

Winmostar tutorial LAMMPS Elongation V7.021

X-Ability Co,. Ltd. <u>question@winmostar.com</u> 2017/7/6



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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.
- Degree of polymerization (chain length), number of molecules, elongation rate, pressure control, Poisson ratio will affect outcomes.
- 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.



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



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Register a monomer

This tutorial will describe how to model a polyethylene.

- 1. Model a monomer of polyethylene (ethane, C_2H_6) on the main window.
- 2. Click MD | Assign Charges | By Acpype | Execute.
- 3. Uncheck User Charge to hide charge information
- 4. Click two hydrogens to be the end point of the monomer.





Register a monomer

- 1. Click MD | Polymer | Register Monomer.
- 2. Set Name to pe, and click OK.

I.

3. Click **OK** on the dialog.



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II. Define a polymer

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- 1. Click MD | Polymer | Homo Polymer Builder.
- 2. Set Polymer Name to pe50, Polymerization Degree to 50, Select pe in Monomer List.
- 3. Click Build.
- 4. Click Close

Edit View Semi-Empirical QM MD Solid Tools Tutorial Help Polymerization Remote Job Submission Rep1 H 1 \vee Chep Polymerization Degree 50 Solvate/Build Cell V Rep1 H 1 \vee Chep Monomer List Pe Insert Molecules 1 Y=1.0401 Z=0.0000 0.000 Lpr Polymerization Degree 50	
Solvate/Build Cell Inost Insert Molecules Generate Ions I Y=1.0401 Z=0.0000 H PP Monomer List Pe pmma_noc PP	
Assign Charges > Gromacs > LAMMPS > Amber > Polymer Register Monomer DPD Homo Polymer Builder Interface Builder Block Polymer Builder	play Delete
Winmostar V7.002	Head/Tail Configuration
saved successfully. New port of the second successfully. OK Build	Head to Tail Head to Head

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Homo Polymer Builder



III. Build Cell

- 1. Click MD | Polymer | Polymer Cell Builder.
- 2. Set Polymers Available to pe50, Number to 20, and click >> Add >>.
- 3. Click **Build**. Save as **pe_elong.mol2**.



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III. Build a simulation cell

Click **OK** on the dialog, then the simulation cell will be displayed on the window.
Click **Close** to close **Polymer Cell Builder**.



- 1. Click MD | LAMMPS | Keywords Setup.
- 2. Click Reset.

6			LAMN	1PS Setup		-	×
Basic Advance	Output Interaction	n Nor	n-equilibrium (1) Non	equilibrium (2) Options	Force Field		
Extending Simul	ation		Time Step [fs]	2.0	✔ Generate Veloc	ity	
Units	real	~	# of Time Steps	5000	Pressure Control	iso	\sim
Atom Style	full	~	Ensemble	minimize 🗸 🗸			
Pair Style	lj/cut/coul/cut	~	Temperature [K]	300.0			
Potential File		\sim	Pressure [atm]	1.0 1.0 1.0			
<pre>units real atom_style full boundary p p p box tilt large pair_style lj/cut/coul/cut 10. 10. pair_modify mix arithmetic special_bonds amber 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% thermo_style custom step time temp pe ke etotal enthalpy press vol density lx ly lx thermo 10 minimize 1e-4 1e-6 5000 1000000 write_restart %RESTFILE%</pre>					lx ly lz pxx	: pj	
<							>
ок	Cancel]		Load Setting	Save Setting		Reset

- 1. Select Force Field tab, Set Force Field to Dreiding, Charge to Use user-defined charges, then click OK.
- 2. Click MD | LAMMPS | Start LAMMPS.

Dasic	Advance	Output	Interaction	Non-equilibrium (1) Non-equi	librium (2) Option	ns Force Field	
۰G	enerate para	meters					_	
	Force field	ł	(General)	Dreiding	✓ Ex			
			(Water)	SPC/E	\vee			
- F	Charge							
	Assign	charges	Method:	AM1-P	~			
	Use us	er-defined	l charges	\langle				
	Add [p	osition re	straints] sec	tion for selected at	oms E	dit		
				Dump N	ow			
	se naramete	rs in the fi	e on the ma	in window				
	se paramete	o in the fi	ie on the ma					
	oporato Simi	dation Coll	Dictar	ace [A]: 12				
40	enerate sinit	lauon Cell	Distai	ICC [A]: 12.				

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- 1. Click MD | LAMMPS | Keywords Setup.
- 2. Check Extending Simulation, Set Ensemble to nvt, Temperature to 500. In Advance tab, check Constrain Hydrogen. Click OK.
- 3. Click MD | LAMMPS | Start LAMMPS.

2	LAMMPS Setup															
	Basic	Advance	Output	Interaction	Non-equ	uilibriu	m (1) N	on-equil	ibrium (2)	Options	Forc					
	✓ Ext	tending Sim	ulation		Ті	me St	ep [fs]	2.0			✓					
	Units		real		× #	ofTin	ne Steps	500	0		Pre					
	Atom S	Style	full		Er	nsemb	le	nvt		~						
	Pair St	yle	lj/cut/c	coul	Te	emper	ature [K]	500								
						8						LAMM	IPS Setup			-
						Ba	asic Ad	vance	0.	n [Non-e	equilibrium (1) Non-	equilibrium (2)	Options	Force Field	
						E	Boundary	Хр	γ γ <mark>ρ</mark>	∀ Z p	~	Reset COM Motion	linear	~	✓ box tilt large	
						E	Energy To	lerance	1e-4			Reset Interval	50		rigid	
						F	Force Tole	rance	1e-6			Random Seed	12345		Constrain Hydr	ogen
						1	Tdamp [fs]]	100.			Tchain	3		Shake Tolerance	1e-4
						F	Pdamp [fs]]	100.			Pchain	3			

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- 1. Click MD | LAMMPS | Keywords Setup.
- 2. Uncheck Generate Velocity in the Basic tab,
- Set Ensemble to npt, Pressure to 200, then click OK.
- 3. Click **MD** | **LAMMPS** | **Start LAMMPS**.

ŝ	0					LÆ	PS Setup				_ □	×	
[Basic	Advance	Output	Interaction	Non-	equilibrium (1)	Non-	equilibrium (2)	Options	Force Field			
	√ Ext	ending Sim	g Simulation			Time Step [fs]		2.0 Generate V			locity		
	Units	nits real		~	✓ # of Time Steps		5000		Pressure Contro	iso		~	
	Atom S	Style	full		٧	Ensemble		npt					
	Pair St	Style lj/cut/coul/cut		~	✓ Temperature [K]		500						
	Potent	ial File			\sim	Pressure [atm]]	200					



- 1. Click MD | LAMMPS | Keywords Setup.
- 2. In **Basic** tab, set **Temperature** to **250**, **Pressure** to **1**, then click **OK**.
- 3. Click **MD | LAMMPS | Start LAMMPS**.

30	LAMMPS Setup										
Basic Advance C	Output Interaction	Non-equilibrium (1)	Non-equilibrium (2)	Options	Force Field						
Extending Simula	ation	Time Step [fs]	2.0		Generate Velocity						
Units	real	✓ # of Time Step	ps 5000	5000		iso		~			
Atom Style	full	✓ Ensemble	npt	~							
Pair Style	lj/cut/coul/cut	✓ Temperature [[K] 250								
Potential File		V Pressure [atm									
	· · ·	-									

Next, calculate elongation to produce strain and stress curve.

- 1. Click MD | LAMMPS | Keywords Setup.
- 2. On Basic tab, set # of Time Steps to 50000, Pressure Control to xy,
- 3. On **Non-equilibrium (1)** tab, check **Enable Elongation**, set **Eng**, set **Strain Rate** to **1e-5**, then click **OK**.
- 4. Click MD | LAMMPS | Start LAMMPS

SS 1	AMMPS Setup	
Basic Advance Output Interaction Non-equilibrium (1)	Non-equilibrium (2) Options Force Field	
Extending Simulation Time Step [fill]	3] 2.0 Generate Velocity	
Units real # of Time St	eps 50000 Pressure Control xy	
Atom Style full Characteristic Ensemble	npt 😻	LAMMPS Setup
Pair Style lj/cut/coul/cut V Temperature	[K] 250 Basic Advance Output In	tgraction Non-equilibrium (1) Non-equilibrium (2) Options
Potential File	m] 1 Snable Elongation	Enable Simulated Annealing
	✓ Affine Transformation	Final Temperature 300.0
	Eng. Strain Rate 1e-5 [1/fs]	Annealing Rate: N/A
	Max Eng. Strain: 1.000	
	Preserve Volume	



- 1. Click MD | LAMMPS | Energy Plot. Open the file by default.
- 2. Check Lz (System size of z direction) and Pzz (Pressure of z direction) in Energy terms. Check Block Average, set Size to 10.
- 3. Click Draw, then Click Excel.



Columns **A**, **B**, and **C** contains MD time steps, **Lz**(System size of z direction) and **Pzz** (Pressure of z direction) respectively. Columns **D** and **E** contain strain and stress respectively, and can be calculated as described below.

To calculate column **D**: Normalize the first value of **Lz** in column **B** (**41.07478**) and subtract 1.

To calculate column E: Multiply -1 to Pzz values in column C.

The graph manifests stress-strain curve by taking values from column **D** for the X-axis and column **E** for the Y-axis. (Graph shown is plotted with a lower limit of 0 in the Y-axis)



reference: Hossain, D., Tschopp, M.A., Ward, D.K., Bouvard, J.L., Wang, P., Horstemeyer, M.F., Polymer, 51 (2010) 6071-6083.

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- 1. Click MD | LAMMPS | Import Trajectory in the main window.
- 2. Open the files selected by default.
- 3. Click 3D in Animation window.



- 1. Click View | Preferences on the Winmostar 3D.
- 2. Check Rainbow in Preferences window.
- 3. Click |> (Play) button to check the polymers are elongating.



