.86813	1	52.7975
843	CG	0.30447	1	87.2366
844	CG	0.56977	1	72.464
845	CG	1	1	104.5355
846	CG	1	1	104.8269
847	CG	0.44378	1	112.9228
848	CG	0.75777	1	102.7709
849	CG	0.60808	1	125.2467
850	CG	0.27888	1	147.7501
834	CG	0.278886	1	60.4903

Debug 1 1

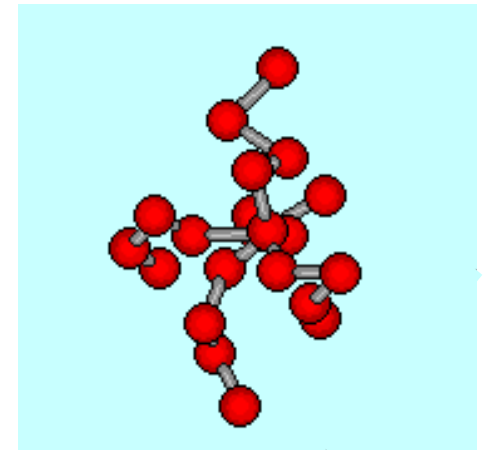
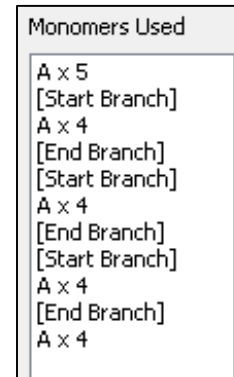
Lamellar phase appears due to microphase separation

Appendix1 : Insert branches

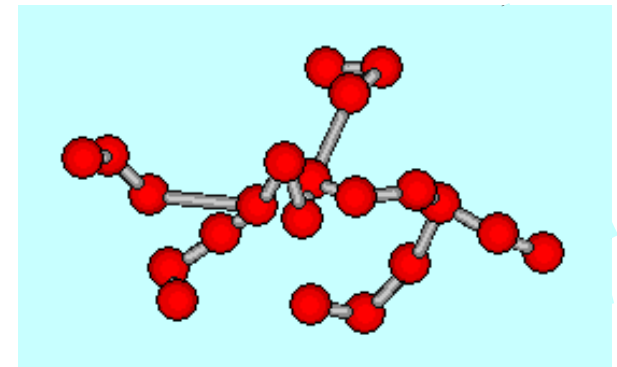
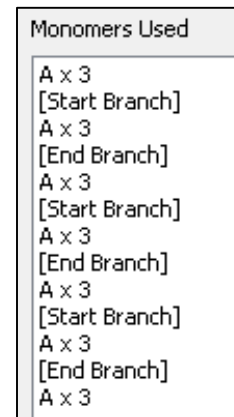
Click **Start** or **End** to insert branches.



e.g.: Star-shaped Polymer



e.g.: Comb-shaped polymer



[Start]: Branching begins from preceding particle

[End]: Ends branching initiated by [Start]

Appendix2: Converting to classical MD coordinates

See following instructions when converting coordinates of DPD to coordinates of classical (all atoms) MD.

1. Click **MD | Polymer | Map monomers**.
2. Set the map of monomers to each particle in the **Monomer** field, input **Density**, then click **Build**.
3. Register the monomer via **MD | Polymer | Register Monomer**
(See Winmostar LAMMPS tutorial: Polymer modeling)

Please note, conversion processing time depends on the number of particles.

