

Network for Computational Nanotechnology (NCN)

Purdue, Norfolk State, Northwestern, MIT, Molecular Foundry, UC Berkeley, Univ. of Illinois, UTEP

Polymer Modeler: User Guide

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PURDUE
UNIVERSITY

OUTLINE

- Polymer Builder (Page 3)
 - » Beginner's Guide
 - » Advanced Guide
- Molecular Dynamics Simulations (Page 30)
 - » Beginner's Guide
 - » Advanced Guide

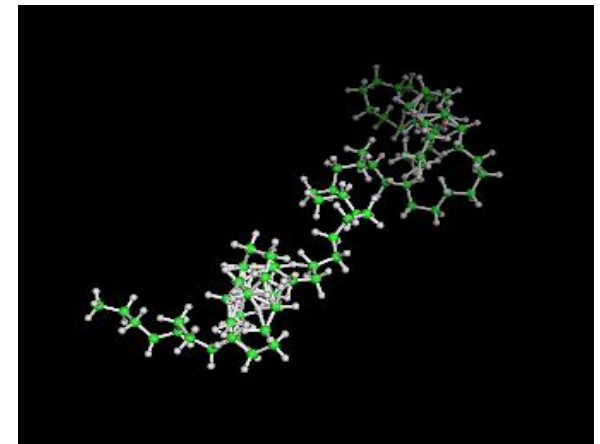
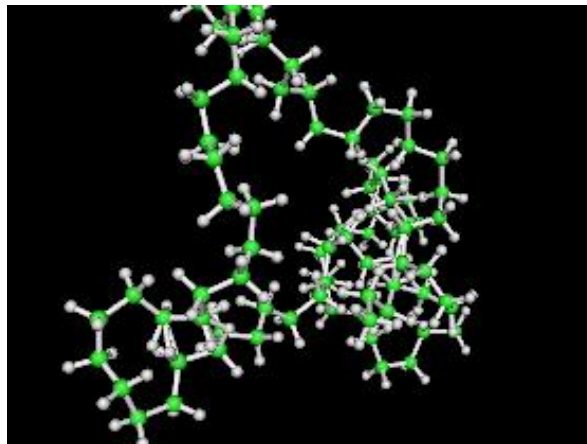
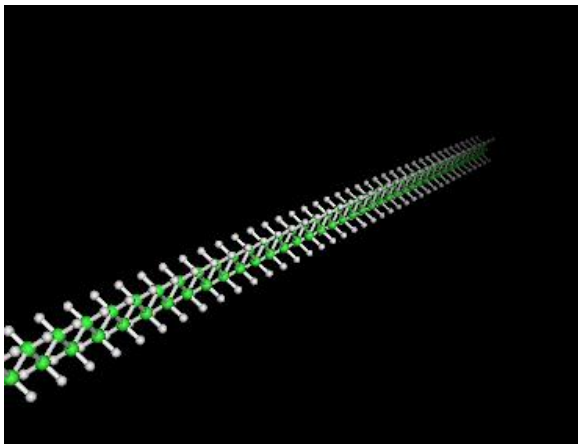
POLYMER BUILDER

OUTLINE: Polymer Builder

- Polymer Builder: An Introduction
- Getting Started: Beginner's Guide
 - » First Step: Choosing a monomer
 - » Number of monomers and chains
 - » Energy Interactions
 - ✓ Torsion angles: all-trans, freely rotating chain
 - » Outputs
- Advanced Options: Expert's Guide
 - » Building a monomer: z-matrix format
 - » Energy Interactions
 - ✓ Torsion angles distribution: energies and probabilities
 - ✓ Long range interactions
 - » Temperature and cell dimensions
 - » Output: Ideal length function
 - » Exploring other options

POLYMER BUILDER: The tool

- The polymer builder tool allows the user to create atomic level structures of linear polymer chains.
- Polymers are made of long chains formed by repeated units called monomers.
- Through the multiple tool options, changes in torsions angles and other energy interactions can be observed.
- Effect of temperature changes in the system may also be noted.



GETTING STARTED

Beginner's Guide

Using the builder

1 Structure → 2 Simulation → 3 Simulate

Structure options: Use pre-built polymers

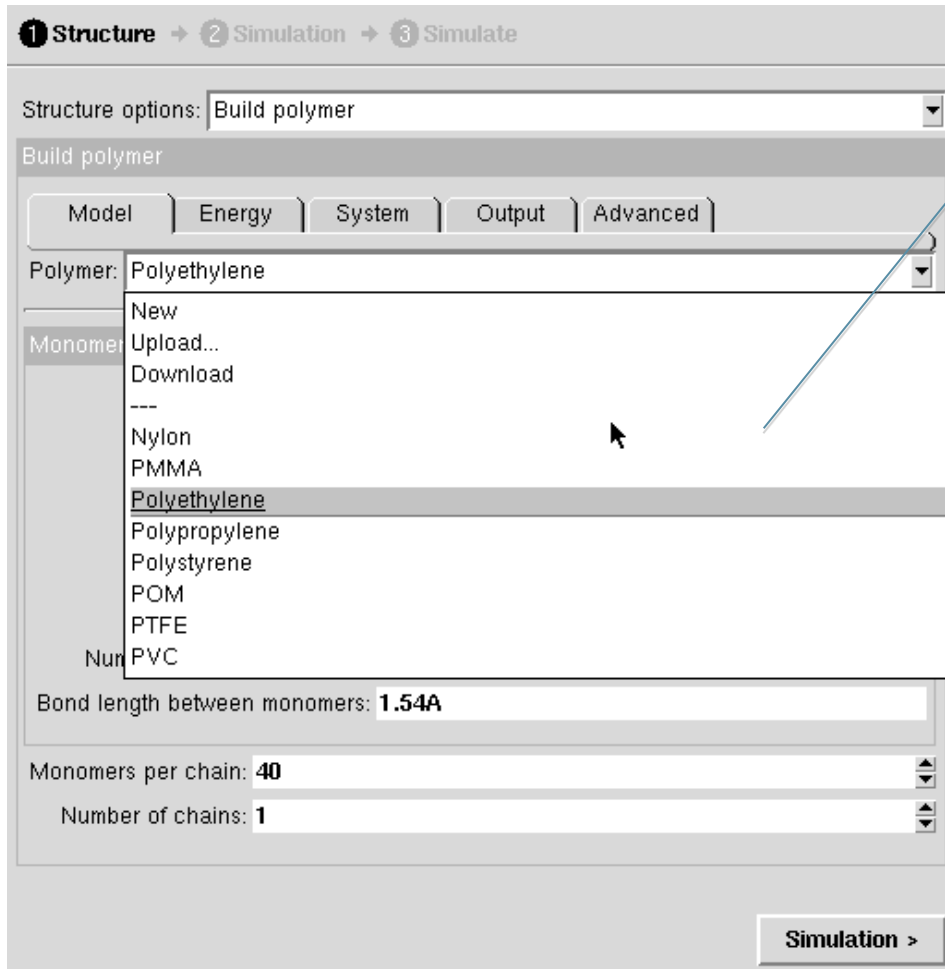
Pre-built polymers: Build polymer
Use pre-built polymers

Choice: Pre-built polymer 1

Simulation >

Select the option stating
“Build Polymer”

First Step: Choosing a monomer.



1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced

Polymer: Polyethylene

Monomer

- New
- Upload...
- Download
-
- Nylon
- PMMA
- Polyethylene
- Polypropylene
- Polystyrene
- POM
- PTFE
- Nur PVC

Bond length between monomers: 1.54A

Monomers per chain: 40

Number of chains: 1

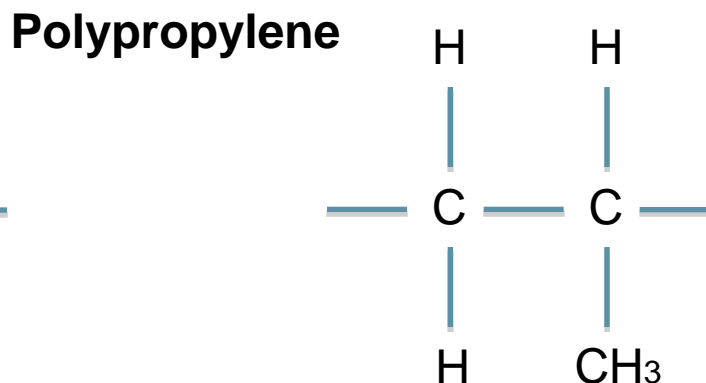
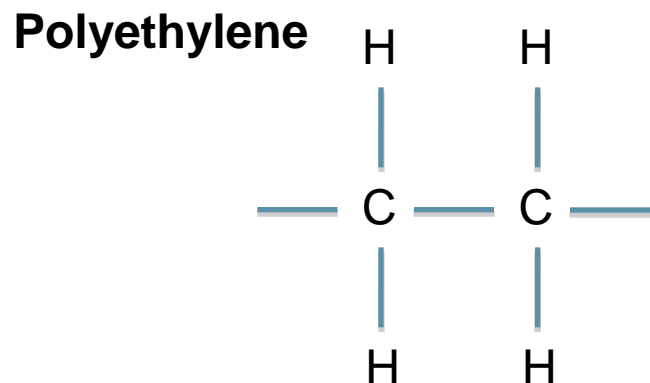
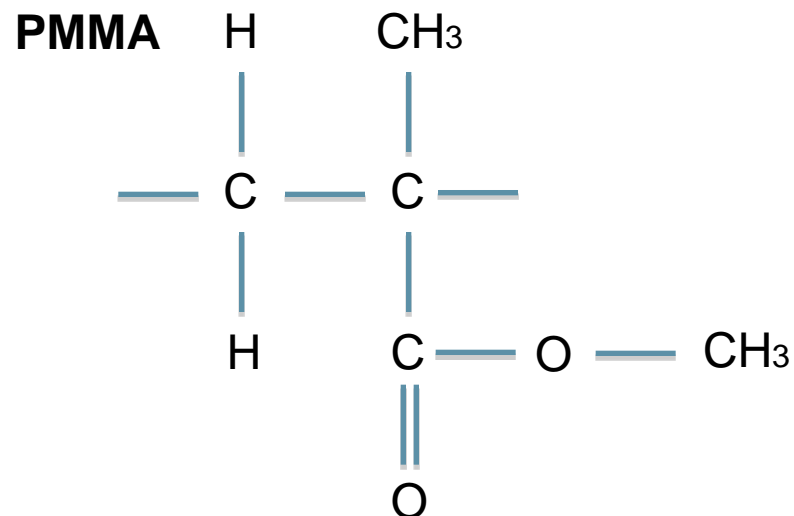
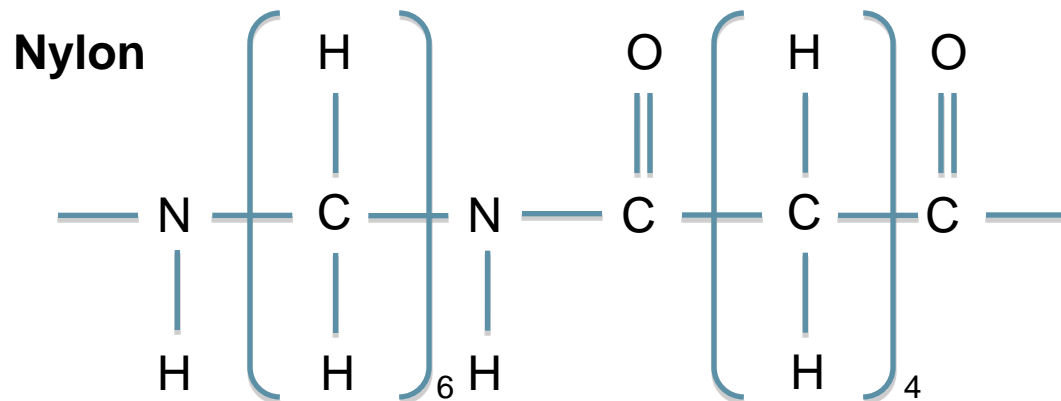
Simulation >

Choosing a built in monomer

If a built-in monomer is chosen, the z-matrix, number of backbone atoms, and bond length between monomers are automatically loaded

Getting Started

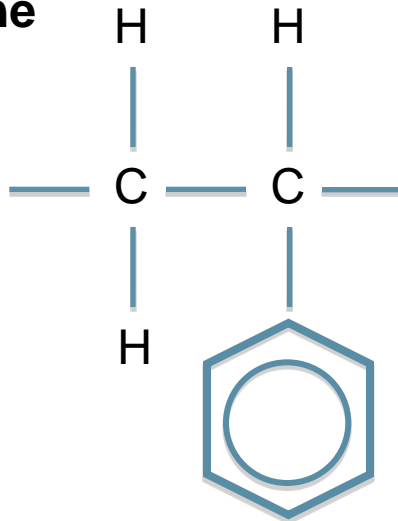
Polymers repeat units (monomers) used:



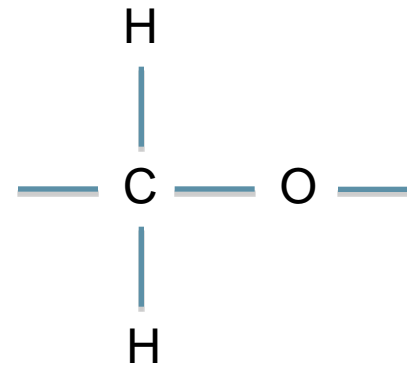
Getting Started

Polymers repeat units (monomers) used:

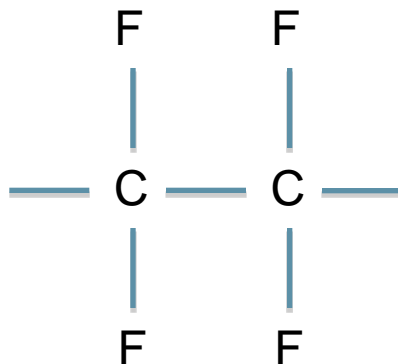
Polystyrene



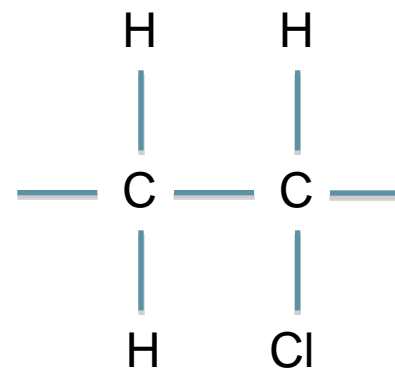
POM



PTFE



PVC



Getting Started

Choose the number of monomers and chains

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced

Polymer: Polyethylene

Monomer z-matrix

z-matrix:

H							
C3	1	1.09					
C3	2	1.54	1	112			
H	3	1.09	2	112	1	180	
H	2	1.09	1	112	3	120	
H	2	1.09	1	112	3	-120	
H	3	1.09	4	112	2	120	
H	3	1.09	4	112	2	-120	

Number of backbone atoms: 4

Bond length between monomers: 1.54Å

Monomers per chain: 40

Number of chains: 1

Simulation >

Specify the number of monomers that each chain will contain

Specify the number of chains to be built, each with the specified number of monomers

Getting Started

Specify the desired distribution of torsion angles

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced

Torsion angles Long-range interactions

Predefined: Freely rotating chain

New

All trans (rodlike)

Freely rotating chain

Format: angle (deg) probability

RIS energies: Enter RIS angles and energies here

Format: angle (deg) energy (eV)

Simulation >

All torsion angles are set to 180°

All angles are equally likely, therefore uniform distribution of angles is selected

Getting Started

Choose the outputs that you want to observe

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced

View constructed chains: ☒ yes

Animate rotation: ☒ yes

Plot theoretical end-to-end length: ☒ yes

Theoretical end-to-end chain length

Theoretical chain length, R , is a power law function of a prefactor, C , the number of backbone atoms, n , and an exponent, p .

$$R = Cn^p$$

Prefactor: 1.0

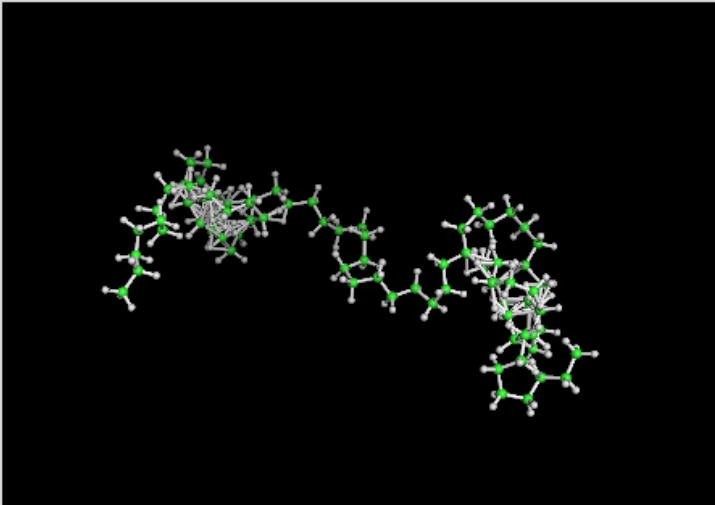
Power: 0.5

Results: Molecular structures.
Displays the chains constructed.
Example shows one freely rotating polyethylene chain of 40 monomers.

Simulation >

1 Input → 2 Simulate

Result: Molecular structures



1 result Parameters... Clear

< Input

Getting Started

Choose the outputs that you want to observe

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model | Energy | System | Output | Advanced

View constructed chains: ☒ yes

Animate rotation: ☒ yes

Plot theoretical end-to-end length: ☒ yes

Theoretical end-to-end chain length

Theoretical chain length, R , is a power law function of a prefactor, C , the number of backbone atoms, n , and an exponent, p .

$$R = Cn^p$$

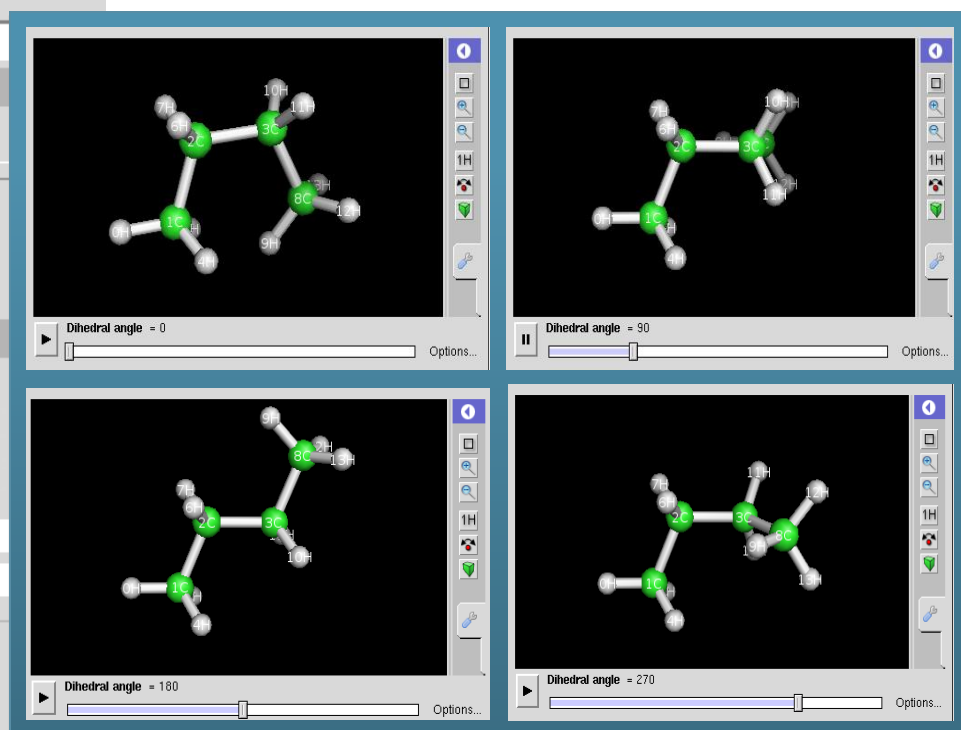
Prefactor: 1.0

Power: 0.5

Results: Monomer rotation.

The animate rotation varies the torsion angles from 0 to 360 degrees between two monomers, showing the effect of the dihedral angle variations

Simulation >



Getting Started

Choose the outputs that you want to observe

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced

View constructed chains: ☒ yes

Animate rotation: ☒ yes

Plot theoretical end-to-end length: ☒ yes

Theoretical end-to-end chain length

Theoretical chain length, R , is a power law function of a prefactor, C , the number of backbone atoms, n , and an exponent, p .

$$R = Cn^p$$

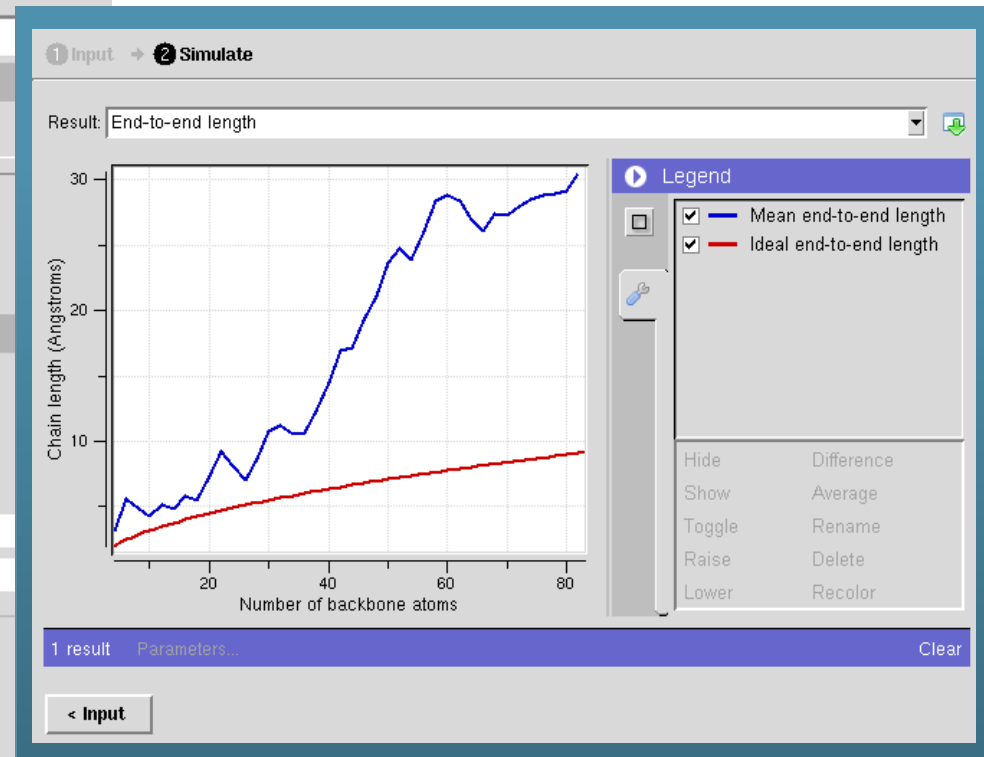
Prefactor: 1.0

Power: 0.5

Results: End-to-end length.

Outputs a graph of the mean end-to-end length of the polymer chain as well as the theoretical length according to the function specified.

Simulation >



Accuracy of mean end-to-end length depends on number of chains built.

Observing the outputs

1 Structure → 2 **Simulation** → 3 Simulate

Simulation choice:

Structure output only

Run LAMMPS on structure

< Structure

Simulate >

In order to output the polymer structure without running MD simulations, select this option

This panel appears after the simulation button, on the bottom right corner of the first panel, is pressed.

ADVANCED OPTIONS

Expert's Guide

Steps to specify a new monomer

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model | Energy | System | Output | Advanced

Polymer: Polyethylene

Monomer z-matrix

z-matrix:

H							
C3	1	1.09					
C3	2	1.54	1	112			
H	3	1.09	2	112	1	180	
H	2	1.09	1	112	3	120	
H	2	1.09	1	112	3	-120	
H	3	1.09	4	112	2	120	
H	3	1.09	4	112	2	-120	

Number of backbone atoms: 4

Bond length between monomers: 1.54Å

Monomers per chain: 40

Number of chains: 1

Simulation >

Step 1: Build the z-matrix

Step 2: Specify backbone atoms

Step 3: Specify bond length

Advanced Options

Step 1: Building the z-matrix

Diagram illustrating the structure of a molecule (likely a branched alkane) with labels for atoms, bond lengths, bond angles, and torsion angles.

Labels:

- First atom
- Line number of the atom it is linked to
- Distance to atom it is linked to
- Atom that defines angle
- Bond angle
- Atom that defines torsion angle
- Torsion (or dihedral) angle

Structure Data:

Atom	Line number	Distance (Å)	Atom	Bond angle (°)	Atom	Torsion angle (°)
H	1	1.09	C3	112	1	180
C3	2	1.54	H	112	3	120
C3	3	1.09	H	112	3	120
H	2	1.09	H	112	3	-120
H	2	1.09	H	112	2	120
H	3	1.09	H	112	2	-120
H	3	1.09	H	112	2	-120

Step 2: Specifying the backbone atoms

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model | Energy | System | Output | Advanced

Polymer: Polyethylene

Monomer z-matrix

z-matrix:

H	1	1.09				
C3	2	1.54	1	112		
C3	3	1.09	2	112	1	180
H	2	1.09	1	112	3	120
H	2	1.09	1	112	3	-120
H	3	1.09	4	112	2	120
H	3	1.09	4	112	2	-120

Number of backbone atoms: 4

Bond length between monomers: 1.54Å

Monomers per chain: 40

Number of chains: 1

Simulation >

Backbone atoms MUST be listed first when creating the z-matrix

Specify the number of atoms that represent the backbone of the monomer

Step 3: Specifying the bond length

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model | Energy | System | Output | Advanced

Polymer: Polyethylene

Monomer z-matrix

z-matrix:

H							
C3	1	1.09					
C3	2	1.54	1	112			
H	3	1.09	2	112	1	180	
H	2	1.09	1	112	3	120	
H	2	1.09	1	112	3	-120	
H	3	1.09	4	112	2	120	
H	3	1.09	4	112	2	-120	

Number of backbone atoms: 4

Bond length between monomers: 1.54Å

Monomers per chain: 40

Number of chains: 1

Simulation >

Specify the bond length between the monomers

When creating the polymer chain the head of one monomer and the tail atom of the other are removed, this length represents the distance of the new bond created.

Setting torsion angles

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced

Torsion angles Long-range interactions

Predefined: New

Torsions: Rotational isomer states, energies

RIS probabilities: Uniform distribution
Rotational isomer states, probabilities
Rotational isomer states, energies

Format: angle (deg) probability

RIS energies: Enter RIS angles and energies here

Format: angle (deg) energy (eV)

Simulation >

Define using probabilities

Define using energies

Specify which torsions angles are energetically favored

Define torsion angles occurrence using probabilities

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced

Torsion angles Long-range interactions

Predefined: New

Torsions: Rotational isomer states, probabilities

RIS probabilities: Enter RIS angles and probabilities here

Format: angle (deg) probability

RIS energies: Enter RIS angles and energies here

Format: angle (deg) energy (eV)

Simulation >

To specify torsion angles using probabilities, enter angle (in degrees) followed by probability, separated by a space

Note: Do NOT include units in input

Define torsion angles occurrence using energies

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced

Torsion angles Long-range interactions

Predefined: New

Torsions: Rotational isomer states, energies

RIS probabilities: Enter RIS angles and probabilities here

Format: angle (deg) probability

RIS energies: Enter RIS angles and energies here

Format: angle (deg) energy (eV)

Simulation >

To specify torsion angles using energies, enter angle (in degrees) followed by its energy (in eV), separated by a space

Probability is calculated from the energies using the Maxwell-Boltzman probability with the temperature specified on the System tab

Advanced Options

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced

Torsion angles Long-range interactions

Self-avoiding chain: ☒ yes

Not self-avoiding chain

Self-avoiding chain

Simulation >

Prevents polymer chains from self intersecting

Advanced Options

Define the system volume

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model | Energy | System | Output | Advanced

Volume

System volume: Specify cell dimensions

Density: Specify polymer density

Cell dimensions: Specify cell dimensions

Format: a b c (Angstroms)

Temperature: 300K

Simulation >

Specify the system's volume using the polymer's density.

Express density in grams per cubic centimeter (g/cm^3)

Specify the cell dimensions of the system in Angstroms

Note: Do NOT include units in input

Advanced Options

Define the system temperature

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model Energy System Output Advanced


Volume

System volume: Specify cell dimensions

Density: Specify polymer density

Cell dimensions: Specify cell dimensions

Format: a b c (Angstroms)

Temperature:  300K

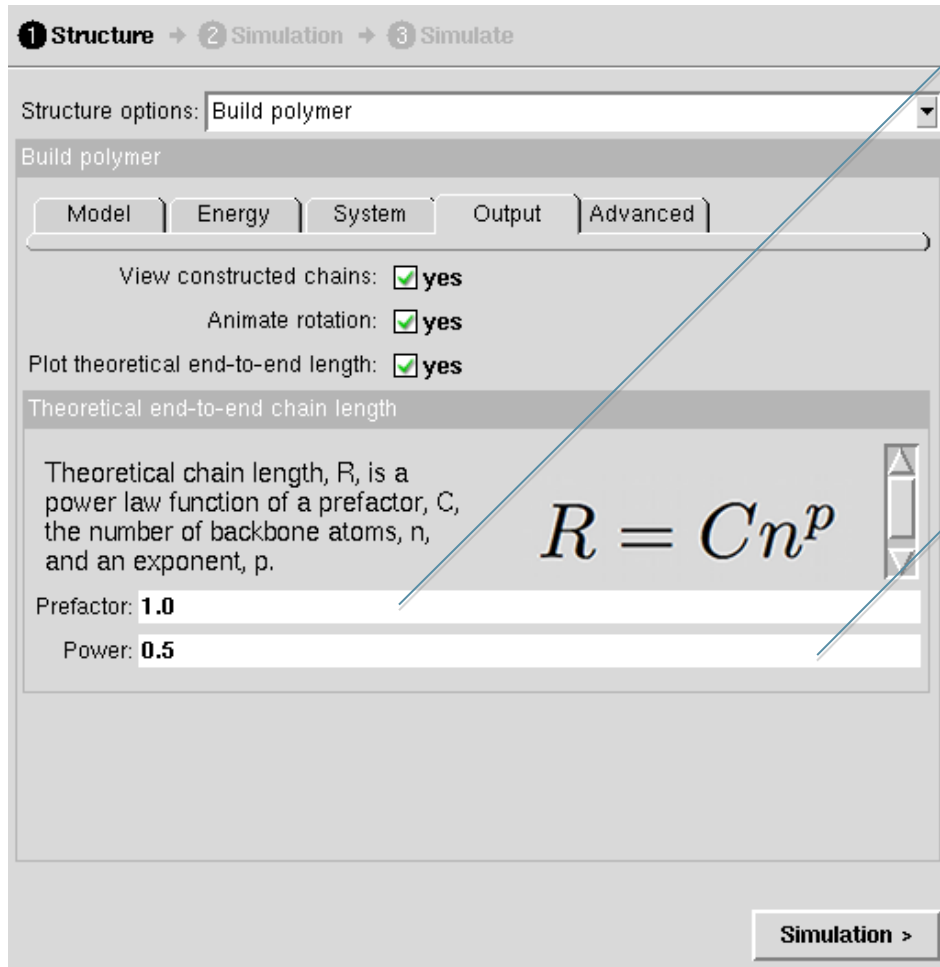
Simulation >

Specify the temperature of the system

This temperature will be used in the calculation of the torsion angles probabilities for the given energies, using the Maxwell-Boltzman probability.

Advanced Options

Defining the theoretical end-to-end length function



1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model | Energy | System | Output | Advanced

View constructed chains: ☒ yes

Animate rotation: ☒ yes

Plot theoretical end-to-end length: ☒ yes

Theoretical end-to-end chain length

Theoretical chain length, R , is a power law function of a prefactor, C , the number of backbone atoms, n , and an exponent, p .

$$R = Cn^p$$

Prefactor: 1.0

Power: 0.5

Simulation >

The prefactor C depends of the polymer being built

For polyethylene:
Rod-like chain $C \rightarrow 1.28$,
Freely-rotating chain $C \rightarrow 2.28$.

The exponent P represents the model used to calculate the theoretical end to end length

For a random walk $P \rightarrow 1/2$,
Rod-like chain $P \rightarrow 1$,
Self-avoiding random walk $P \rightarrow 3/5$,
Strong Attraction $P \rightarrow 1/3$.

Advanced Options

Exploring other options

1 Structure → 2 Simulation → 3 Simulate

Structure options: Build polymer

Build polymer

Model | Energy | System | Output | Advanced

Random number generator seed: 0

Write z-matrices: ☐ no

Simulation >

Assign a number generator seed to exactly reproduce results later

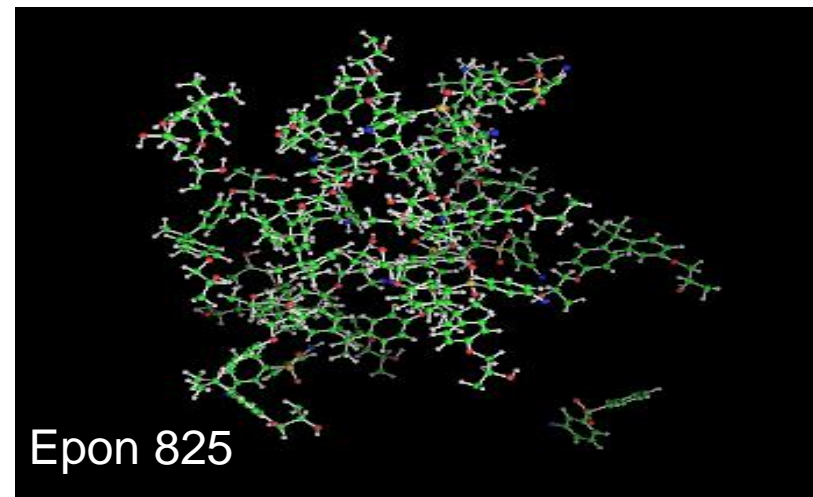
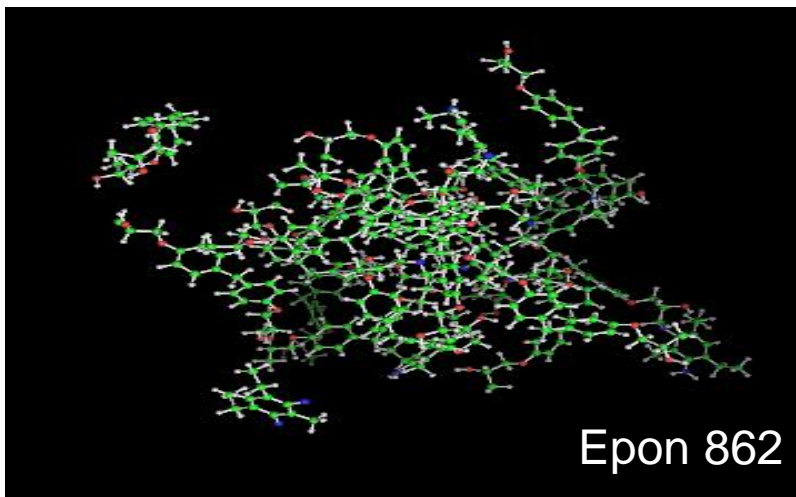
MOLECULAR DYNAMIC SIMULATIONS

OUTLINE: Molecular Dynamic Simulations

- MD Simulations: An Introduction
- Getting Started: Beginner's Guide
 - » Running LAMMPS on structure
 - » Energy Expression
 - » Drivers
 - ✓ Setting the ensemble
 - ✓ Strain Rate
 - ✓ Periodic Tasks
- Advanced Options: Expert's Guide
 - » Thermalizing system

Molecular Dynamic Simulations

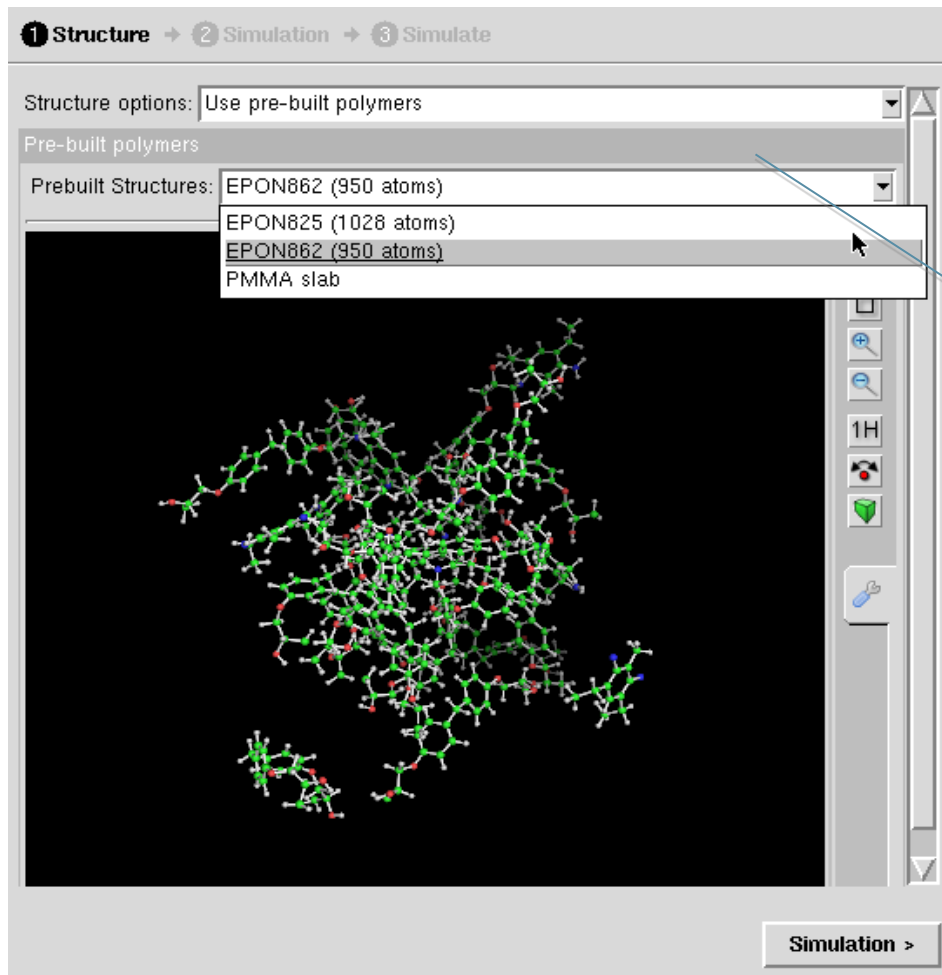
- Molecular dynamics consists in following the motion of all the atoms in your material.
- The tool provides an easy to understand interface to allow users to set up molecular dynamic simulations.
- Using the open source code LAMMPS, different polymeric samples can be deformed and different outputs can be observed.



GETTING STARTED

Beginner's Guide

Using pre-built polymers

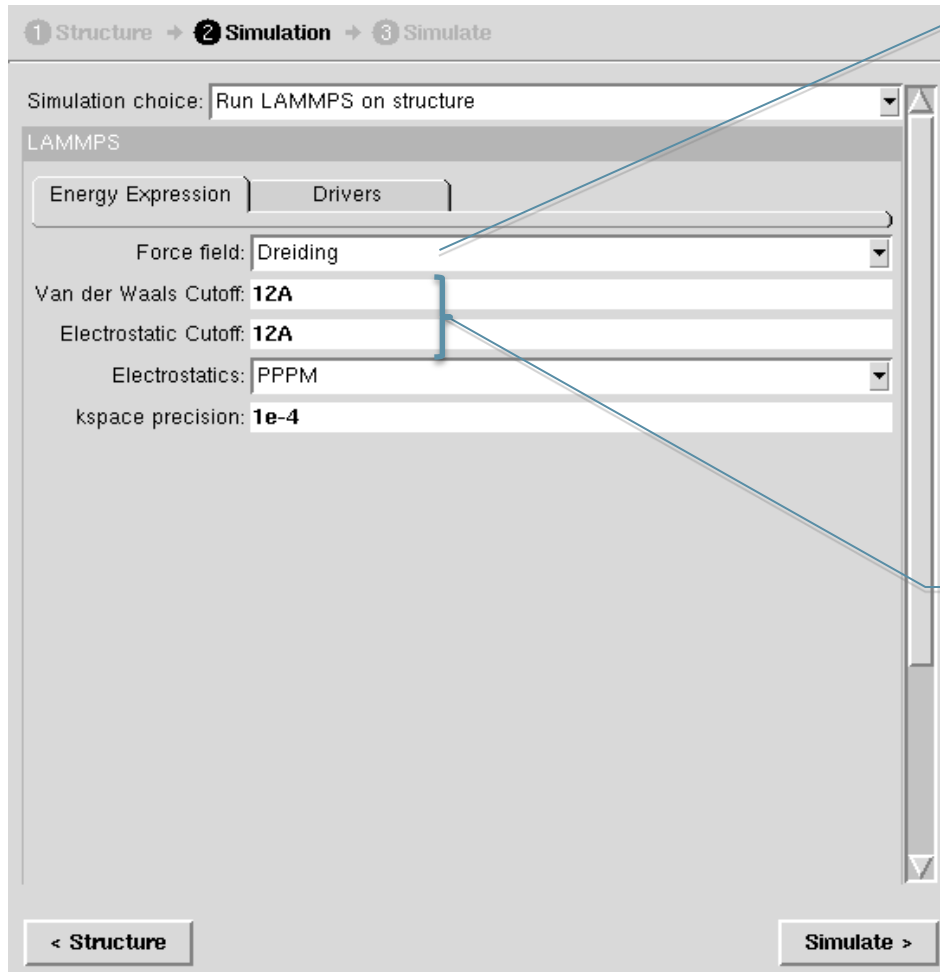


Select any of the polymer pre-built structures

You may also build your own polymer structure using the builder presented previously.

Getting Started

Running LAMMPS on structure



The screenshot shows the nanoHUB interface for running LAMMPS simulations. At the top, there are three tabs: 1 Structure, 2 Simulation (selected), and 3 Simulate. Below the tabs, the 'Simulation choice' dropdown is set to 'Run LAMMPS on structure'. Under the 'LAMMPS' section, there are two tabs: 'Energy Expression' (selected) and 'Drivers'. The 'Energy Expression' tab contains several settings: 'Force field' is set to 'Dreiding', 'Van der Waals Cutoff' is set to '12A', 'Electrostatic Cutoff' is set to '12A', 'Electrostatics' is set to 'PPPM', and 'k-space precision' is set to '1e-4'. At the bottom of the interface, there are two buttons: '< Structure' and 'Simulate >'. Two blue lines point from the text boxes on the right to the 'Force field' and 'Van der Waals Cutoff' settings.

Force fields dictate how the forces between atoms are approximated.

Currently Dreiding is the only option offered and is a good generic force field. More application specific force fields exist and may be added later

These two cutoffs dictate after what distance the interactions between atoms are no longer calculated.

Getting Started

Running LAMMPS on structure

1 Structure → 2 Simulation → 3 Simulate

Simulation choice: Run LAMMPS on structure

LAMMPS

Energy Expression Drivers

Force field: Dreiding

Van der Waals Cutoff: 12A

Electrostatic Cutoff: 12A

Electrostatics: PPPM

kspace precision: 1e-4

< Structure Simulate >

The PPPM and ewld options will calculate electrostatic interactions beyond the cutoff specified above

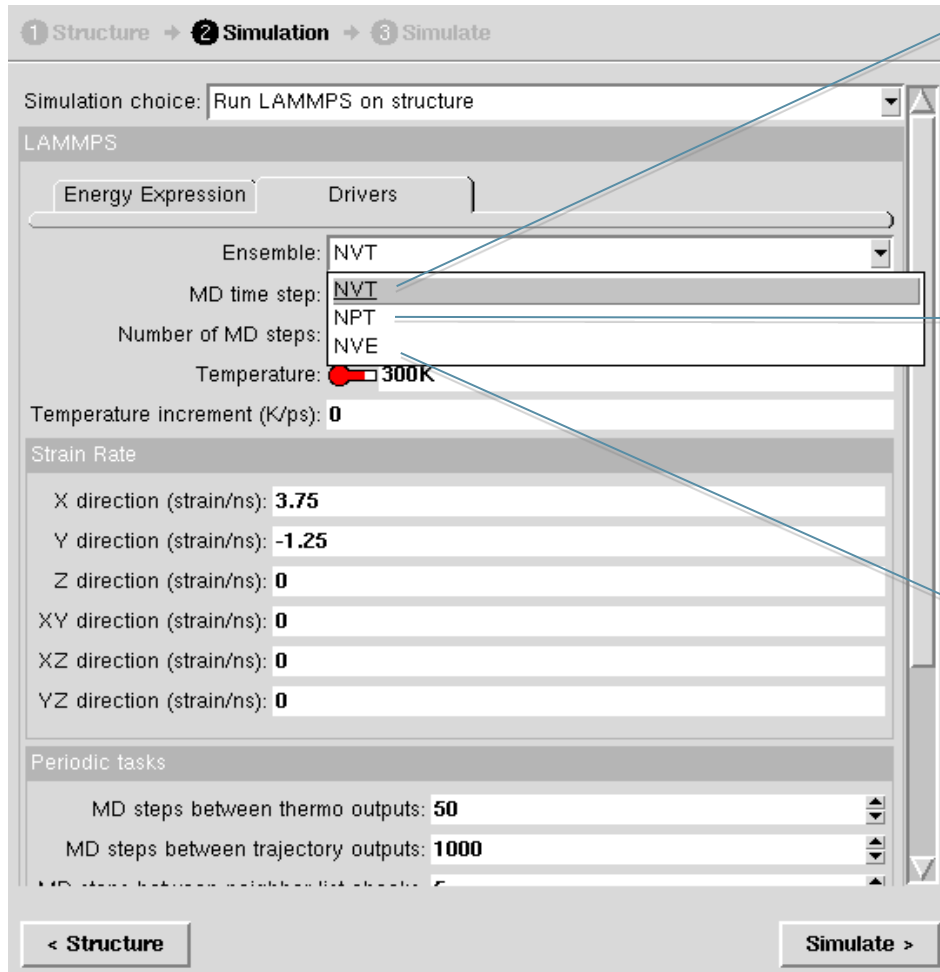
The cutoff option will ignore all long range interactions.

This specifies how many kspace vectors are present in the ewld option or FFT grid size in PPPM.

1e-4 corresponds to 1 part in a million

Getting Started

Setting the ensemble



1 Structure → 2 Simulation → 3 Simulate

Simulation choice: Run LAMMPS on structure

LAMMPS

Energy Expression Drivers

Ensemble: NVT

MD time step: NVT

Number of MD steps: NPT

Temperature: 300K

Temperature increment (K/ps): 0

Strain Rate

X direction (strain/ns): 3.75

Y direction (strain/ns): -1.25

Z direction (strain/ns): 0

XY direction (strain/ns): 0

XZ direction (strain/ns): 0

YZ direction (strain/ns): 0

Periodic tasks

MD steps between thermo outputs: 50

MD steps between trajectory outputs: 1000

< Structure Simulate >

This ensemble controls the number of atoms, volume, and temperature of the system.

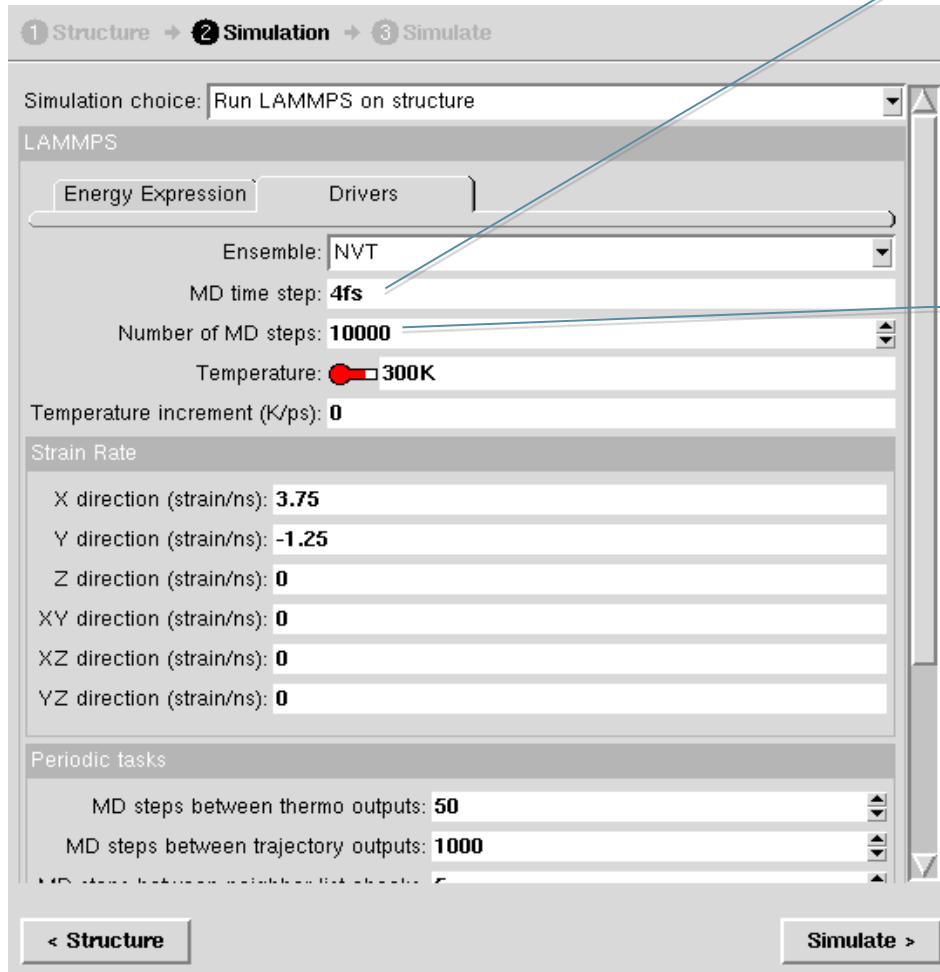
This ensemble controls the number of atoms, pressure, and temperature of the system.

This ensemble controls the number of atoms, volume, and total energy of the system.

If a strain is to be applied NVT or NVE should be selected.

Getting Started

Specify the different drivers



1 Structure → 2 Simulation → 3 Simulate

Simulation choice: Run LAMMPS on structure

LAMMPS

Energy Expression Drivers

Ensemble: NVT

MD time step: 4fs

Number of MD steps: 10000

Temperature: 300K

Temperature increment (K/ps): 0

Strain Rate

X direction (strain/ns): 3.75

Y direction (strain/ns): -1.25

Z direction (strain/ns): 0

XY direction (strain/ns): 0

XZ direction (strain/ns): 0

YZ direction (strain/ns): 0

Periodic tasks

MD steps between thermo outputs: 50

MD steps between trajectory outputs: 1000

MD steps between virial stress outputs: 1000

< Structure Simulate >

Length of time between MD steps.

Shorter time steps give more accurate results but increases computation time.

Total number of time steps in the simulation.

Specify the different drivers

1 Structure → 2 Simulation → 3 Simulate

Simulation choice: Run LAMMPS on structure

LAMMPS

Energy Expression Drivers

Ensemble: NVT

MD time step: 4fs

Number of MD steps: 10000

Temperature: 300K

Temperature increment (K/ps): 0

Strain Rate

X direction (strain/ns): 3.75

Y direction (strain/ns): -1.25

Z direction (strain/ns): 0

XY direction (strain/ns): 0

XZ direction (strain/ns): 0

YZ direction (strain/ns): 0

Periodic tasks

MD steps between thermo outputs: 50

MD steps between trajectory outputs: 1000

MD steps between neighbor list checks: 5

< Structure Simulate >

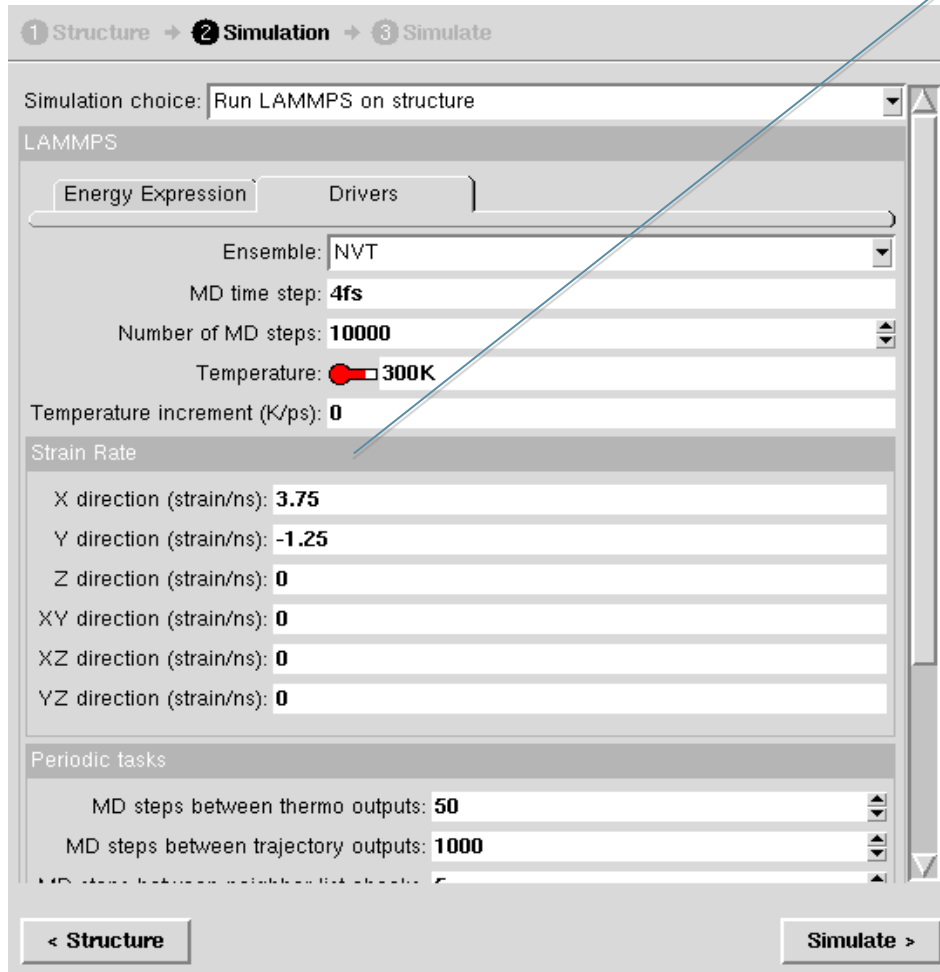
Sets the temperature of the system.

System temperature is regulated using a Nose/Hoover thermostat.

Controls the rate at which the temperature is changed over the course of the simulation.

Getting Started

Set the strain rate for the different directions



The screenshot shows the 'Simulation' tab of the nanoHUB interface. The 'Simulation choice' is 'Run LAMMPS on structure'. Under the 'LAMMPS' section, the 'Ensemble' is set to 'NVT', 'MD time step' is '4fs', 'Number of MD steps' is '10000', and 'Temperature' is '300K'. The 'Strain Rate' section is highlighted with a blue box and a line pointing to the text 'Set the strain rate for the different directions'. The strain rates are: X direction (3.75), Y direction (-1.25), Z direction (0), XY direction (0), XZ direction (0), and YZ direction (0). The 'Periodic tasks' section shows 'MD steps between thermo outputs' as 50 and 'MD steps between trajectory outputs' as 1000. Navigation buttons '< Structure' and 'Simulate >' are at the bottom.

The strain rate controls the rate of deformation performed on the system. Deformation can be applied in any combination of the principle and shear directions.


Note: All Strain rates are in engineering strain.

When using large negative strain rates, if the strain rate combined with the simulation length make the sample contract more than physically possible, an error will be encountered and a smaller strain rate or shorter simulation length will be necessary.

Getting Started

Periodic Tasks

1 Structure → 2 Simulation → 3 Simulate

Temperature:  300K

Temperature increment (K/ps): 0

Strain Rate

X direction (strain/ns): 3.75

Y direction (strain/ns): -1.25

Z direction (strain/ns): 0

XY direction (strain/ns): 0

XZ direction (strain/ns): 0

YZ direction (strain/ns): 0

Periodic tasks

MD steps between thermo outputs: 50

MD steps between trajectory outputs: 1000

MD steps between neighbor list checks: 5

Thermalization

Thermalize system before MD run?: ☐ no

Ensemble: NVT

Number of thermalization steps: 1000

< Structure Simulate >


How many steps between output writings

Computer will perform calculations to update the atoms every MD step.

How often the program will write atom positions to the trajectory file.

Periodic Tasks

1 Structure → 2 Simulation → 3 Simulate

Temperature:  300K

Temperature increment (K/ps): 0

Strain Rate

X direction (strain/ns): 3.75

Y direction (strain/ns): -1.25

Z direction (strain/ns): 0

XY direction (strain/ns): 0

XZ direction (strain/ns): 0

YZ direction (strain/ns): 0

Periodic tasks

MD steps between thermo outputs: 50

MD steps between trajectory outputs: 1000

MD steps between neighbor list checks: 5

Thermalization

Thermalize system before MD run?: ☐ no

Ensemble: NVT

Number of thermalization steps: 1000

< Structure Simulate >

Controls how often LAMMPS creates a new list of nearby atoms for each atom in the system.

If an error stating an atom has been lost occurs, decreasing this number will create a new neighbor list more often. However, lower values increase computation time.


ADVANCED OPTIONS

Expert's Guide

Advanced Options

Check the box to thermalize system before running simulations

1 Structure → 2 Simulation → 3 Simulate

Temperature:  300K

Temperature increment (K/ps): 0

Strain Rate

X direction (strain/ns): 3.75

Y direction (strain/ns): -1.25

Z direction (strain/ns): 0

XY direction (strain/ns): 0

XZ direction (strain/ns): 0

YZ direction (strain/ns): 0

Periodic tasks

MD steps between thermo outputs: 50

MD steps between trajectory outputs: 1000

MD steps between neighbor list checks: 5

Thermalization

Thermalize system before MD run?: ☒ no

Ensemble: NVT

Number of thermalization steps: 1000

< Structure Simulate >

Heats the system to 600K for a period of time in order to allow atoms to shift positions and reach an overall lower energy configuration.


Note: Output data is not reported during thermalization.

After thermalization another simulation is performed using the conditions specified in the options below.

Advanced Options

Check the box to thermalize system before running simulations

1 Structure → 2 Simulation → 3 Simulate

Temperature:  300K

Temperature increment (K/ps): 0

Strain Rate

X direction (strain/ns): 3.75

Y direction (strain/ns): -1.25

Z direction (strain/ns): 0

XY direction (strain/ns): 0

XZ direction (strain/ns): 0

YZ direction (strain/ns): 0

Periodic tasks

MD steps between thermo outputs: 50

MD steps between trajectory outputs: 1000

MD steps between neighbor list checks: 5

Thermalization

Thermalize system before MD run?: ☐ no

Ensemble: NVT

Number of thermalization steps: 1000

< Structure Simulate >

Ensemble options are the same as earlier and do not have to match the ensemble used later in the simulation.

The thermalization will run for this number of MD steps.

Note: The time of each step is the same as selected earlier.