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Winmostar Tutorial
LAMMPS
Basics
V8.007

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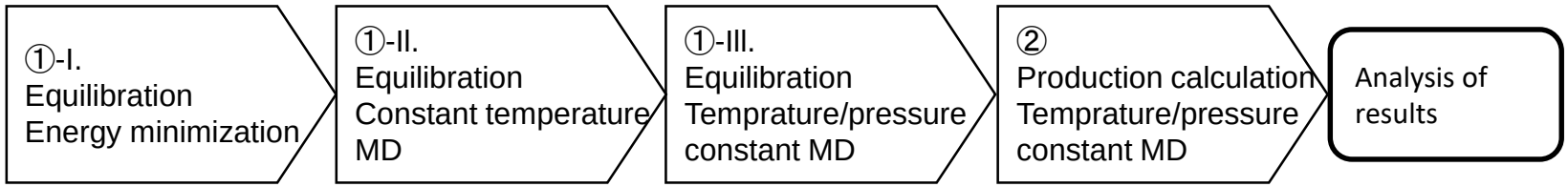
Summary

- We will create a water system with constant temperature and constant pressure, then execute equilibration and production calculations for a basic analysis.



Notes:

- The number of steps required for equilibration depends on the type of molecule and initial density varies and may be different from this example.
- To obtain accurate and reproducible results, the calculation requires long simulation times.
- The method for interaction calculations and/or the force field also affect simulation results.

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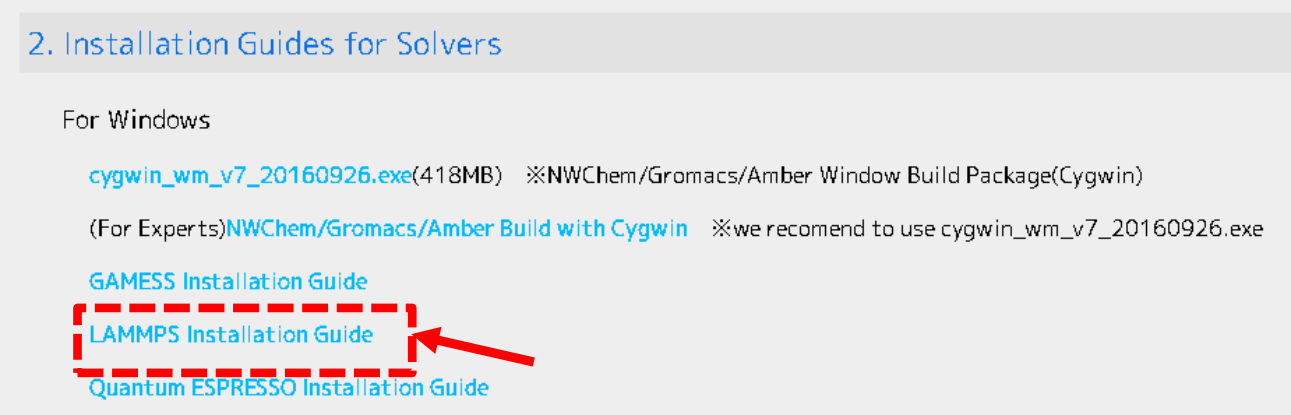
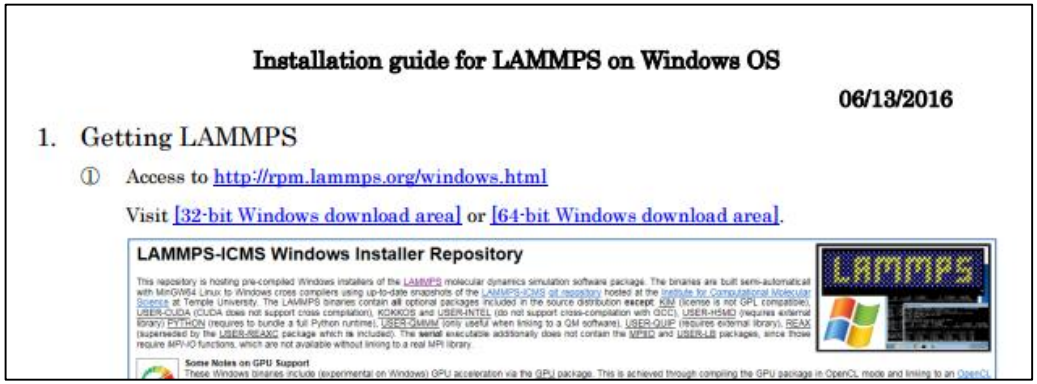
I. Configuration

You must set up both LAMMPS and Cygwin ahead.

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




Installation guide for LAMMPS on Windows OS

06/13/2016

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

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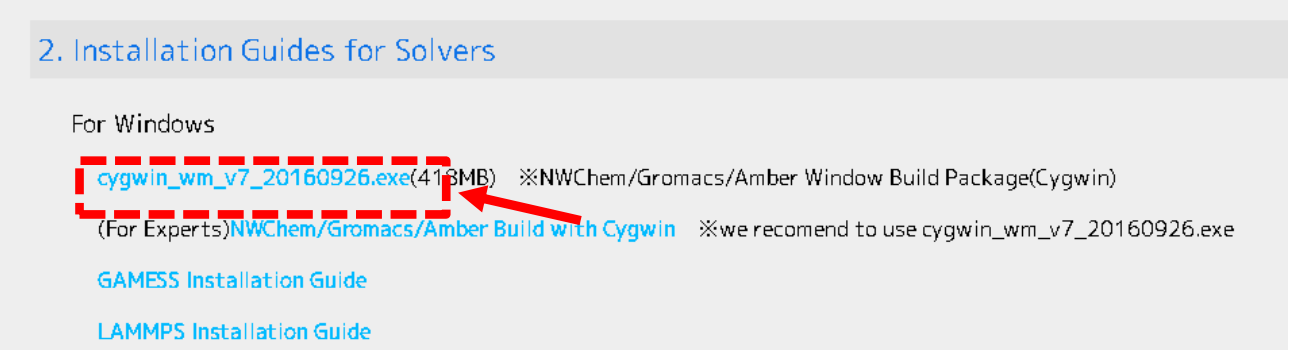
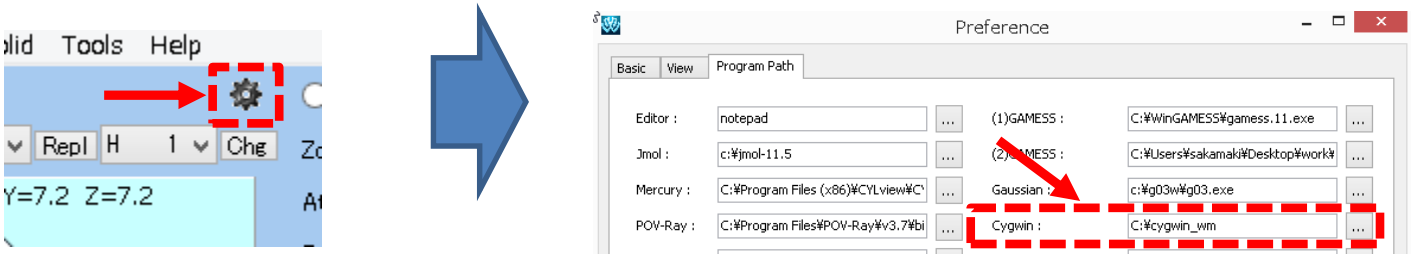
I. Configuration

You must set up both LAMMPS and Cygwin ahead.

- Obtain the installer for Cygwin, which contains the several programs needed by Winmostar, at https://winmostar.com/en/manual_en.html.



- When you change the installation path for Cygwin from the default one, specify it on the preference panel.



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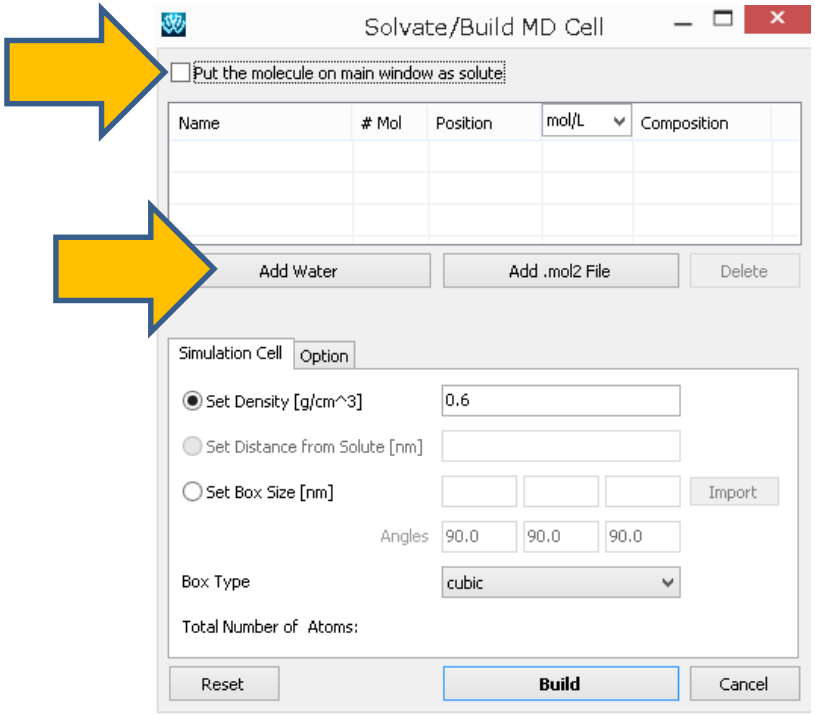
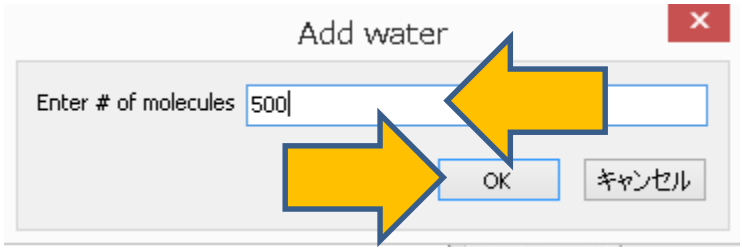
I. Build Simulation Cell

1. Click **MD | Solvate/Build Cell**.
2. Check box for **Put the molecule on main window as solute** and click **Add water**.
3. Enter "**500**" for **Enter # of molecules** text box.
4. Click **OK**.





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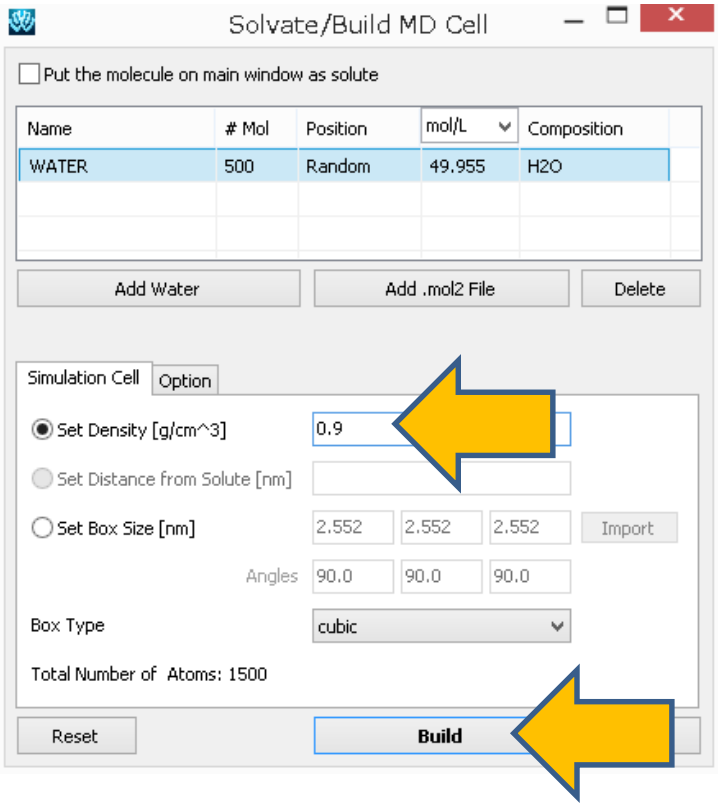
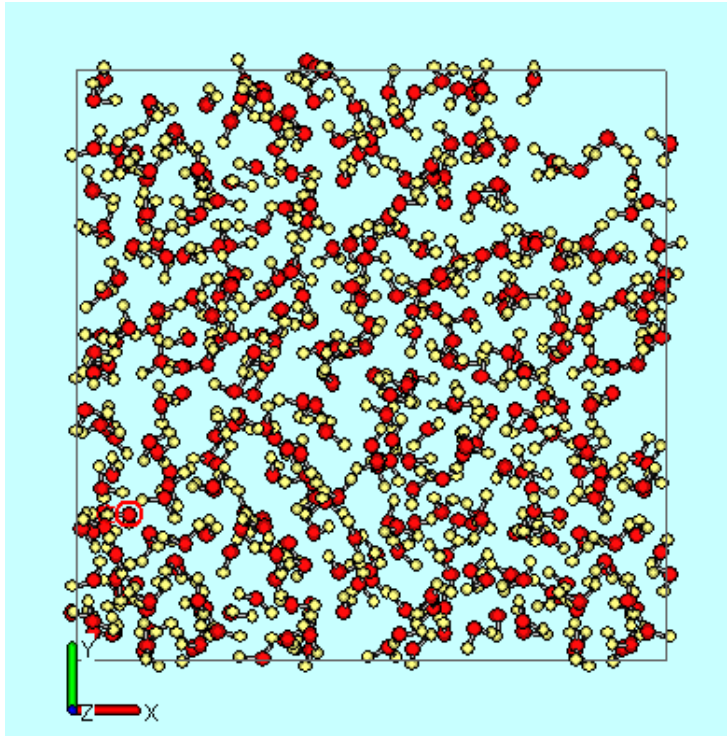
I. Build Simulation Cell

Enter “**0.9**” for **Set Density** and click **Build** to retrieve system shown below.





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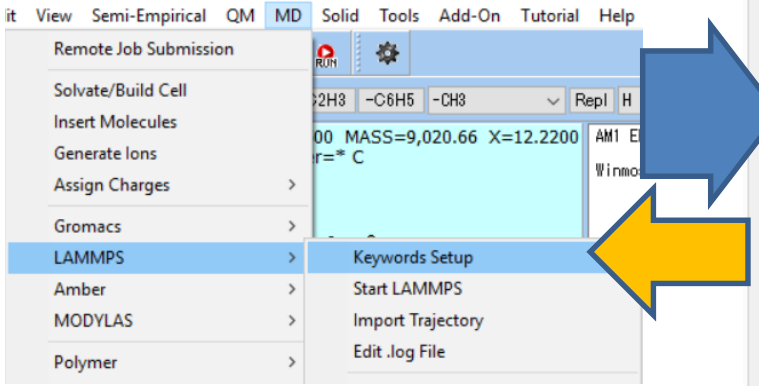
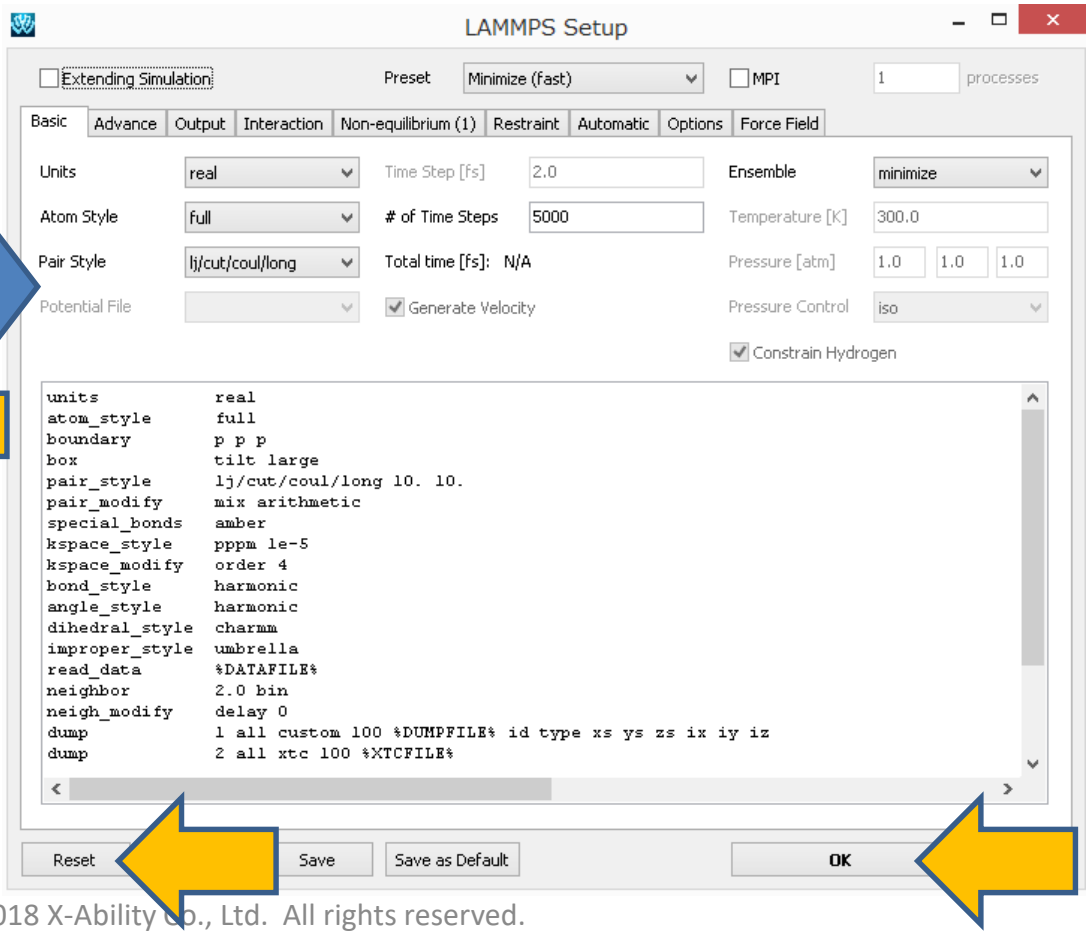
II. Equilibration (Energy Minimization)

Click **MD** | **LAMMPS** | **Keyword Setup**. Click **Reset** if keywords have been modified. Then click **OK**.





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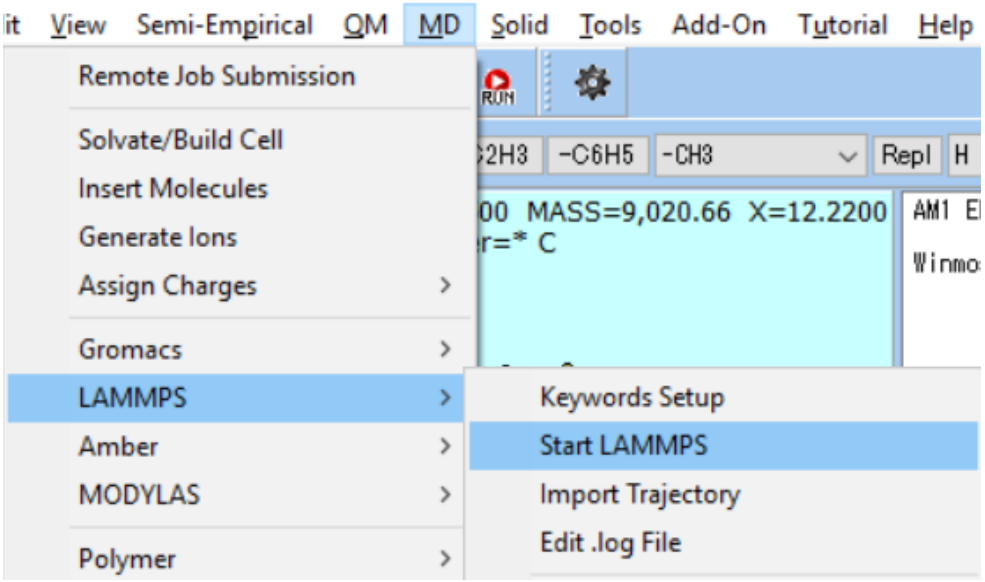
II. Equilibration (Energy Minimization)

Select **MD** | **LAMMPS** | **Start LAMMPS**. After entering the file name for LAMMPS .data file, LAMMPS will start.



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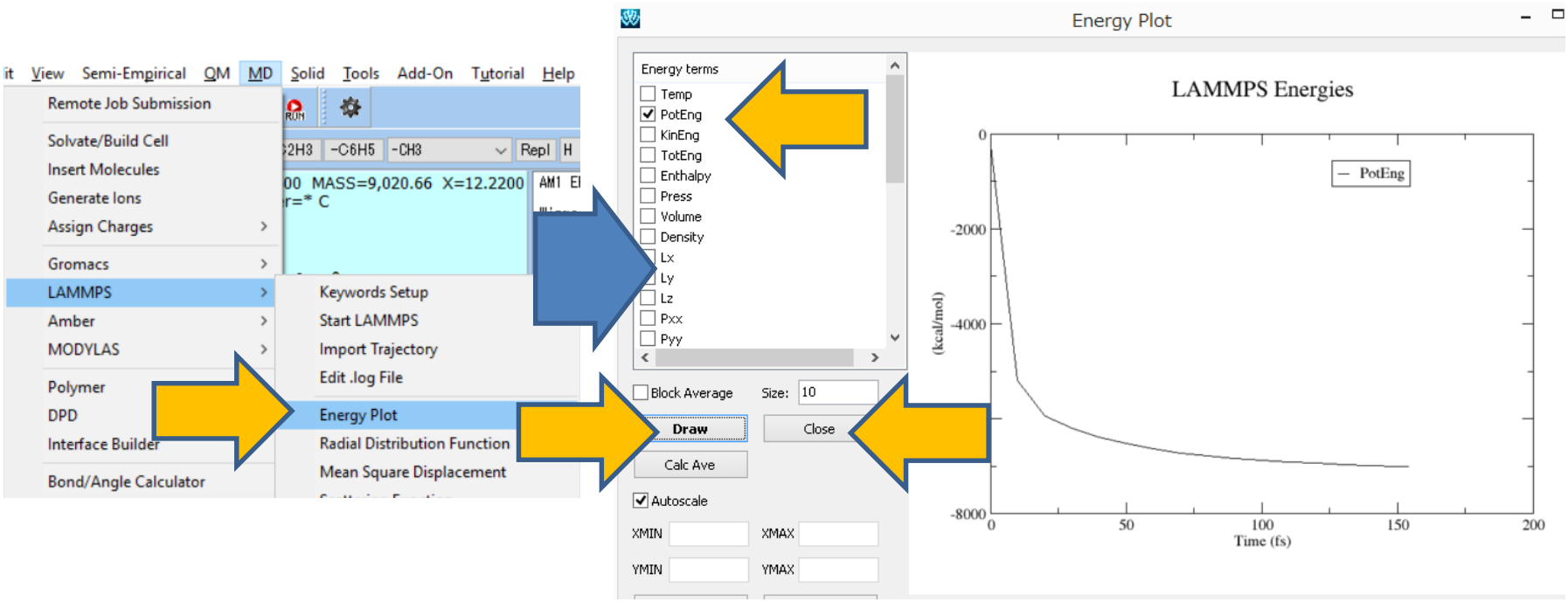
II. Equilibration (Energy Minimization)

Select **MD** | **LAMMPS** | **Energy Plot** and open the file selected by default. Check **PotEng** in **Energy term** and click **Draw** to view change in potential energy. Click close when done.



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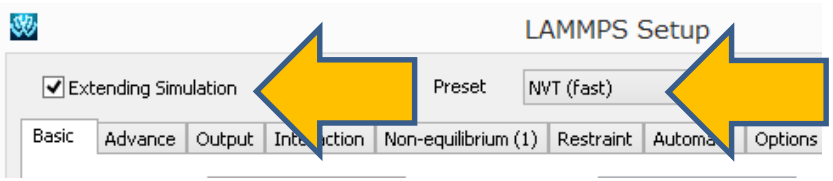
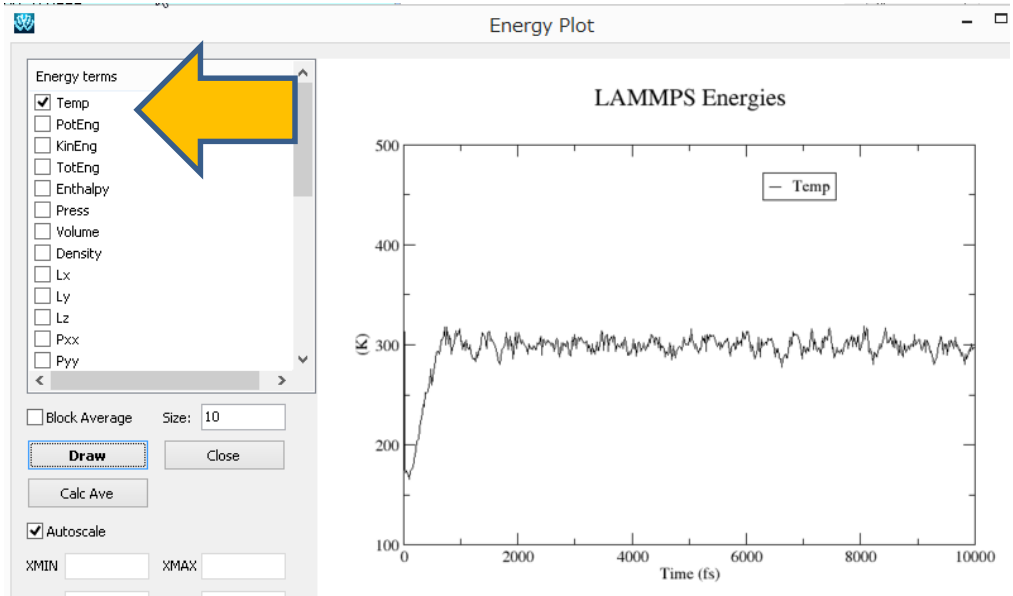
II. Equilibration (Constant Temperature)

1. Select **MD** | **LAMMPS** | **Keyword Setup**. Check the box for **Extending Simulation**, set **Preset** to **NVT (fast)** and click **OK**.
2. Select **MD** | **LAMMPS** | **Start LAMMPS**.
3. After the calculation select **MD** | **LAMMPS** | **Energy Plot**. Check the box for **Temp** (Temperature) then click **Draw** to display changes in temperature. Click **Close** when done.





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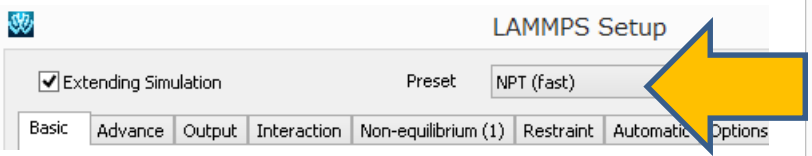
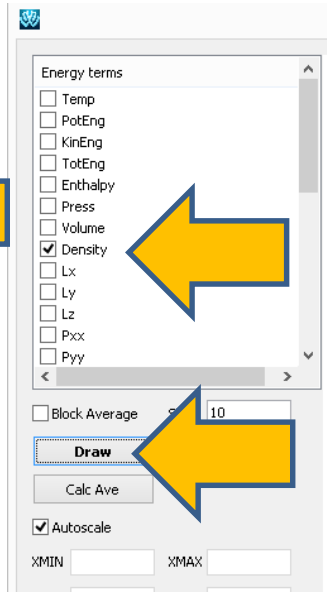
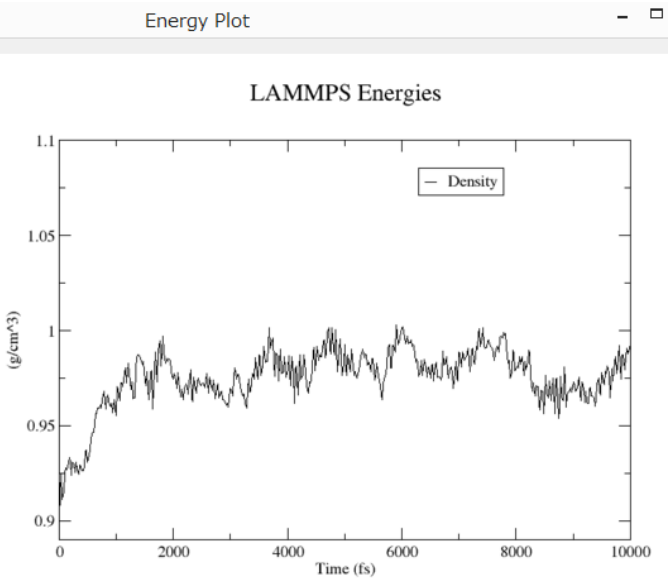
II. Equilibration (Constant Temperature/Pressure)

1. Select **MD** | **LAMMPS** | **Keyword Setup**. Check the box for **Extending Simulation**, set **Preset** to **NPT (fast)** and click **OK**.
2. Select **MD** | **LAMMPS** | **Start LAMMPS**.
3. After the calculation select **MD** | **LAMMPS** | **Energy Plot**. Check the box for Density, then click **Draw** to display changes in density. Click **Close** when done.







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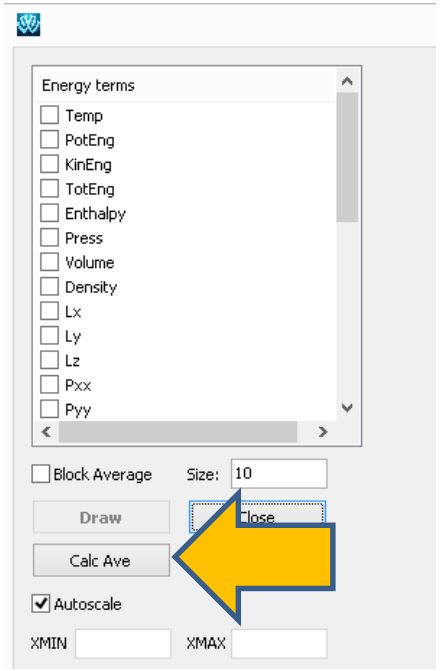
III. Product Run

1. With the same keywords, select **MD** | **LAMMPS** | **Start LAMMPS**.
2. After the calculation select **MD** | **LAMMPS** | **Energy Plot**.
3. Click **Calc Ave**, and select coordinate file suggested by default to display averages of various statistical values.



# data	Average	Standard error
Temp (K)	299.835444231536485	0.327788167594984
PotEng (kcal/mol)	-5544.767736526945560	1.348629955017838
KinEng (kcal/mol)	892.858752455089757	0.976097180514877
TotEng (kcal/mol)	-4651.908982634735370	1.644125872677692
Enthalpy (kcal/mol)	-4651.697317964072680	5.200100384349269
Press (atm)	3.122773844510978	22.346024184835606
Volume (A^3)	15055.435726546909800	7.289356913733757
Density (g/cm^3)	0.993621123532934	0.000482677087822
Lx (A)	24.692141984031920	0.003989345835806
Ly (A)	24.692141984031920	0.003989345835806
Lz (A)	24.692141984031920	0.003989345835806
Pxx (atm)	6.033117067844310	35.197060641085216
Pyy (atm)	-47.875726259481084	35.819951158445115
Pzz (atm)	51.210931500997987	34.105345932735254
Pxy (atm)	-19.311790480039935	22.050771267739162
Pxz (atm)	-2.152596176447073	21.187953566794391
Pyz (atm)	116.175317359666693	23.786597504576520
gamma (mN/m)	18.017179333732543	10.050334052860517
E_pair (kcal/mol)	-5544.767736526945560	1.348629955017838
E_vdwl (kcal/mol)	1063.448844890219330	1.605651126850460
E_coul (kcal/mol)	24008.761293413175700	2.368927929489807
E_long (kcal/mol)	-30616.977882235540200	0.106573159470741
E_tail (kcal/mol)	0.000000000000000	0.000000000000000
E_mol (kcal/mol)	0.000000000000000	0.000000000000000
E_bond (kcal/mol)	0.000000000000000	0.000000000000000
E_angle (kcal/mol)	0.000000000000000	0.000000000000000
E_dihed (kcal/mol)	0.000000000000000	0.000000000000000
E_impro (kcal/mol)	0.000000000000000	0.000000000000000

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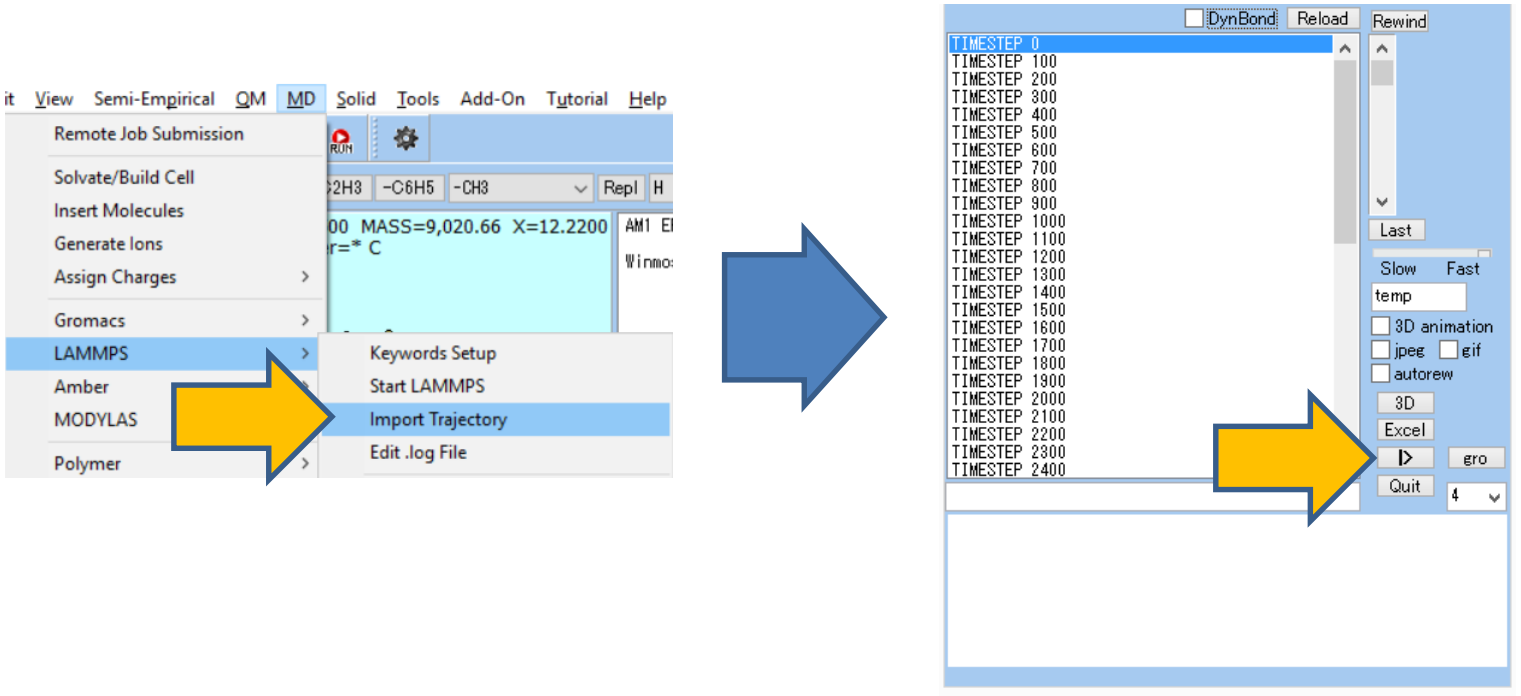
IV. Analysis

① Display Animation

- Select **MD** | **LAMMPS** | **Import Trajectory** and open the data (file extension .data) and dump (file extension .dump) files selected by default.
- On **Animation** window, click the **|>**(Play) button to start an animation



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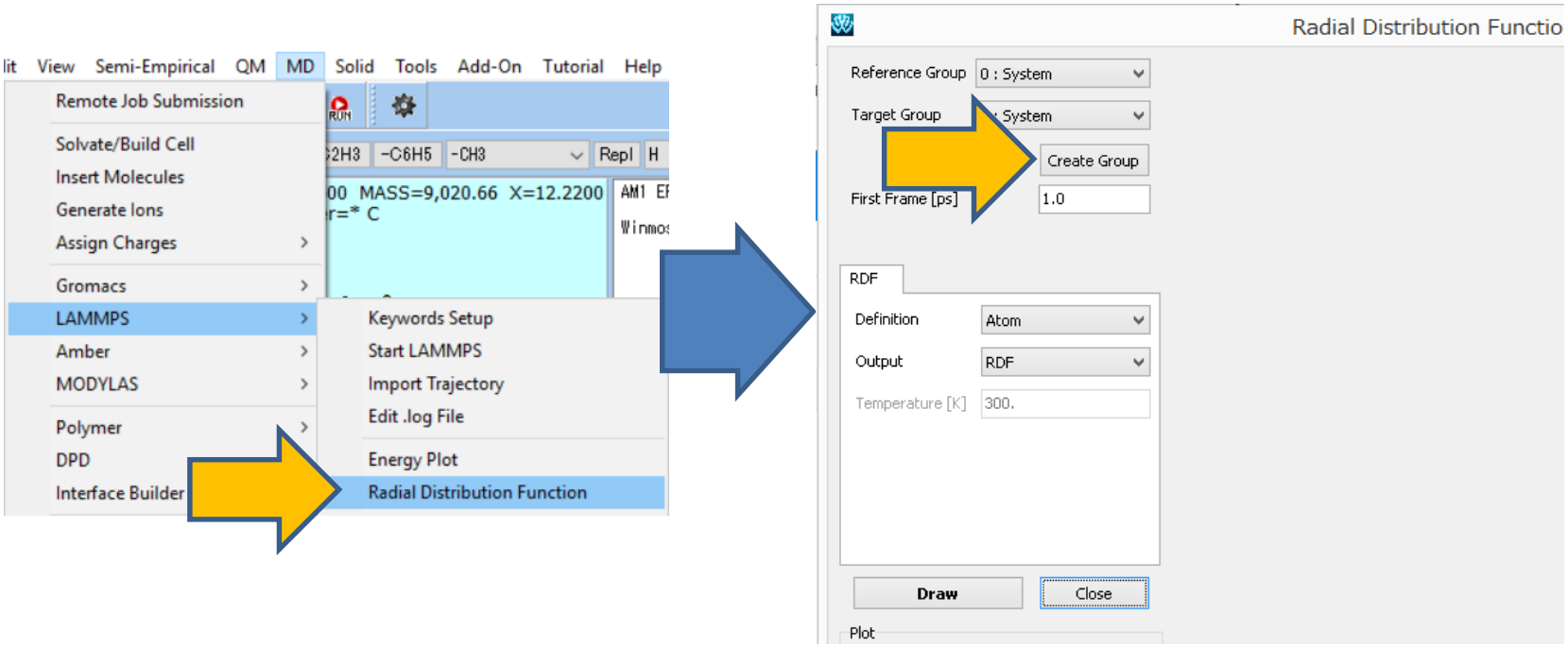
IV. Analysis

② Radial Distribution Function

- Select **MD** | **LAMMPS** | **Radial Distribution Function**. Select the following files suggested by default: trajectory file (extension .xtc), coordinate file (extension .gro), and index file (extension .ndx).
- Click Create Group and select the .gro file suggested by default.



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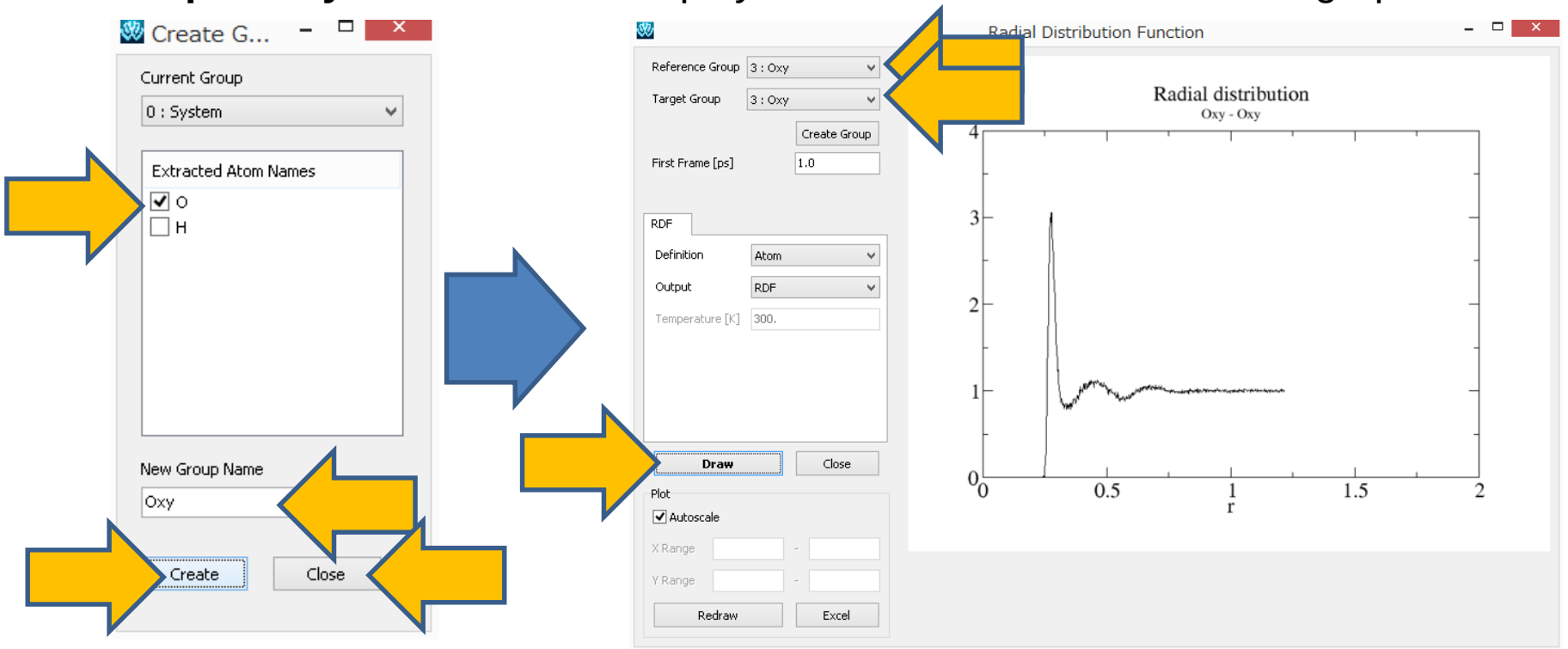
IV. Analysis

② Radial Distribution Function

Set **Extracted Atom Names** for "**O**" by checking the box and enter "**Oxy**" in the text box for **New Group Name**. Click **Create**, then click **Close**.

In the **Radial Distribution Function window**, set **Reference Group** and **Target Group** to **Oxy**. Click **Draw** to display the radial distribution function graph.



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IV. Analysis of Results

③ Mean Square Displacement

- Select **MD** | **LAMMPS** | **Mean Square Displacement**. Select the following files suggested by default: trajectory file (file extension .xtc), coordinate file (file extension .gro), and index file (file extension .ndx).
- Click **Draw** to display the mean square displacement graph. Self diffusion coefficient is shown in the box below.