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Winmostar tutorial

LAMMPS

Dissipative Particle Dynamics（DPD）

V7.021

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Contents

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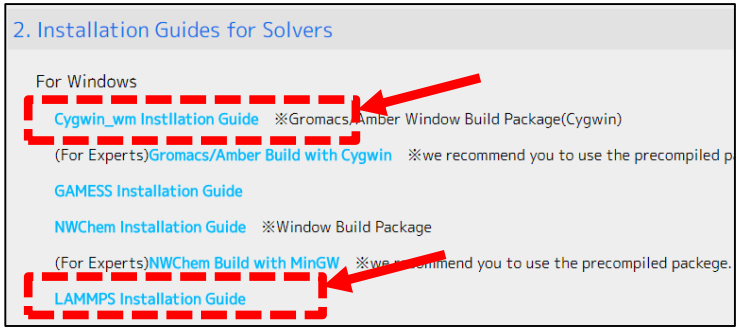
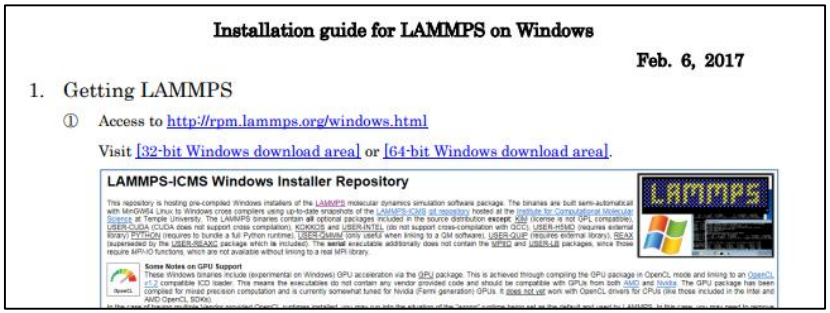
Configure

Set up LAMMPS and Cygwin in advance.

Set up LAMMPS by following **LAMMPS Installation Guide** located at https://winmostar.com/en/manual_en.html.





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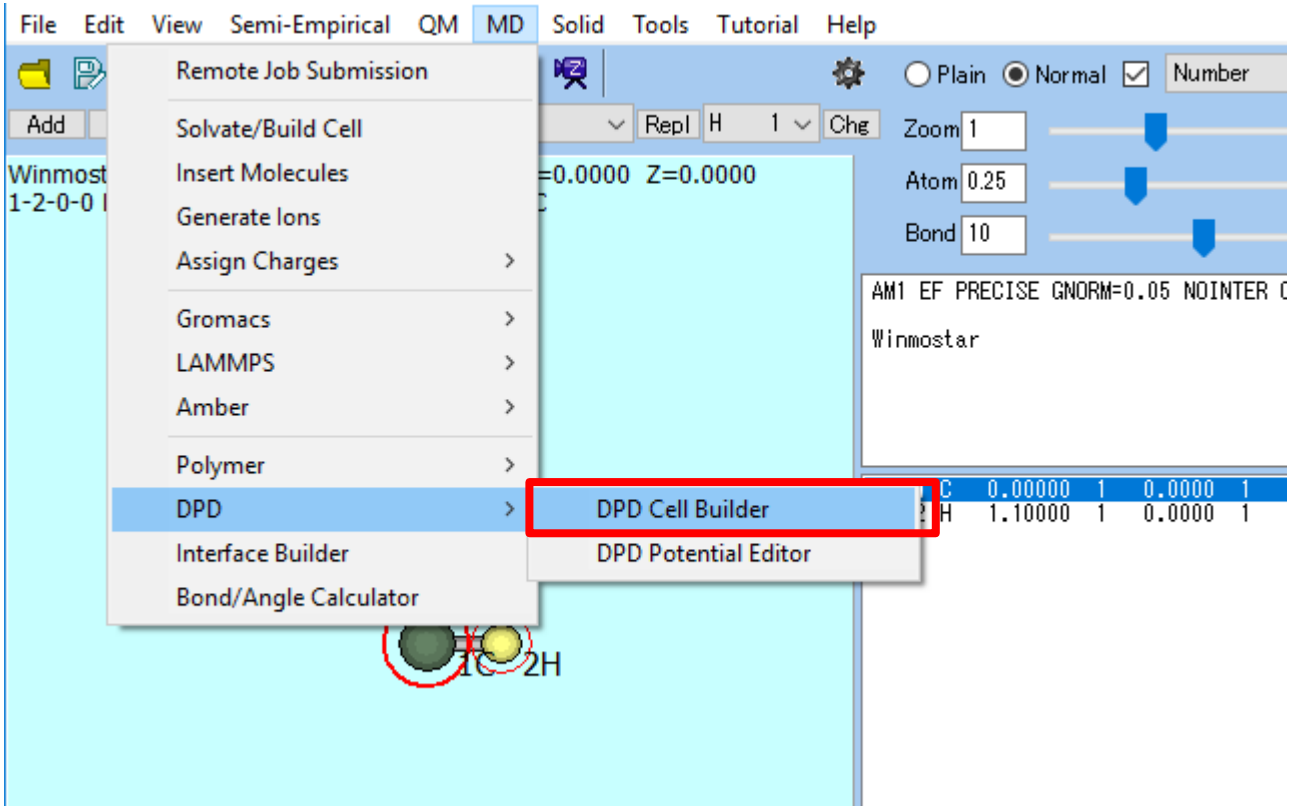
I. Build a simulation cell

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



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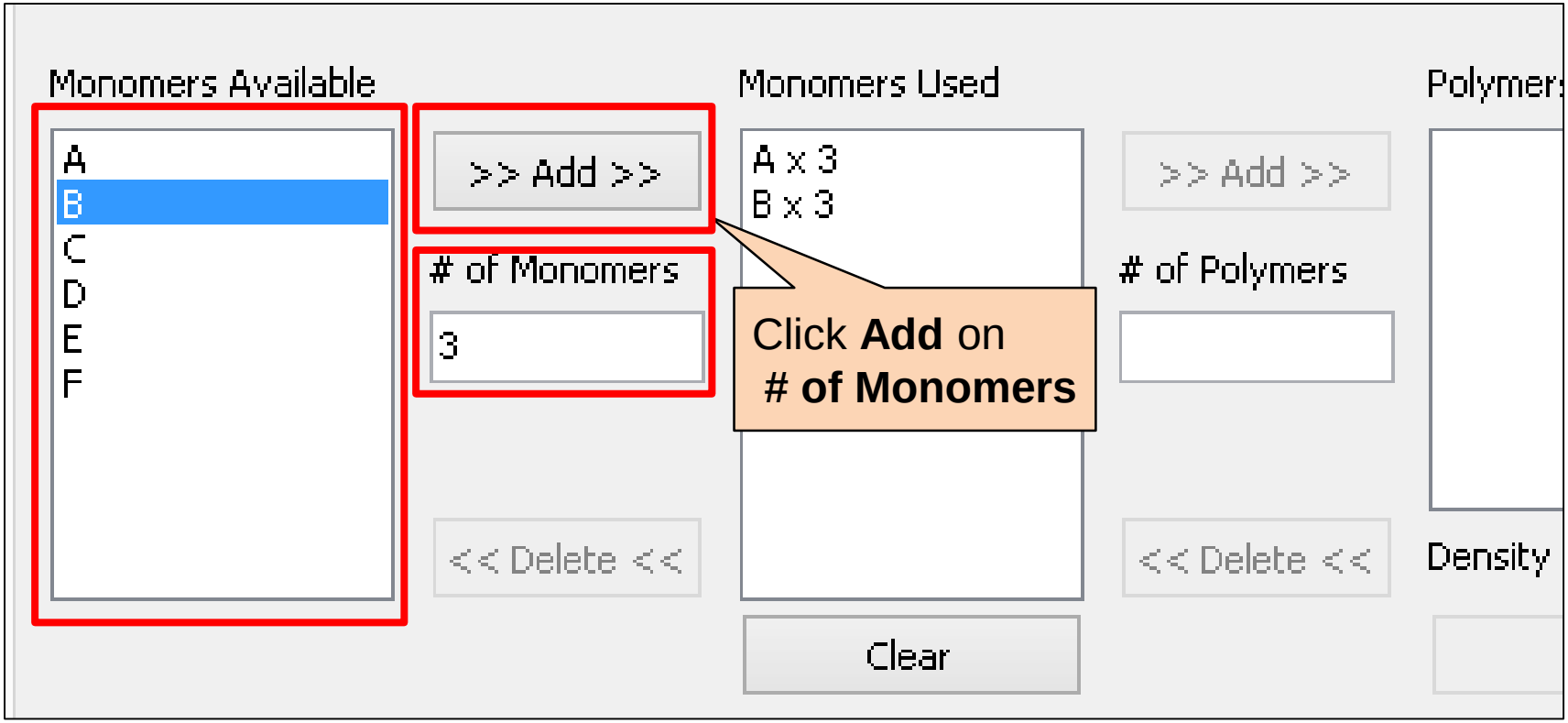
I. Build a simulation cell

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**.



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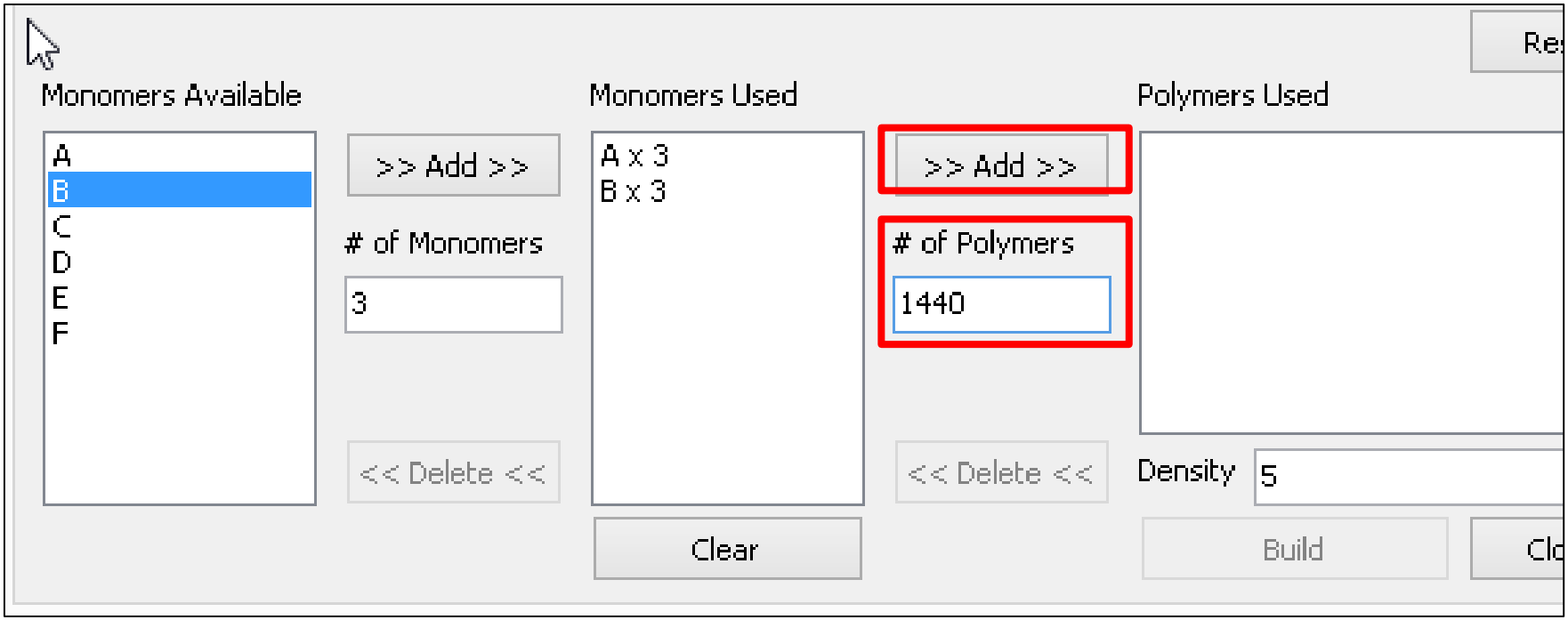
I. Build a simulation cell

Set # **of Polymers** to **1440**. Click **Add**.



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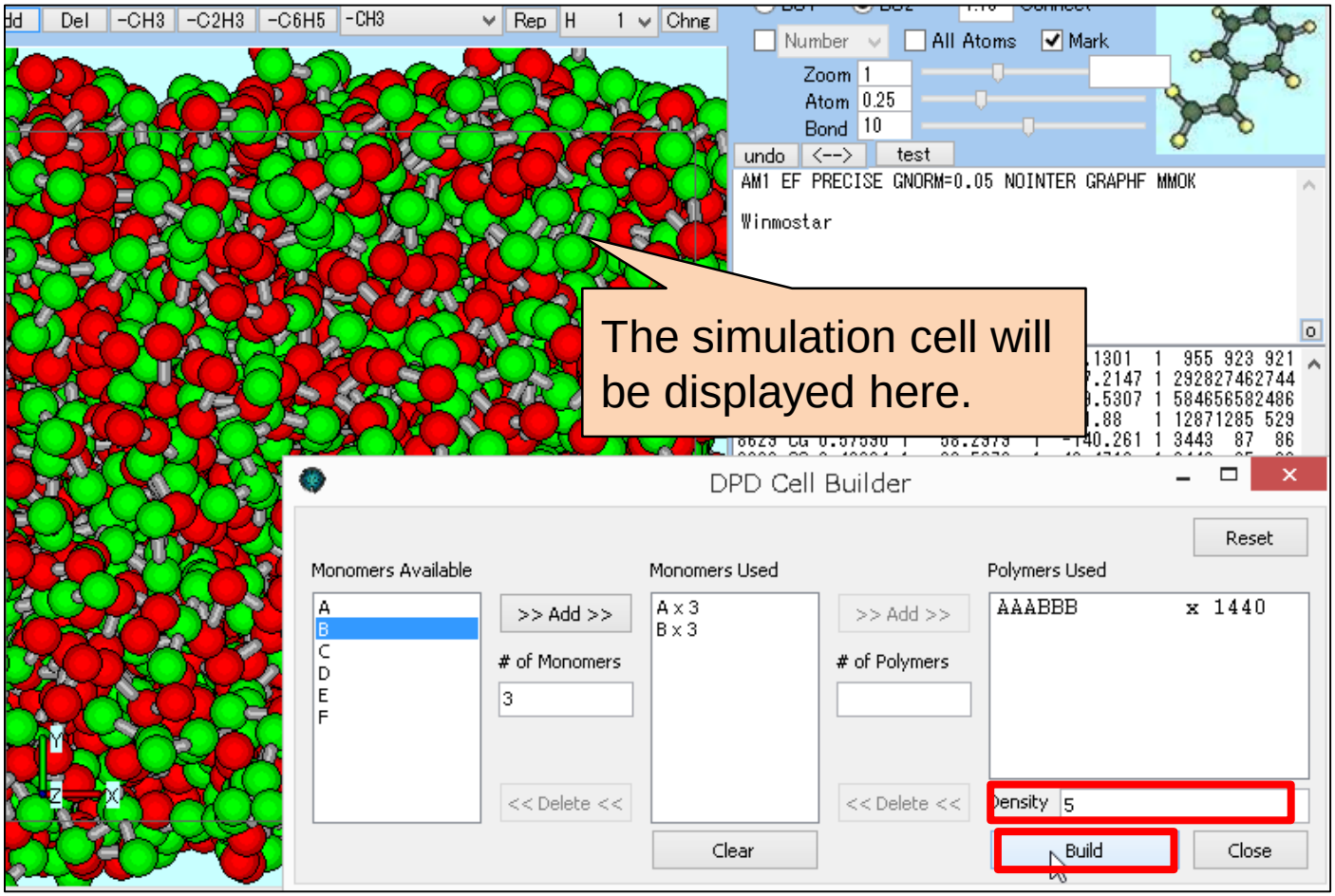
I. Build a simulation cell

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



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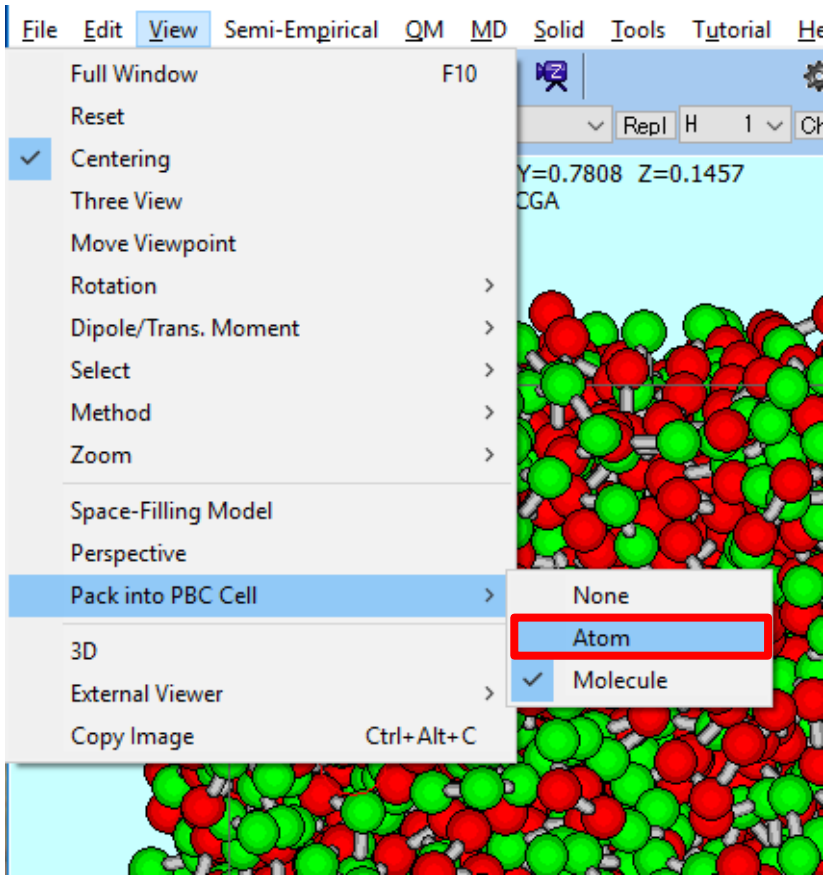
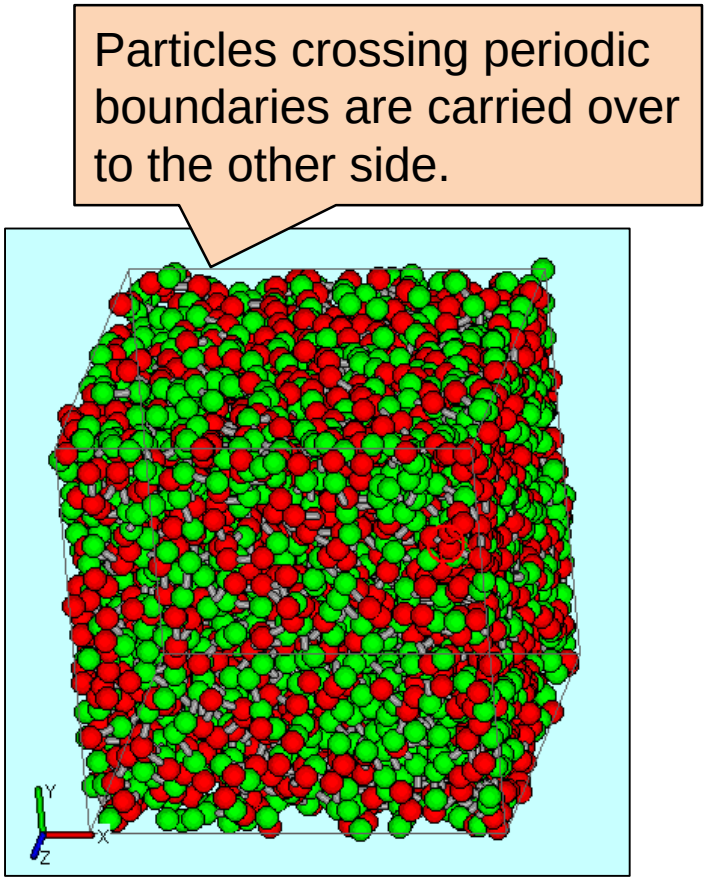
I. Build a simulation cell

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





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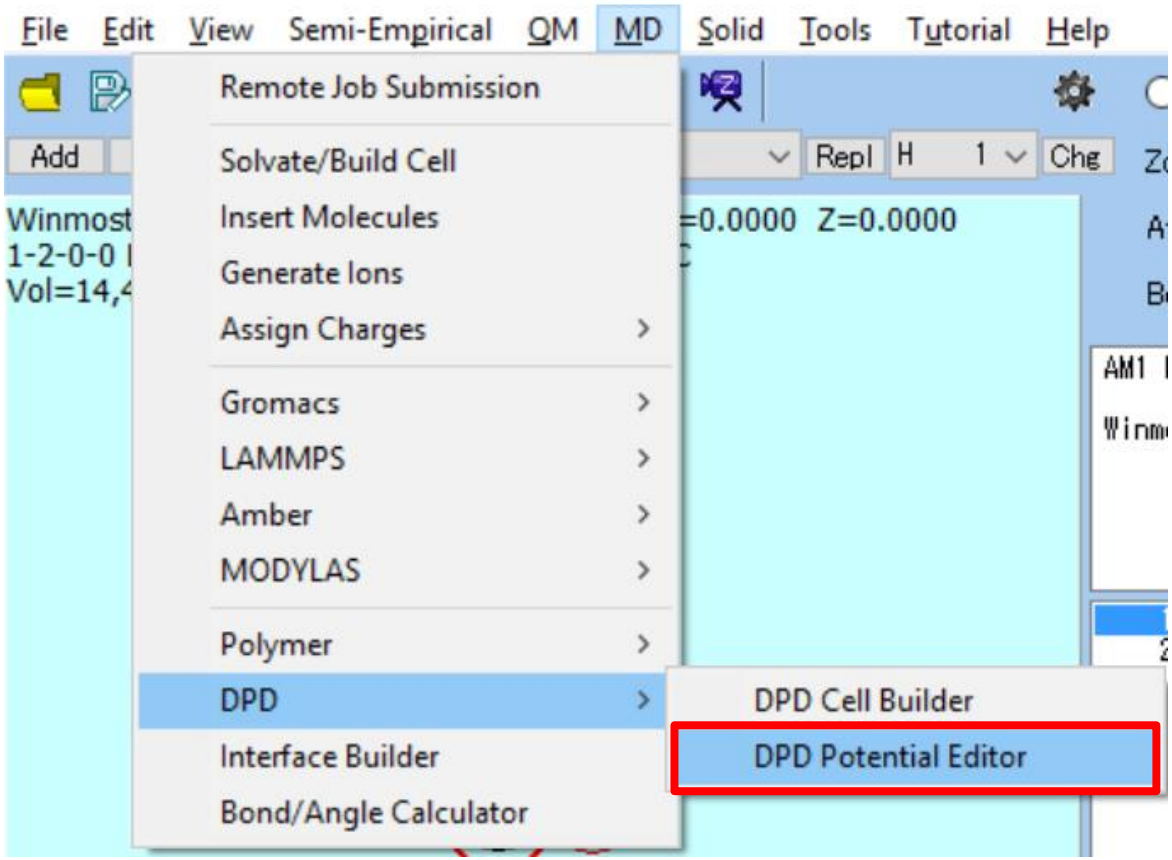
II. Potential setting

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



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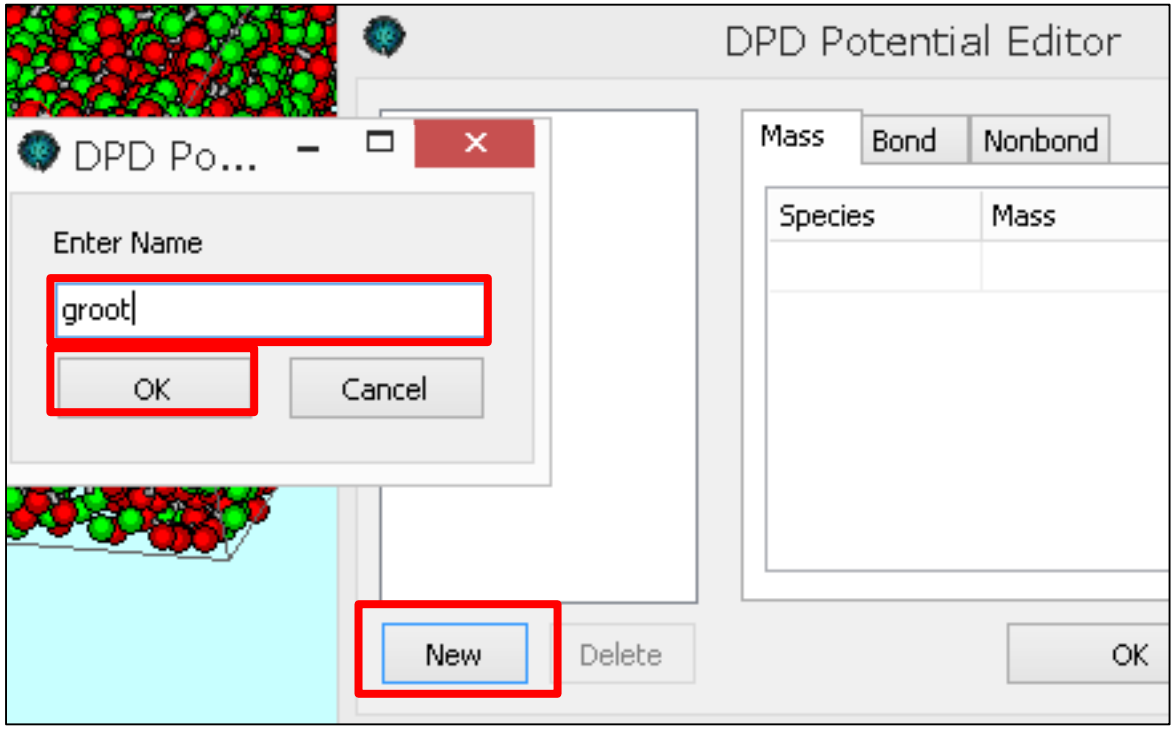
II. Potential setting

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



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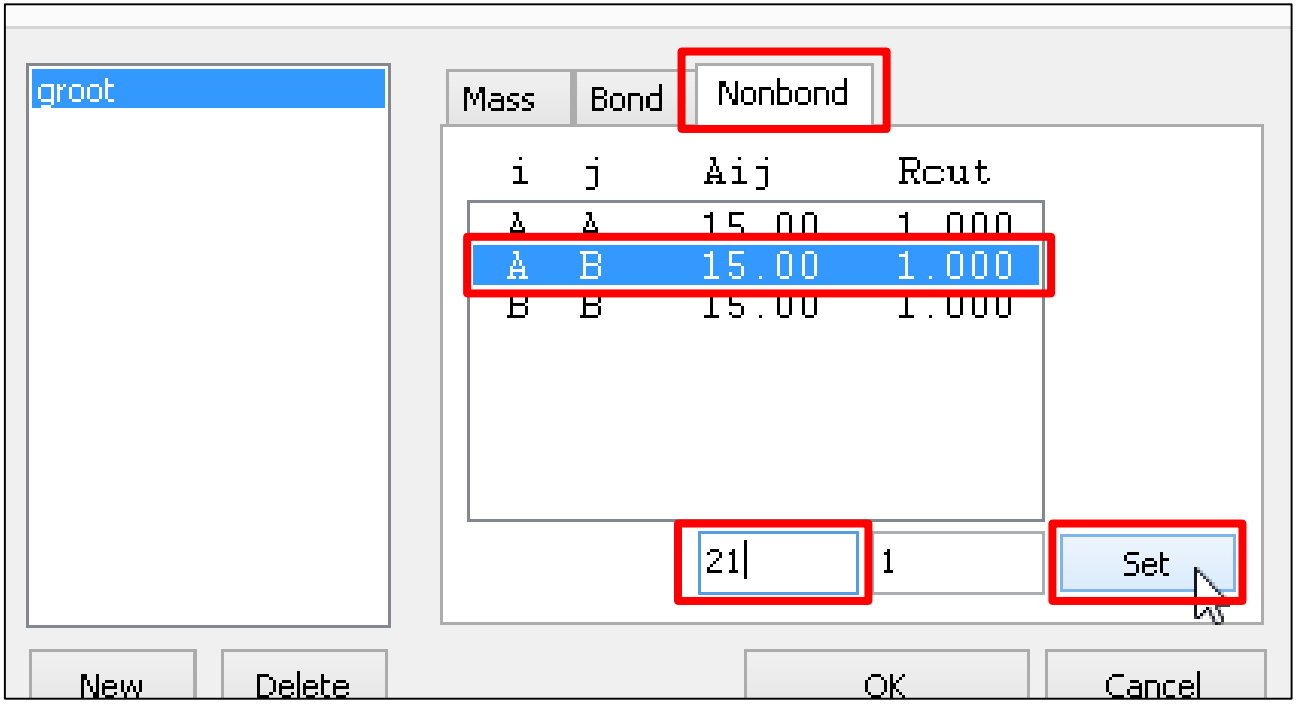
II. Potential setting

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 Aij and Rcut has no dimension.)

There are several ways to determine Aij for any monomers.
For example, see Winmostar Gromacs tutorial “Solubility/χ/DPD Parameters”



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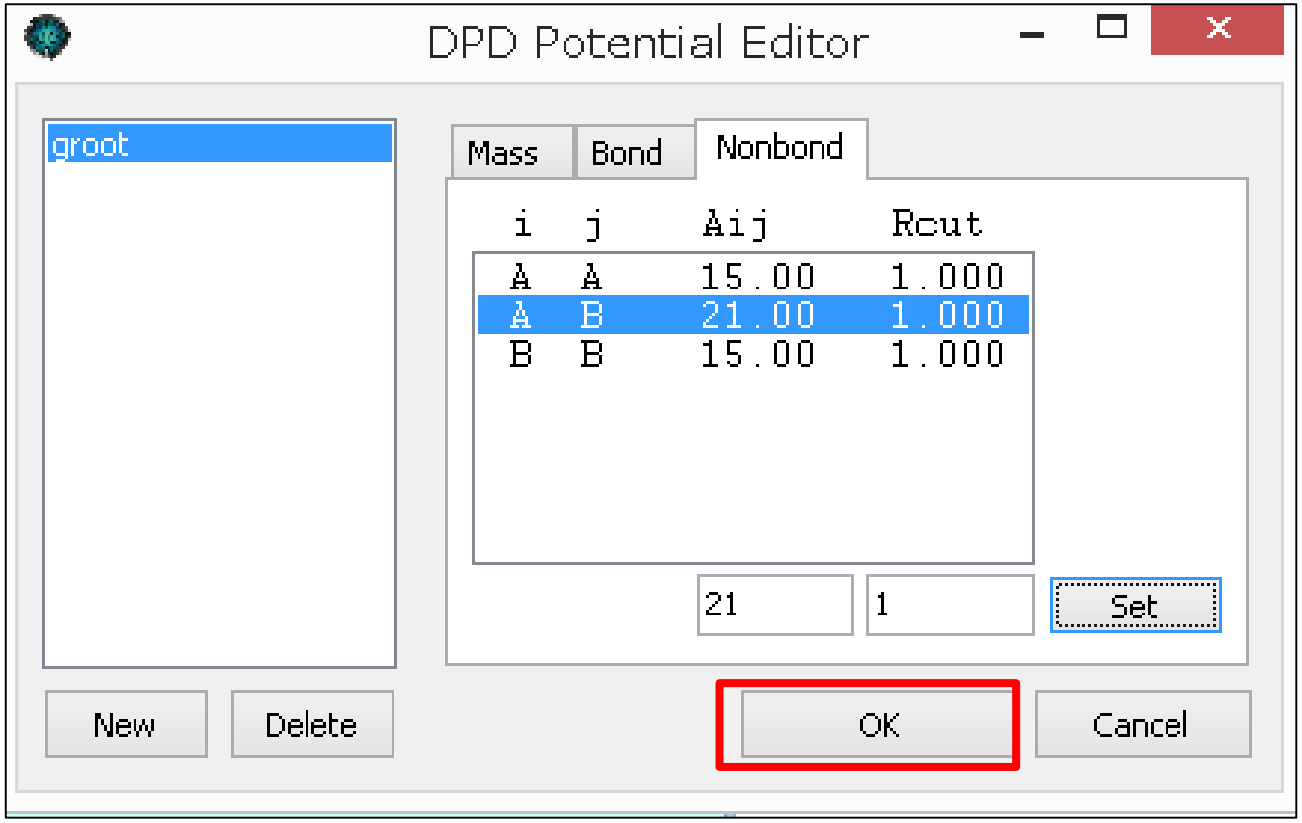
II. Potential setting

Click **OK** to **Potential Editor**.



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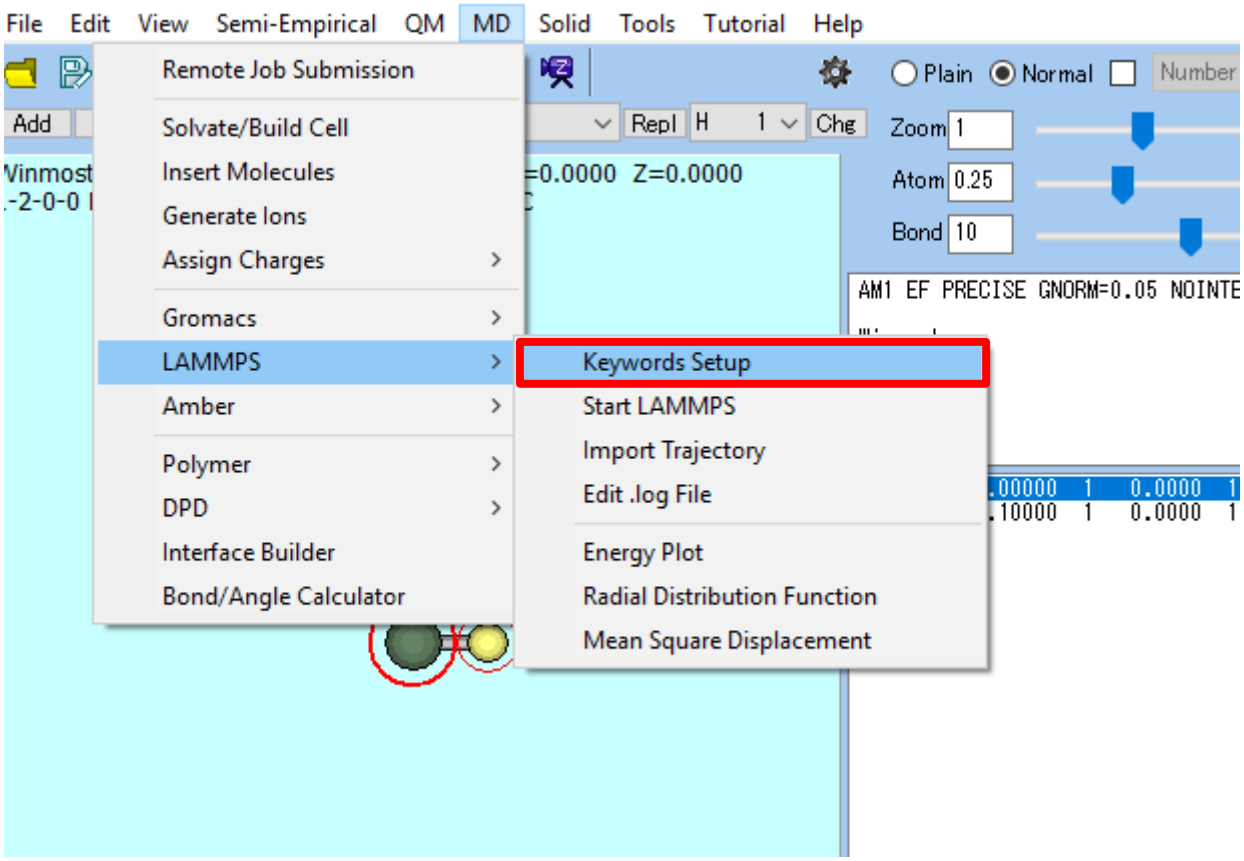
III. LAMMPS setting

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



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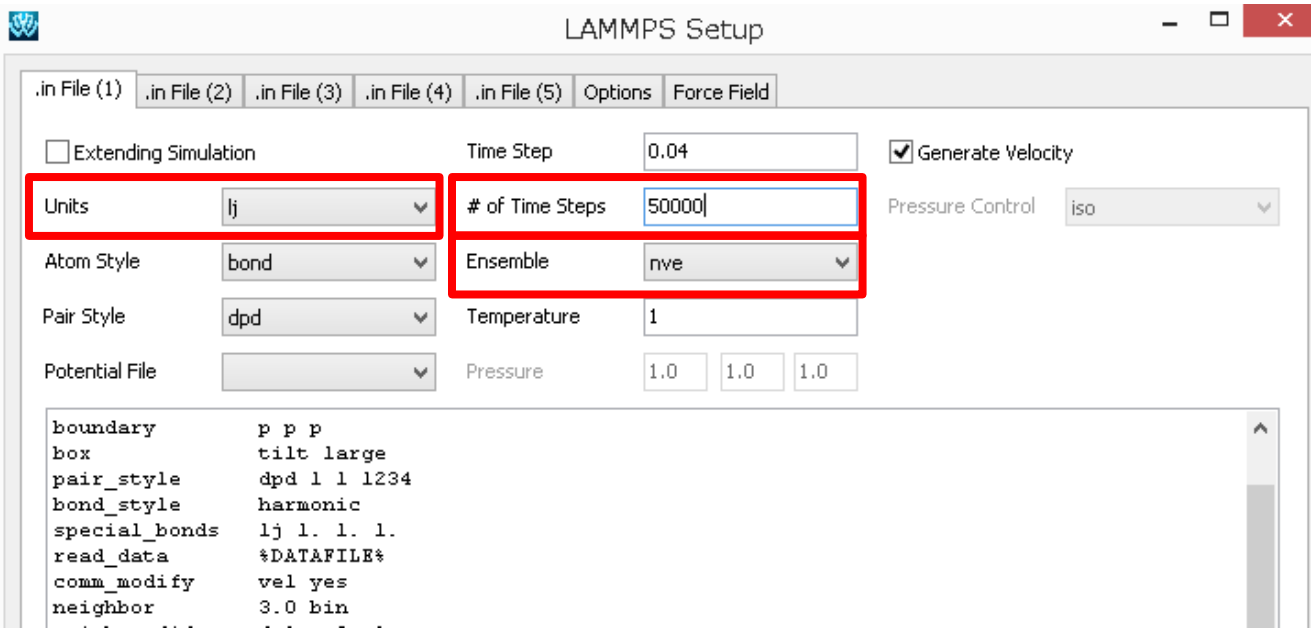
III. LAMMPS setting

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



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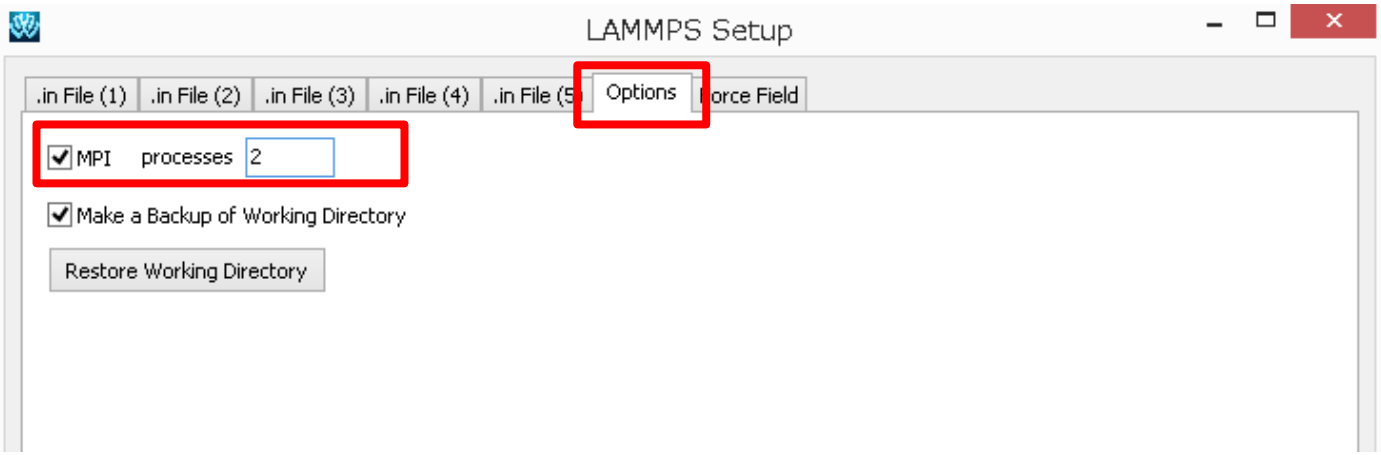
III. LAMMPS setting

Set MPI processes in the Option tab as needed.



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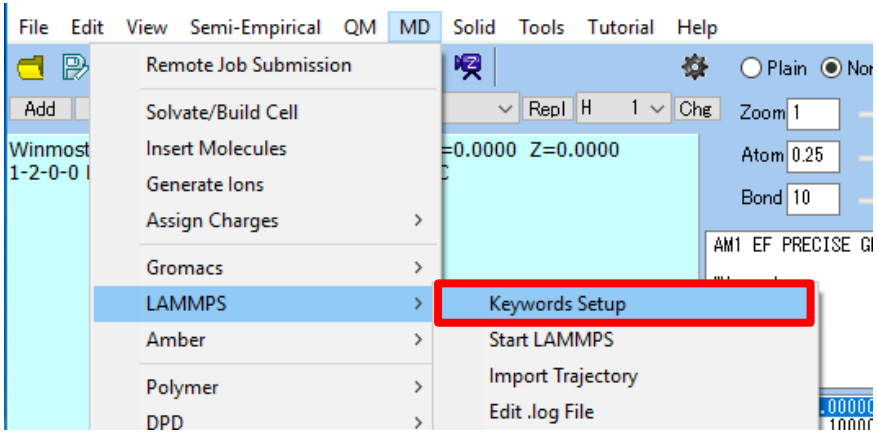
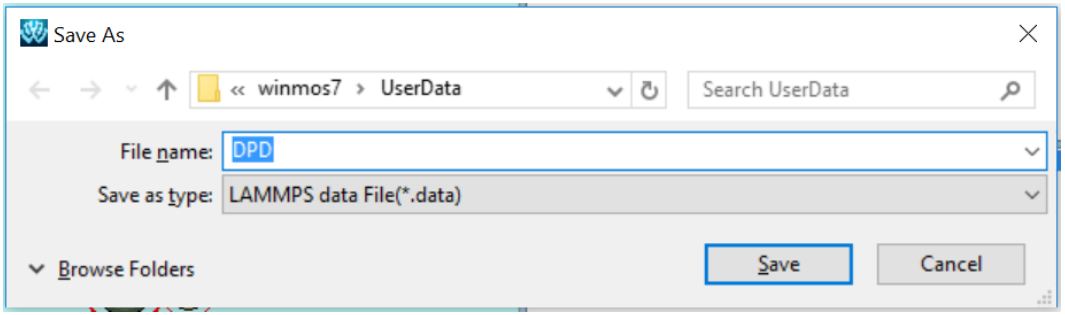
IV. Execute simulations

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



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



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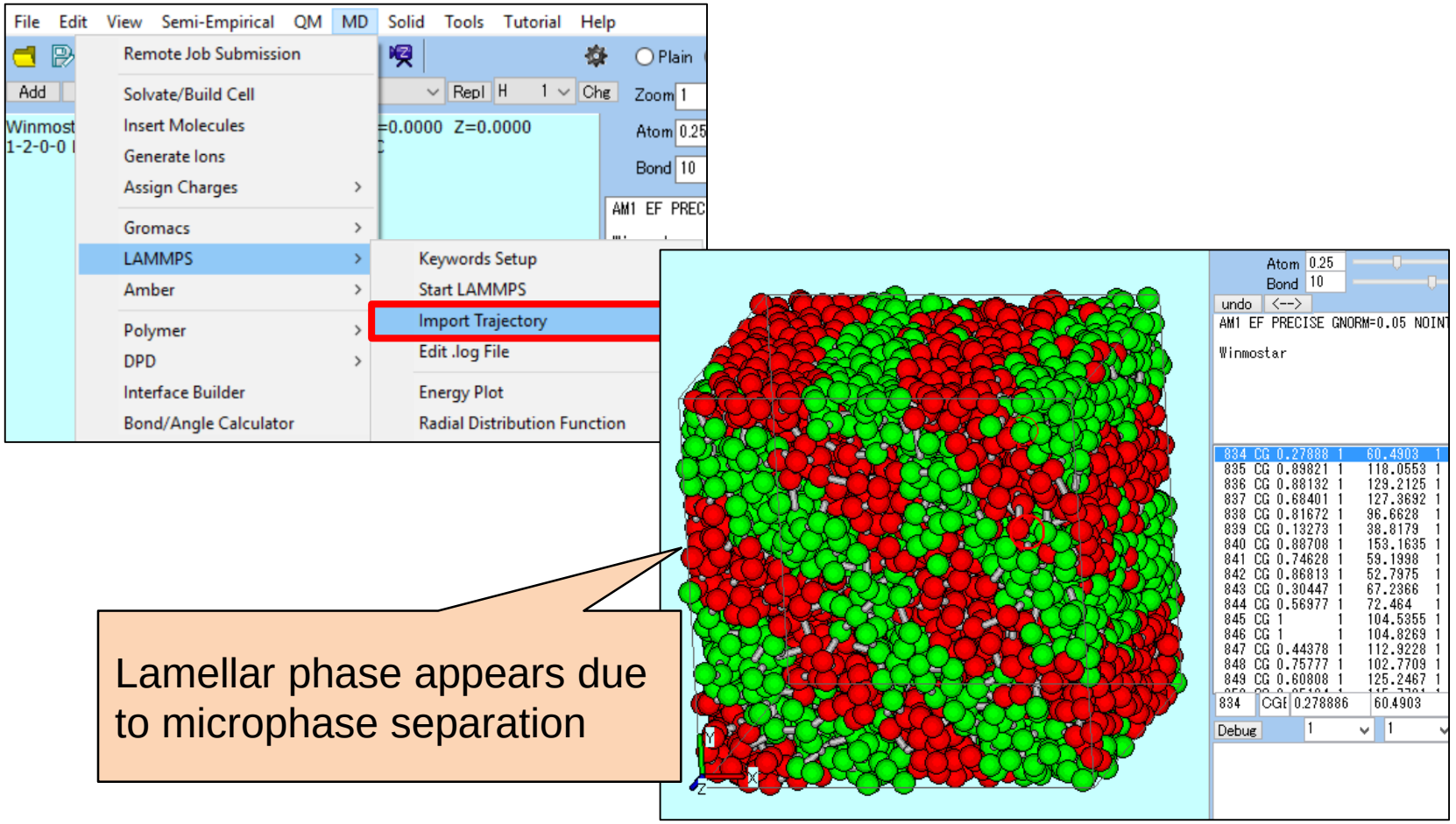
V. Analyze

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



Lamellar phase appears due to microphase separation

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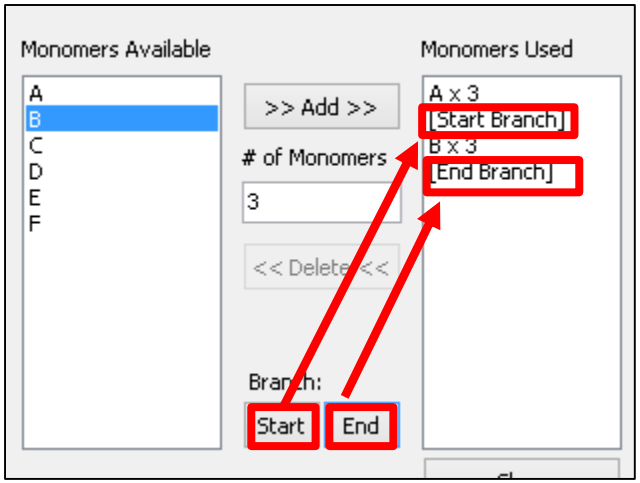
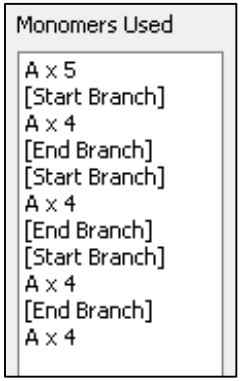
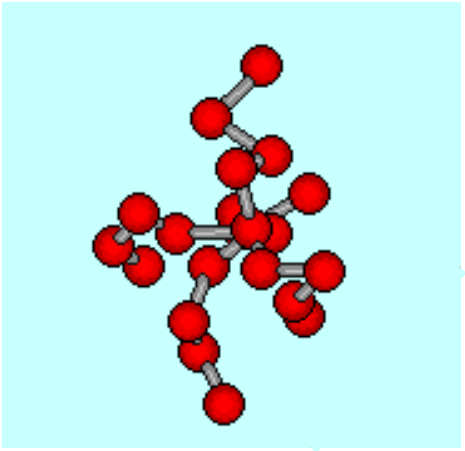
Appendix1： Insert branches

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

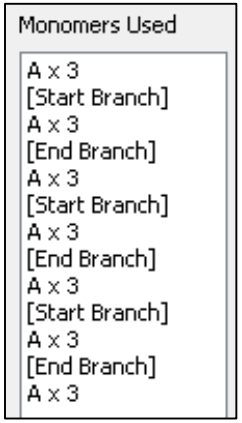


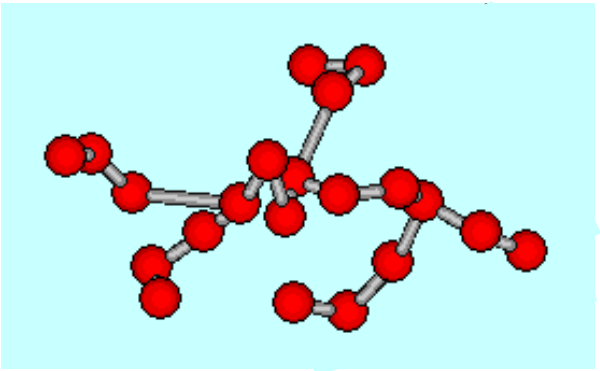
e.g.: Star-shaped Polymer





e.g.: Comb-shaped polymer





[Start]：Branching begins from preceding particle
[End]：Ends branching initiated by [Start]

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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.