

Winmostar Tutorial

LAMMPS

Basics

V8.007

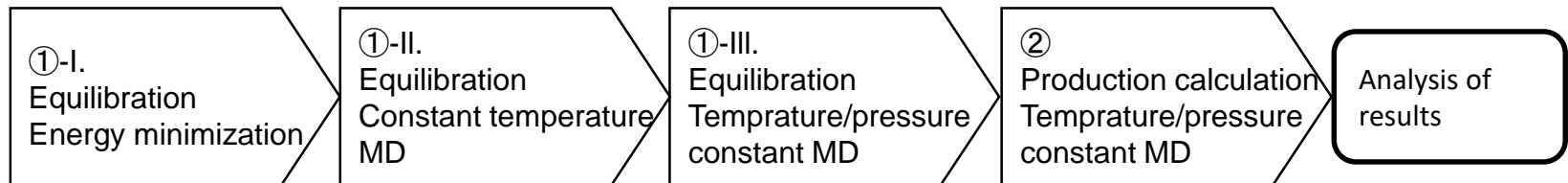
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2018/01/15

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.

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.

2. Installation Guides for Solvers

For Windows

[cygwin_wm_v7_20160926.exe](#)(418MB) ※NWChem/Gromacs/Amber Window Build Package(Cygwin)

(For Experts)[NWChem/Gromacs/Amber Build with Cygwin](#) ※we recomend to use [cygwin_wm_v7_20160926.exe](#)

[GAMESS Installation Guide](#)

[LAMMPS Installation Guide](#)

[Quantum ESPRESSO Installation Guide](#)

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

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 git 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 `atom` (license is not GPL compatible), `USER-CUDA` (CUDA does not support cross-compiler), `ICMS-OPENMP` and `USER-OPENMP` (do not support cross-compiler with GCC), `USER-OPENMP` (requires external library), `PYTHON` (requires to bundle a full Python runtime), `USER-CUBUMI` (only useful when linking to a GM software), `USER-QUIP` (requires external library), `REAX` (supported by the `USER-OPENMP` package which it includes). The `winexec` executable additionally does not contain the `WINDL` and `USER-LJ` packages, since those require GPU functions, which are not available without linking to a real GPU 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

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.

2. Installation Guides for Solvers

For Windows

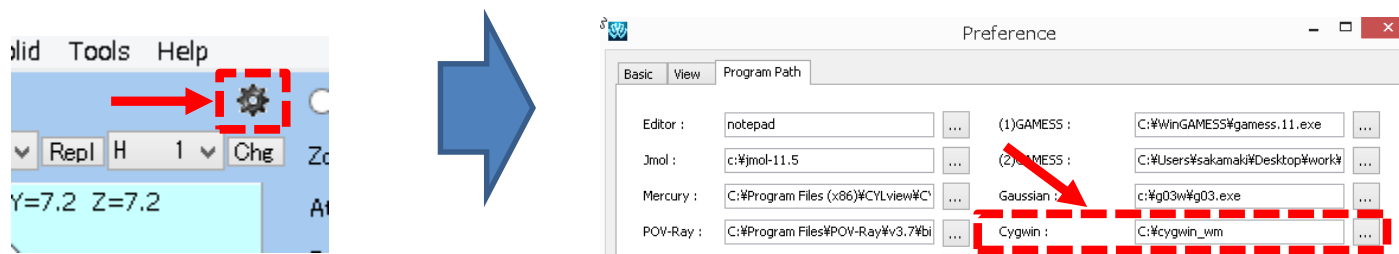
[cygwin_wm_v7_20160926.exe](#) (413MB) ※NWChem/Gromacs/Amber Window Build Package(Cygwin)

(For Experts) [NWChem/Gromacs/Amber Build with Cygwin](#) ※we recomend to use cygwin_wm_v7_20160926.exe

[GAMESS Installation Guide](#)

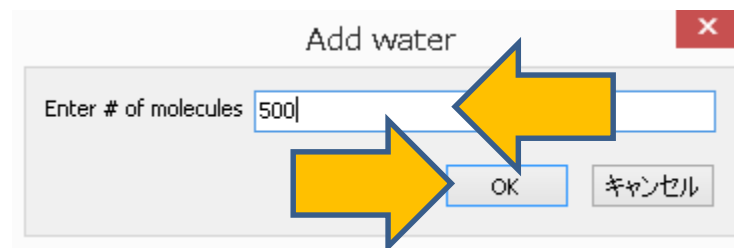
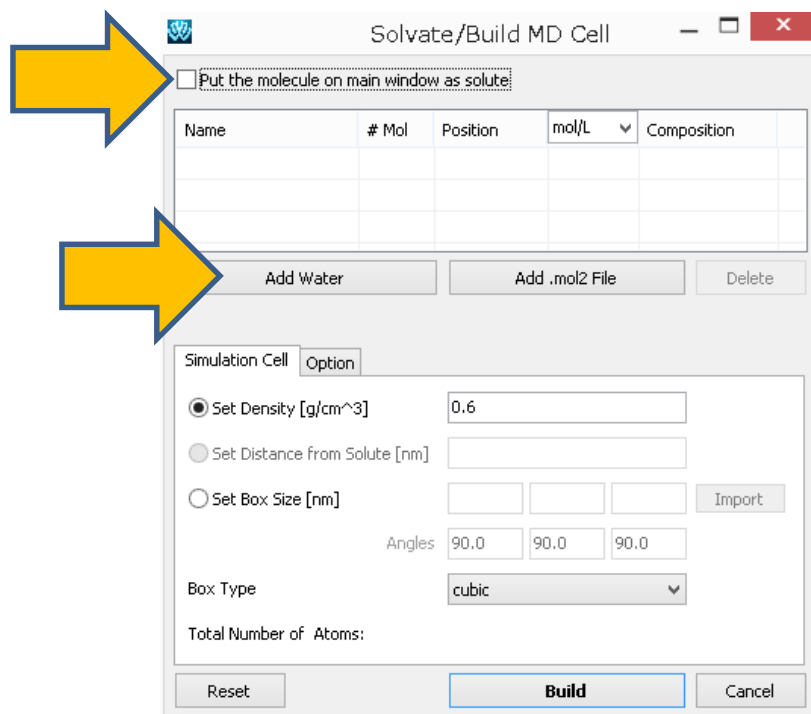
[LAMMPS Installation Guide](#)

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



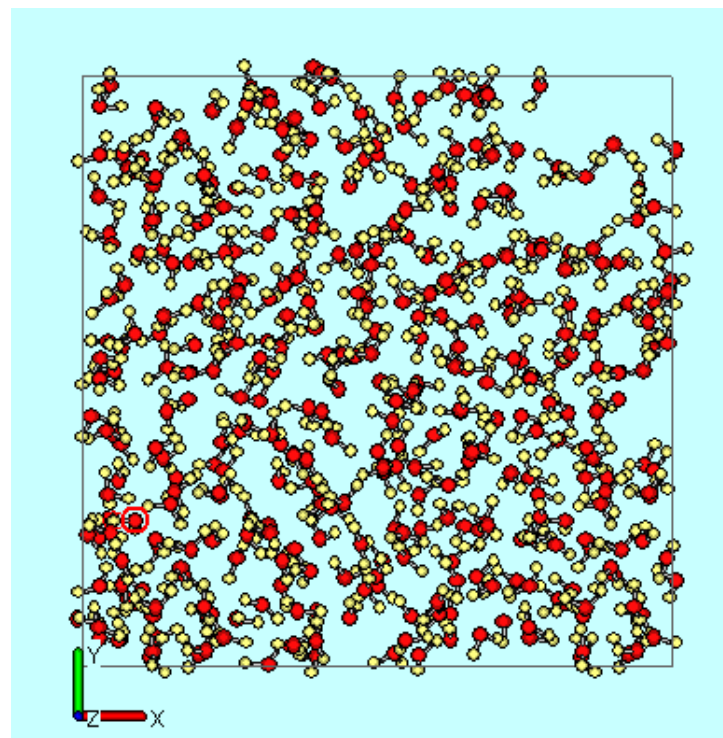
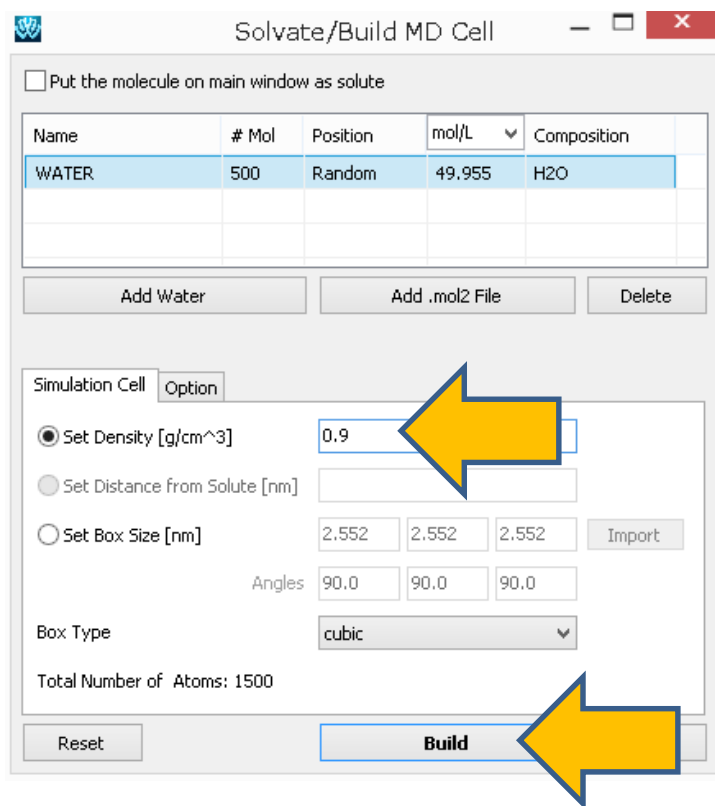
I. Build Simulation Cell

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**.



I. Build Simulation Cell

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



II. Equilibration (Energy Minimization)

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

The screenshot shows the LAMMPS Setup window with the following configuration:

- Extending Simulation:**
- Preset:** Minimize (fast)
- MPI:**
- processes:** 1

Basic Tab Settings:

- Units:** real
- Time Step [fs]:** 2.0
- Ensemble:** minimize
- Atom Style:** full
- # of Time Steps:** 5000
- Temperature [K]:** 300.0
- Pair Style:** lj/cut/coul/long
- Total time [fs]:** N/A
- Pressure [atm]:** 1.0, 1.0, 1.0
- Potential File:** (empty)
- Generate Velocity**
- Pressure Control:** iso
- Constrain Hydrogen**

Keyword List:

```

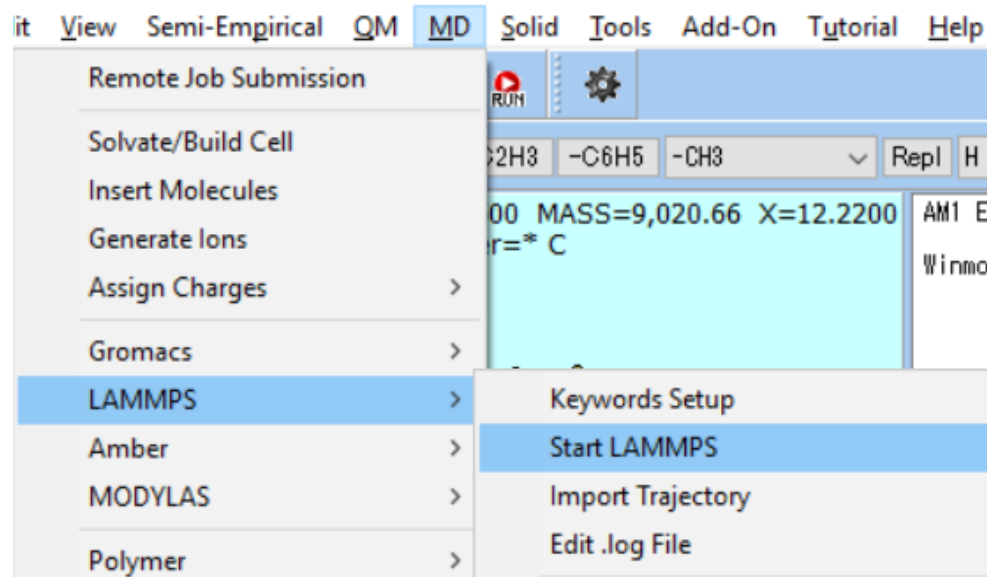
units real
atom_style full
boundary p p p
box tilt large
pair_style lj/cut/coul/long 10. 10.
pair_modify mix arithmetic
special_bonds amber
kspace_style ppm le-5
kspace_modify order 4
bond_style harmonic
angle_style harmonic
dihedral_style charmm
improper_style umbrella
read_data %DATAFILE%
neighbor 2.0 bin
neigh_modify delay 0
dump 1 all custom 100 %DUMPFILe% id type xs ys zs ix iy iz
dump 2 all xtc 100 %XTCFILE%
  
```

Navigation Path: MD | LAMMPS | Keyword Setup

Buttons: Reset, Save, Save as Default, OK

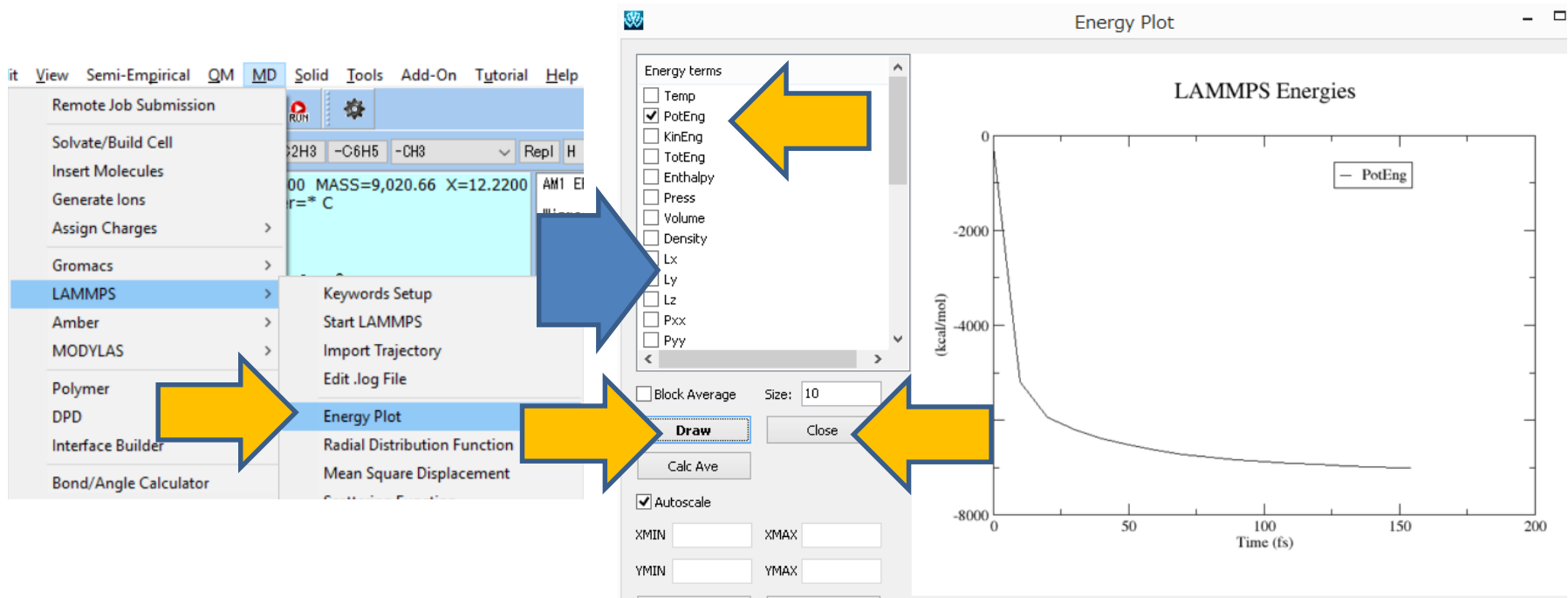
II. Equilibration (Energy Minimization)

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



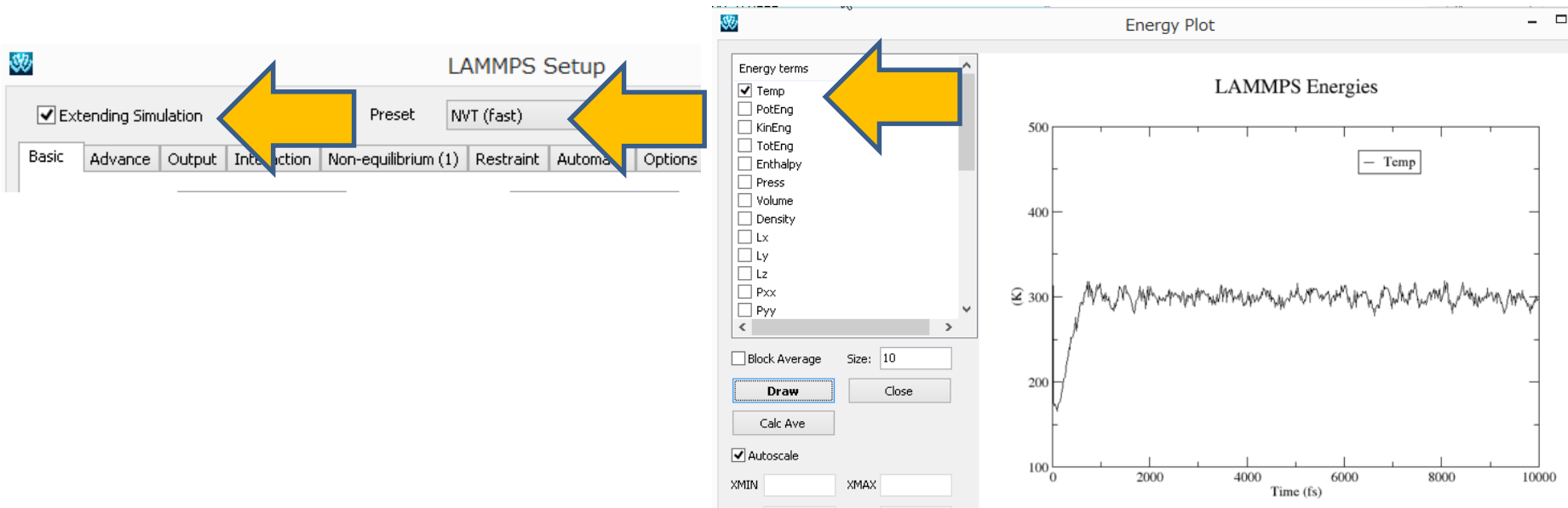
II. Equilibration (Energy Minimization)

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.



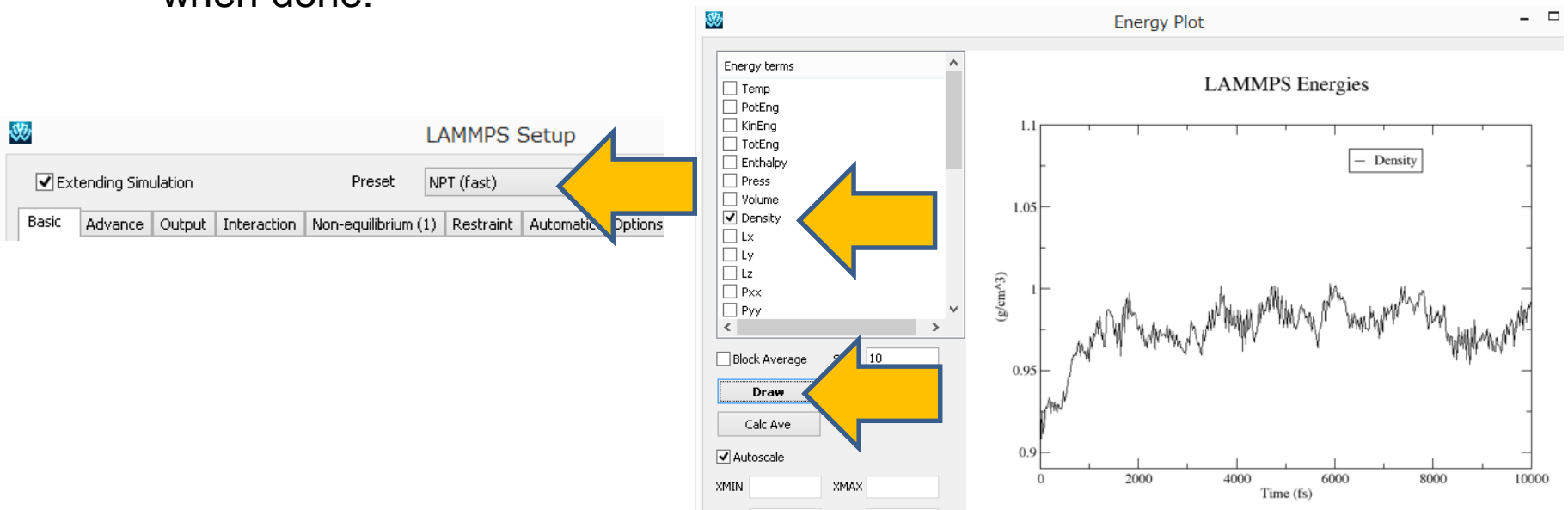
II. Equilibration (Constant Temperature)

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.



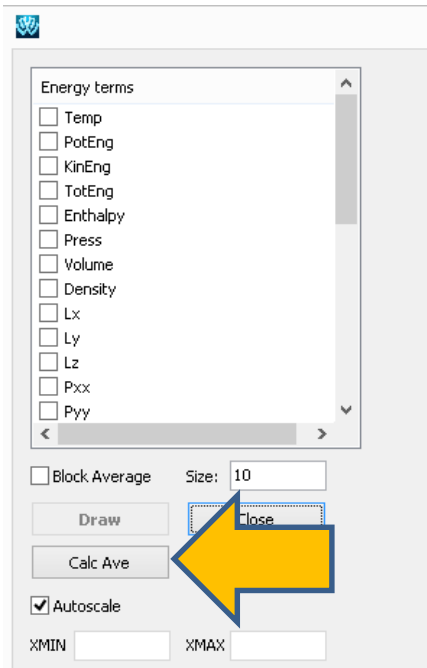
II. Equilibration (Constant Temperature/Pressure)

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.



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.

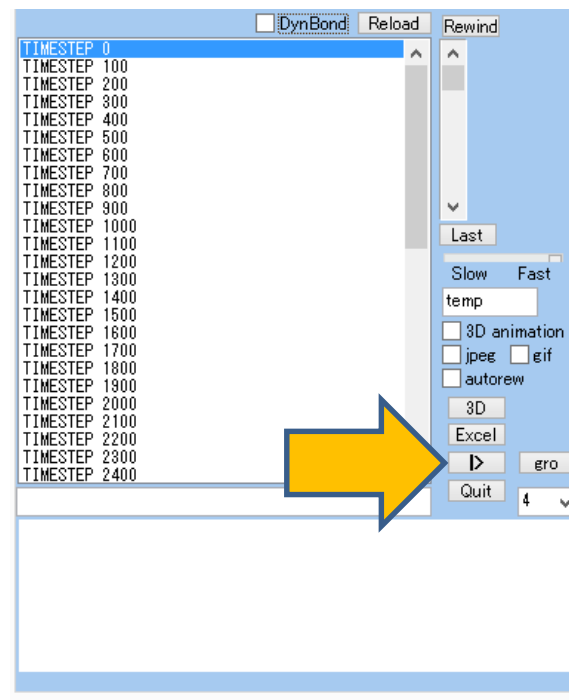
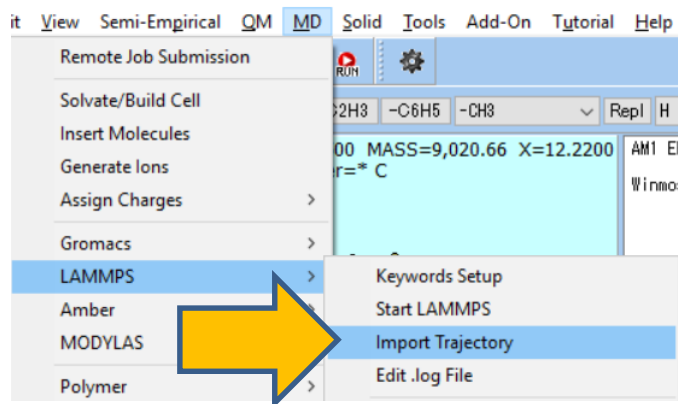


# data	Average	Standard error
Temp (K)	299.835444231536485	0.327788167594984
PotEng (kcal/mol)	-5544.767736526945560	1.348629955017838
KinEng (kcal/mol)	892.858752455089757	0.976097180514877
TotEng (kcal/mol)	-4651.908982634735370	1.644125872677692
Enthalpy (kcal/mol)	-4651.697317964072680	5.200100384349269
Press (atm)	3.122773844510978	22.346024184835806
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

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



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.

The screenshot illustrates the steps to access the Radial Distribution Function (RDF) analysis tool. On the left, the 'MD' menu is open, and 'Radial Distribution Function' is highlighted. A yellow arrow points to this option. A blue arrow points from the menu to the 'Radial Distribution Function' dialog box on the right. In the dialog box, the 'Create Group' button is highlighted with a yellow arrow. The dialog box shows the following settings:

- Reference Group: 0 : System
- Target Group: System
- First Frame [ps]: 1.0
- RDF Definition: Atom
- Output: RDF
- Temperature [K]: 300.

Buttons for 'Draw' and 'Close' are visible at the bottom of the dialog box.

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.

The image displays three sequential screenshots of a software interface, illustrating the steps to generate a Radial Distribution Function (RDF) plot. The first screenshot shows the 'Create Group' dialog box. The 'Current Group' is set to '0 : System'. Under 'Extracted Atom Names', the checkbox for 'O' is checked, and 'H' is unchecked. The 'New Group Name' field contains 'Oxy'. The 'Create' button is highlighted with a yellow arrow. The second screenshot shows the 'Radial Distribution Function' dialog box. The 'Reference Group' and 'Target Group' are both set to '3 : Oxy'. The 'First Frame [ps]' is set to '1.0'. The 'RDF' section has 'Definition' set to 'Atom', 'Output' set to 'RDF', and 'Temperature [K]' set to '300.'. The 'Draw' button is highlighted with a yellow arrow. The third screenshot shows the resulting RDF plot titled 'Radial distribution Oxy - Oxy'. The plot shows a sharp peak at approximately 0.3 nm and a smaller peak at approximately 0.5 nm. The x-axis is labeled 'r' and ranges from 0 to 2. The y-axis ranges from 0 to 4. Yellow arrows indicate the flow from the first window to the second, and from the second to the third. A blue arrow points from the 'Create Group' window towards the 'Radial Distribution Function' window.

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.

The screenshot illustrates the software interface for calculating Mean Square Displacement (MSD). On the left, the 'MD' menu is open, with 'LAMMPS' and 'Mean Square Displacement' highlighted. A blue arrow points from the 'Mean Square Displacement' option to the MSD dialog box. In the dialog box, the 'Draw' button is highlighted with a yellow arrow. The MSD graph shows a linear increase in displacement over time, with a diffusion constant of 2.9352 (+/- 1.2963) (1e-5 cm²/s) displayed at the bottom. A yellow arrow points from the diffusion constant box to the right.