Polymer Modeler: User Guide

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OUTLINE

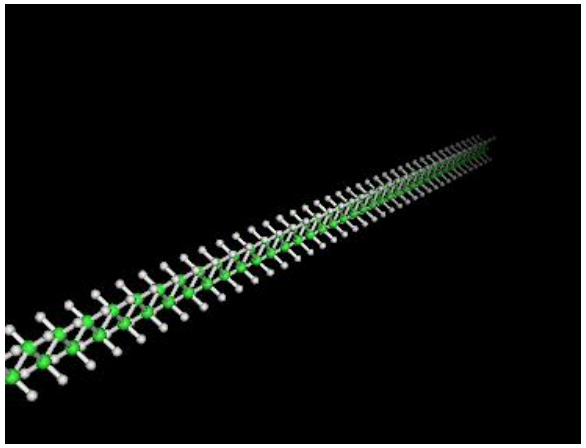
POLYMER BUILDER

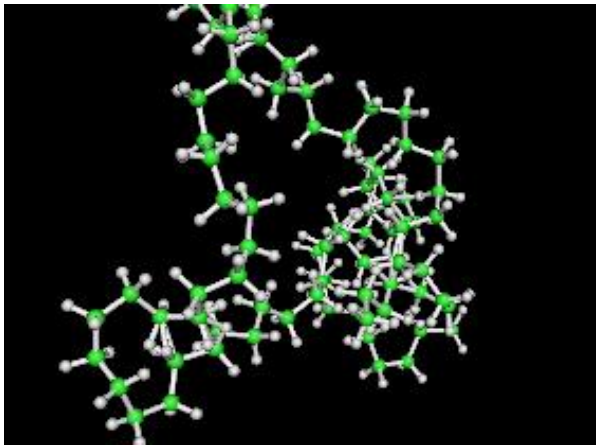
OUTLINE: Polymer Builder

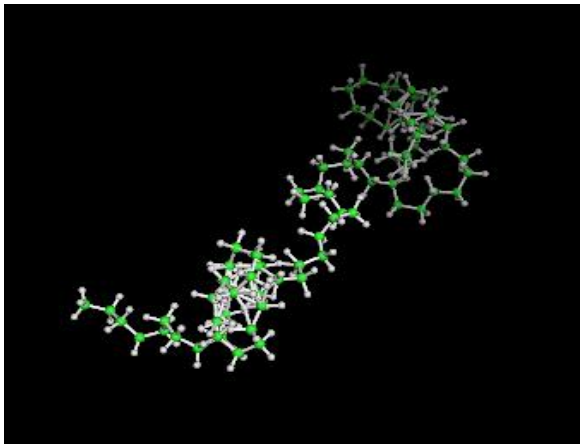
- Polymer Builder: An Introduction
- Getting Started: Beginner's Guide
  - » First Step: Choosing a monomer
  - » Number of monomers and chains
  - » Energy Interactions
    - ✓ Torsion angles: all-trans, freely rotating chain
  - » Outputs
- Advanced Options: Expert's Guide
  - » Building a monomer: 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.



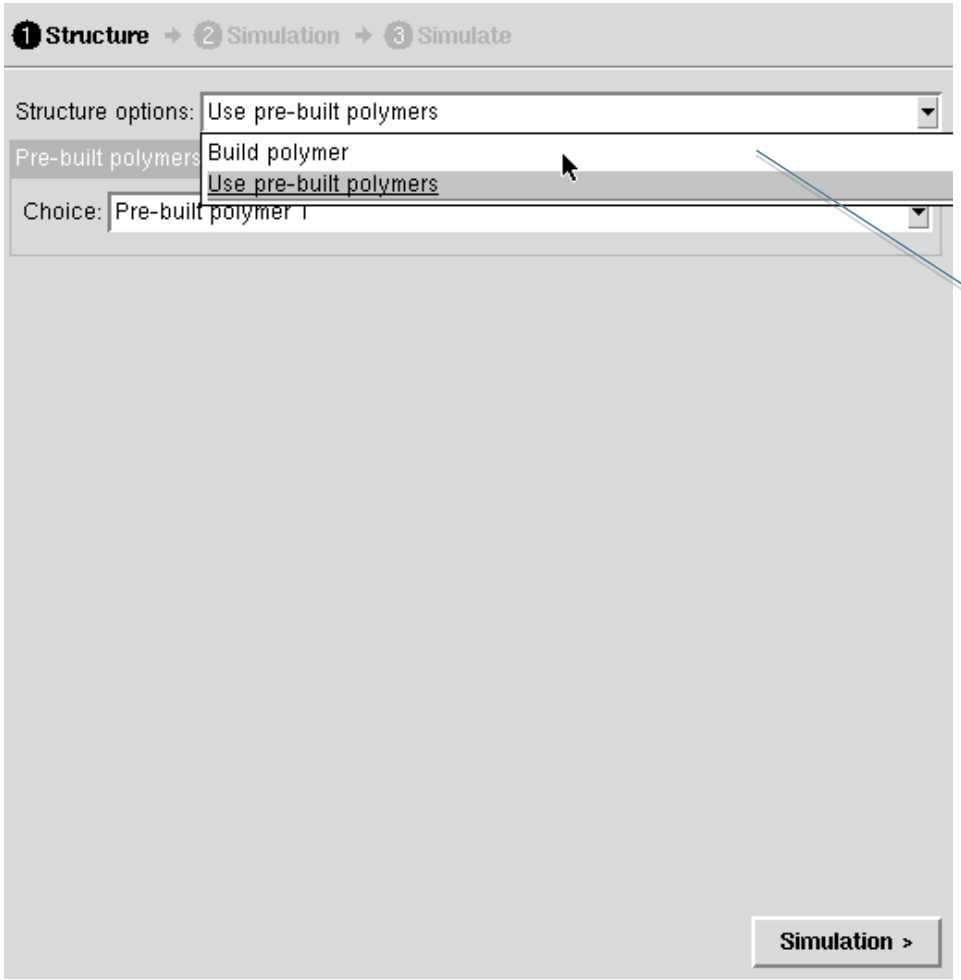




GETTING STARTED

Beginner's Guide

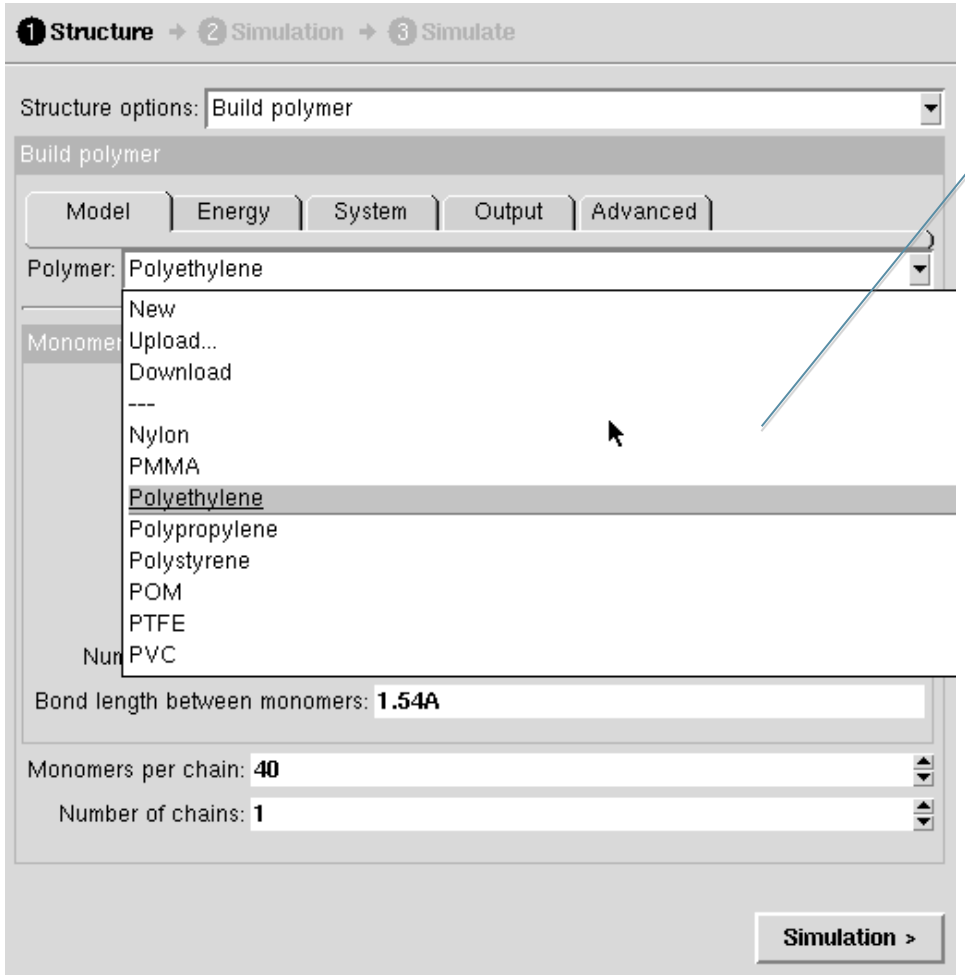
Using the builder



Select the option stating "Build Polymer"

Getting Started

First Step: Choosing a monomer.

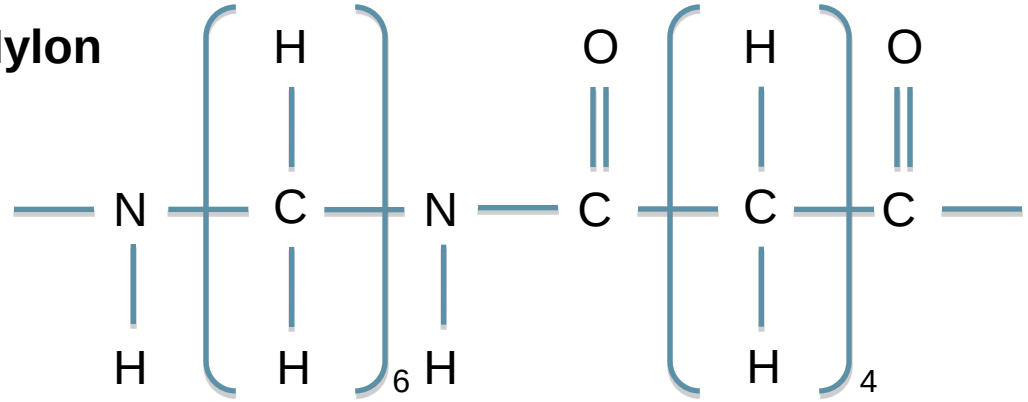


Choosing a built in monomer

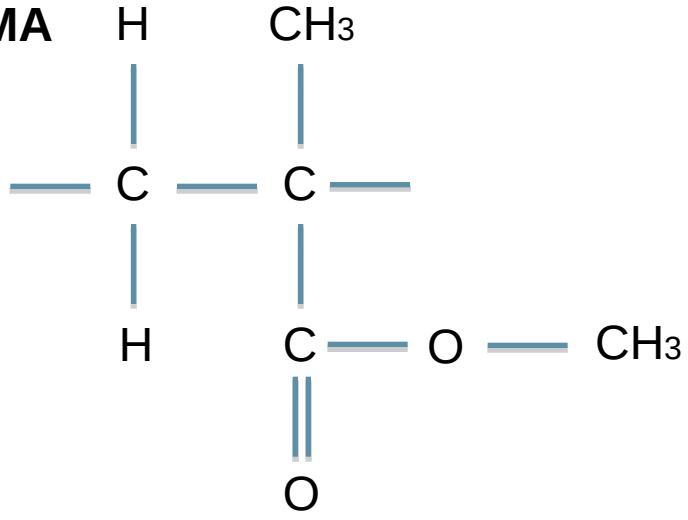
If a built-in monomer is chosen, the z-matrix, number of backbone atoms, and bond length between monomers are automatically loaded

Polymers repeat units (monomers) used:

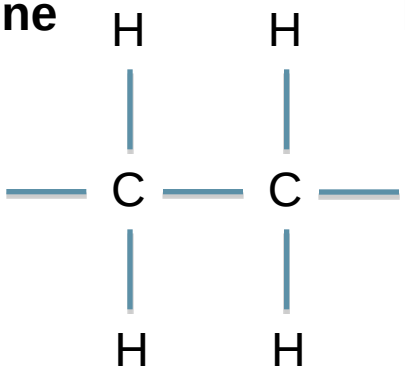
Nylon



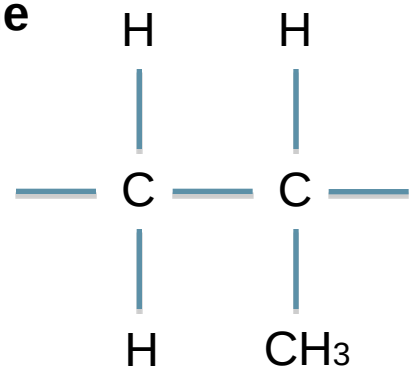
PMMA



Polyethylene

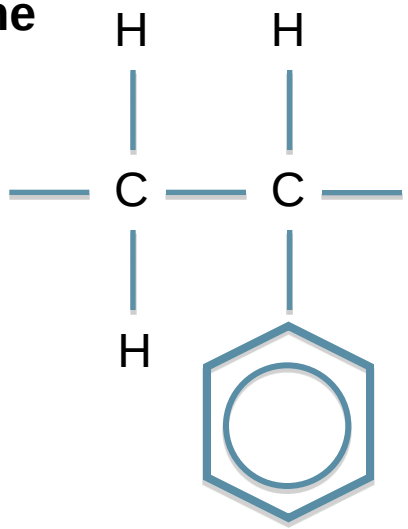


Polypropylene

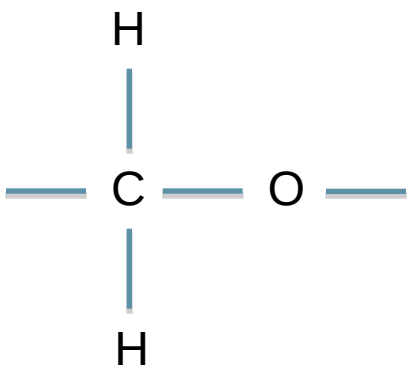


Polymers repeat units (monomers) used:

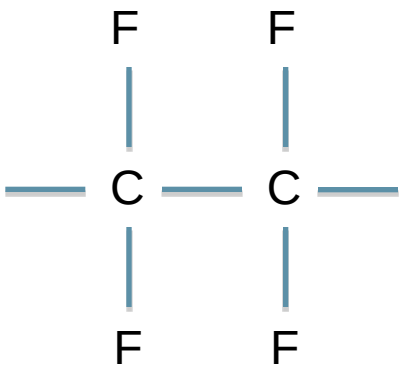
Polystyrene



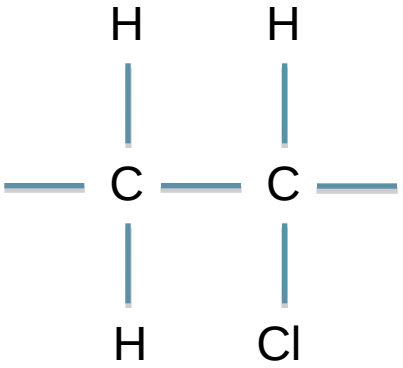
POM



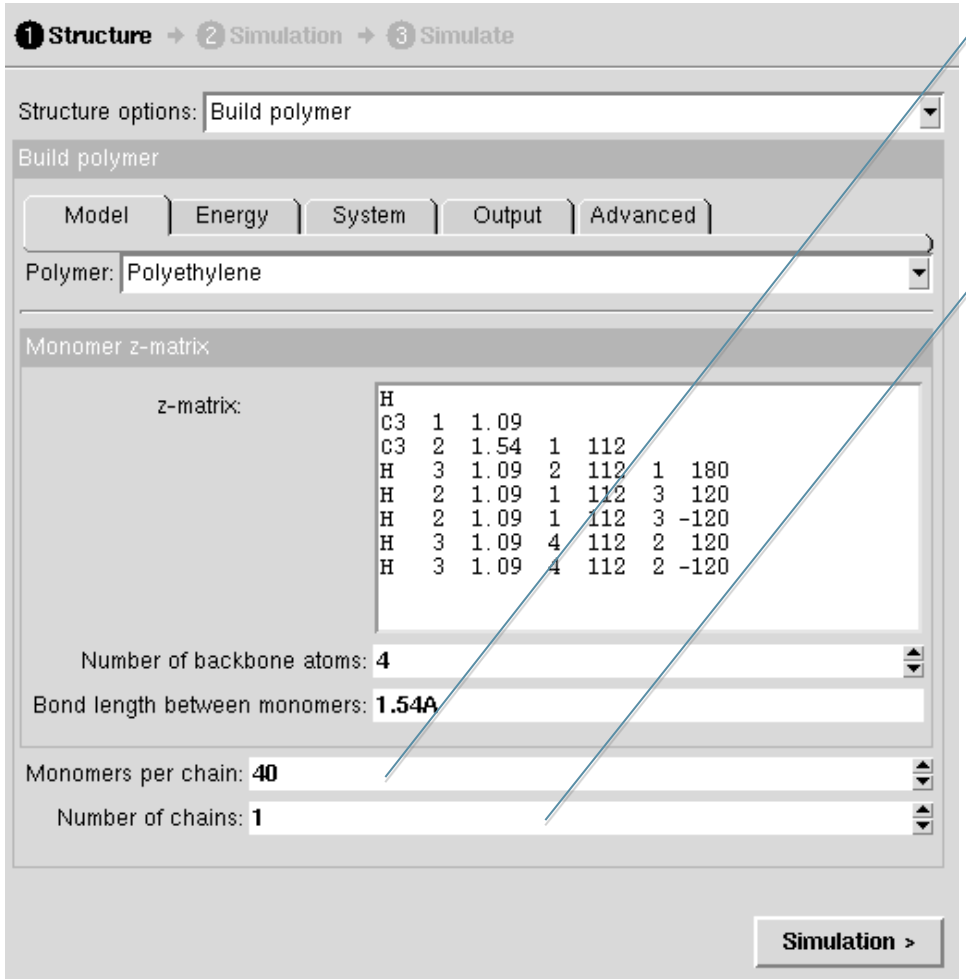
PTFE



PVC



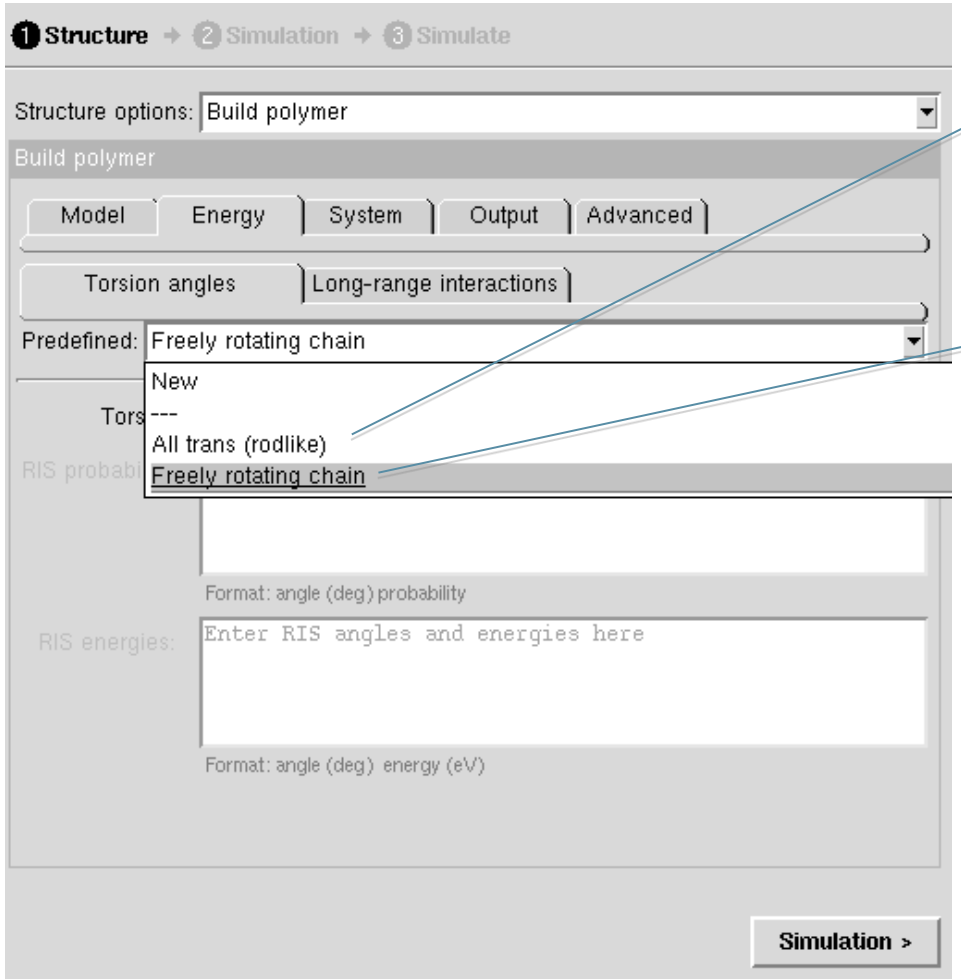
Choose the number of monomers and chains



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

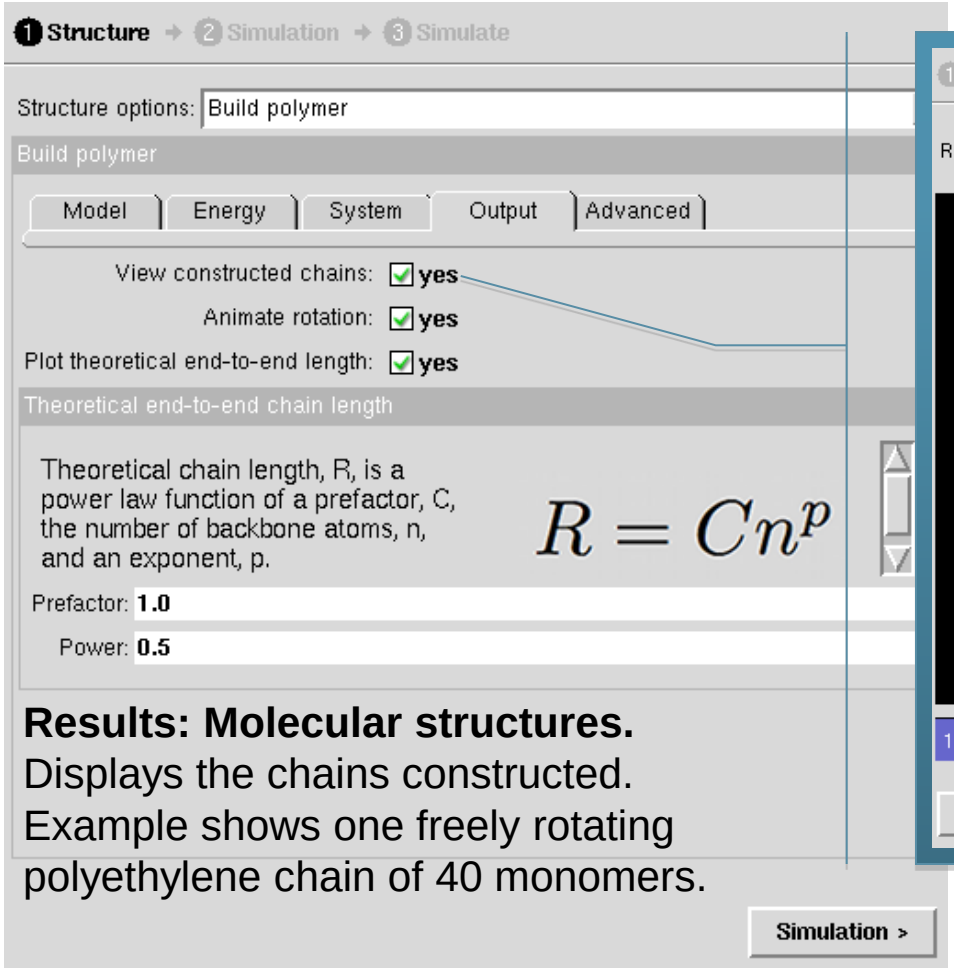
Specify the desired distribution of torsion angles

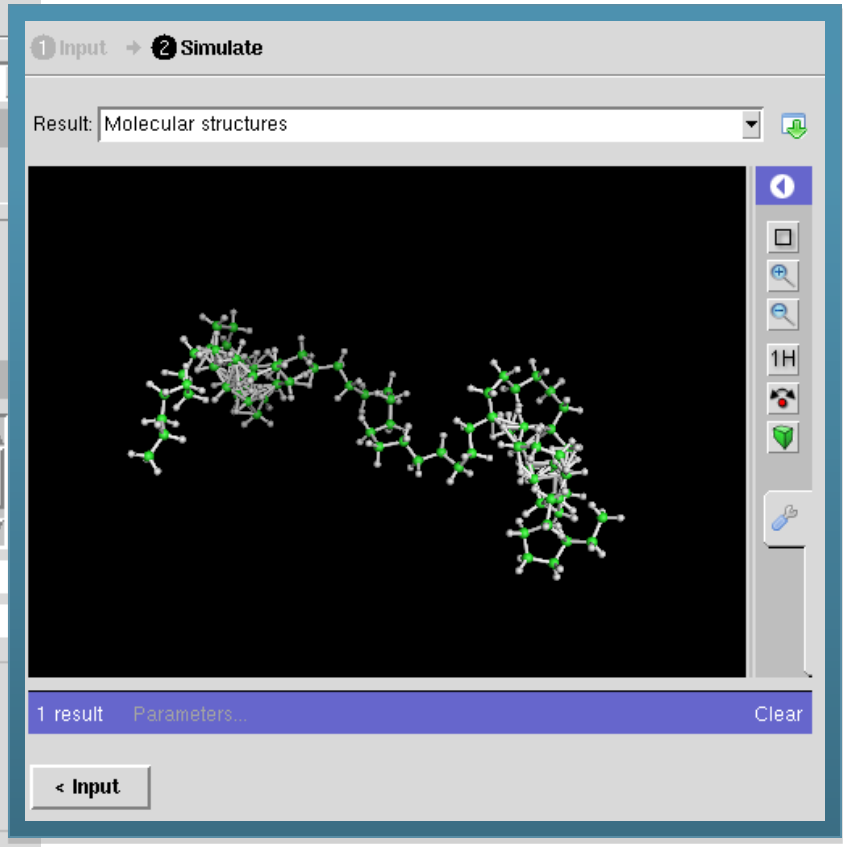


All torsion angles are set to 180°

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

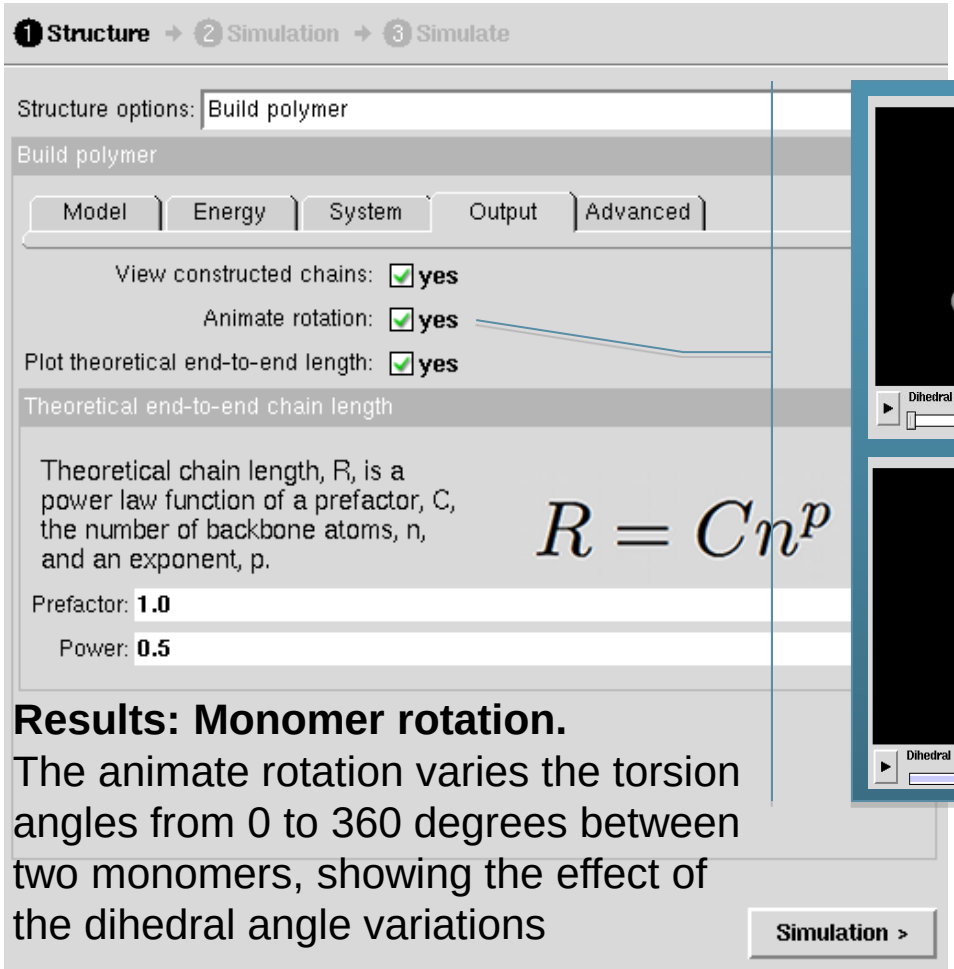
Choose the outputs that you want to observe

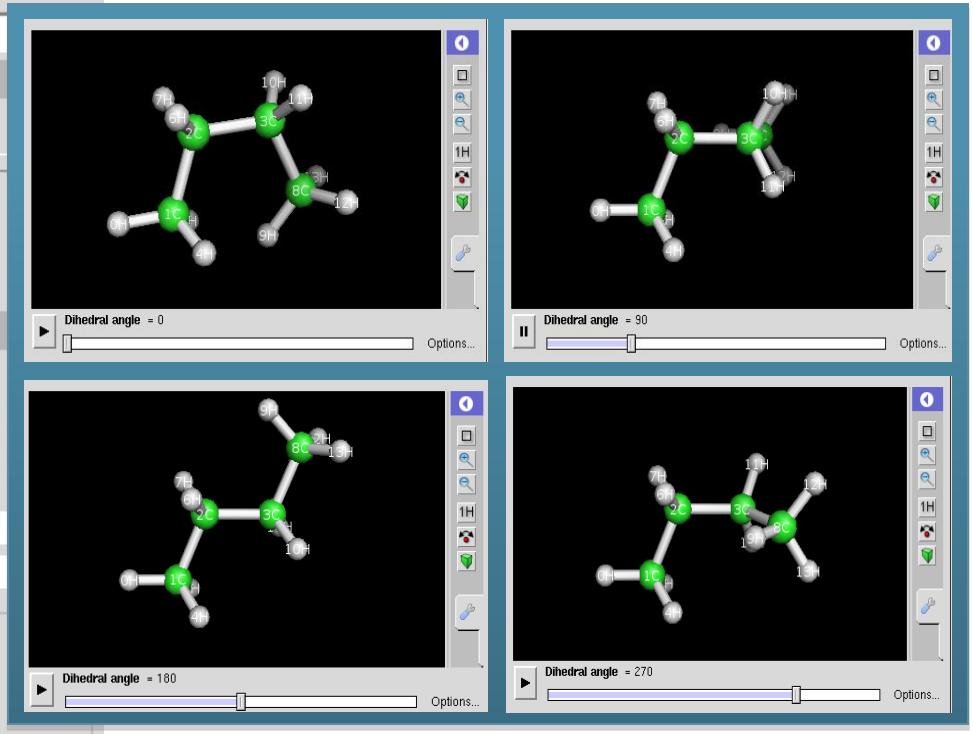




Results: Molecular structures.
Displays the chains constructed.
Example shows one freely rotating polyethylene chain of 40 monomers.

Choose the outputs that you want to observe



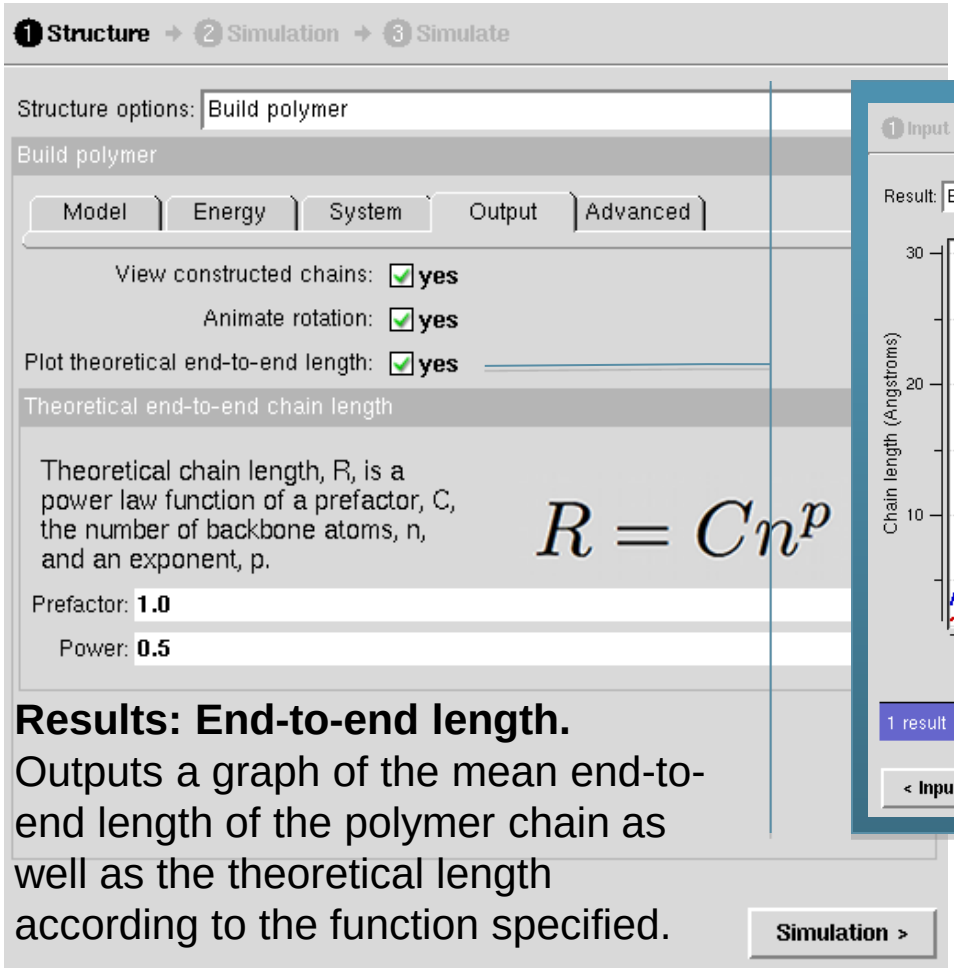


Results: Monomer rotation.

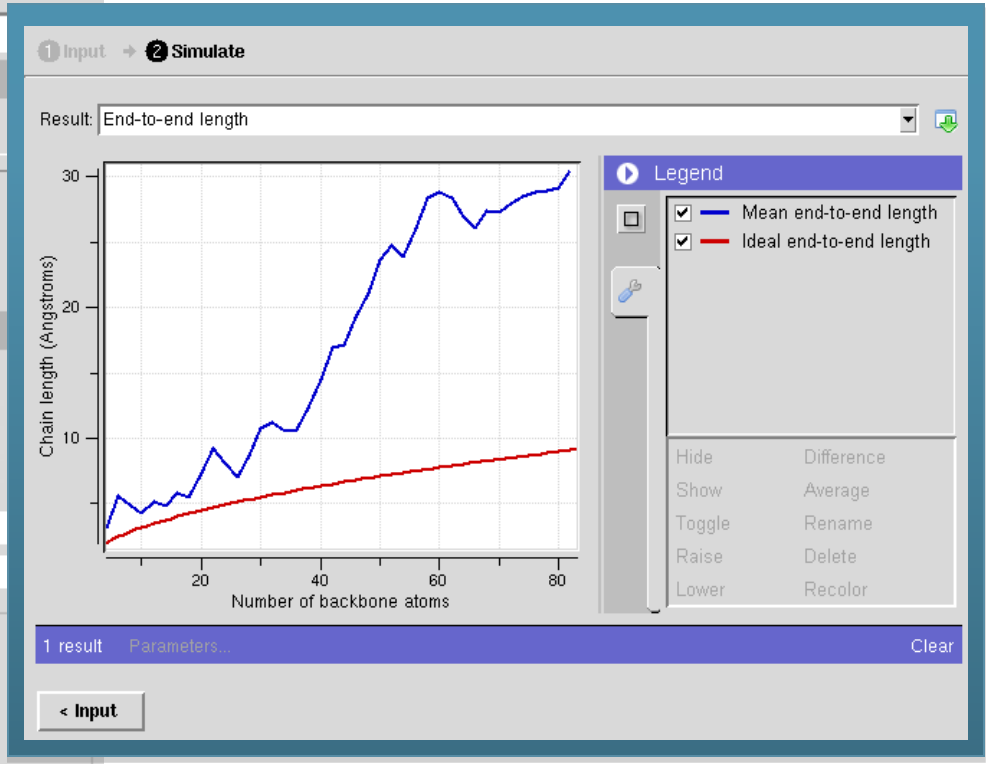
The animate rotation varies the torsion angles from 0 to 360 degrees between two monomers, showing the effect of the dihedral angle variations

Getting Started

Choose the outputs that you want to observe

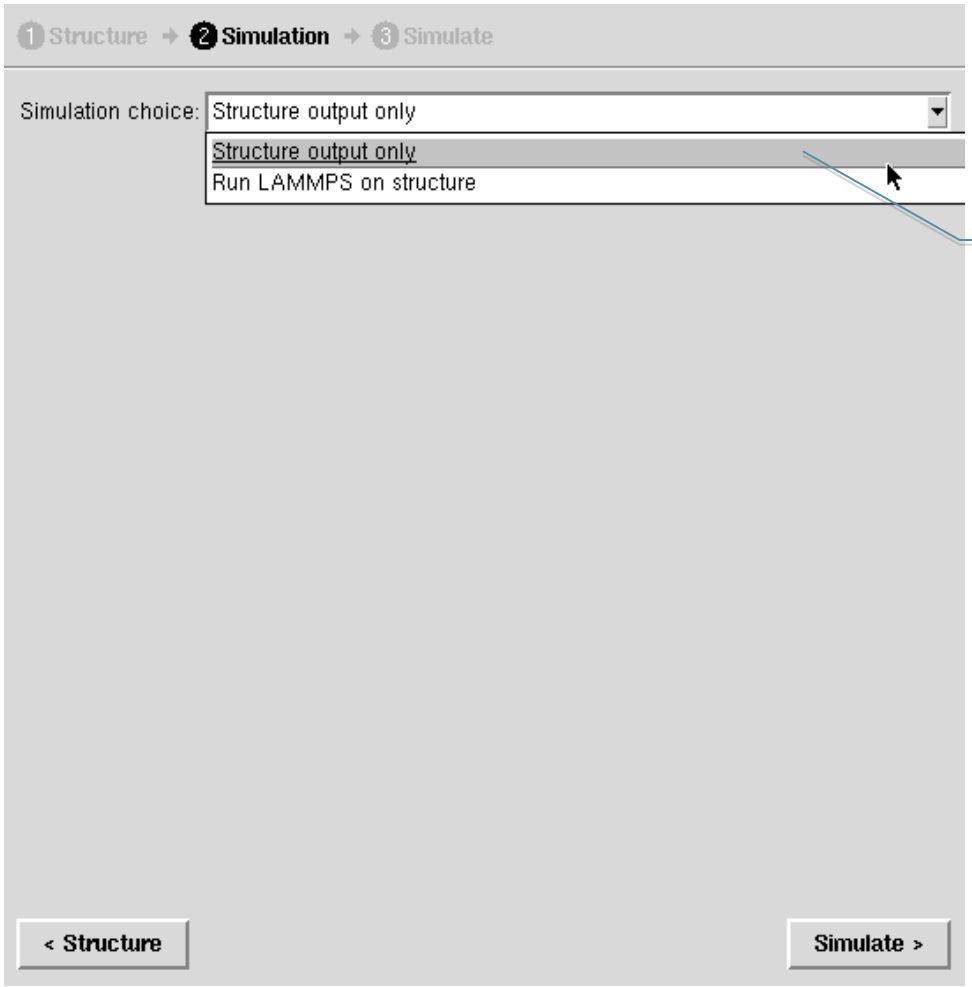


Results: End-to-end length.
Outputs a graph of the mean end-to-end length of the polymer chain as well as the theoretical length according to the function specified.



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

Observing the outputs



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

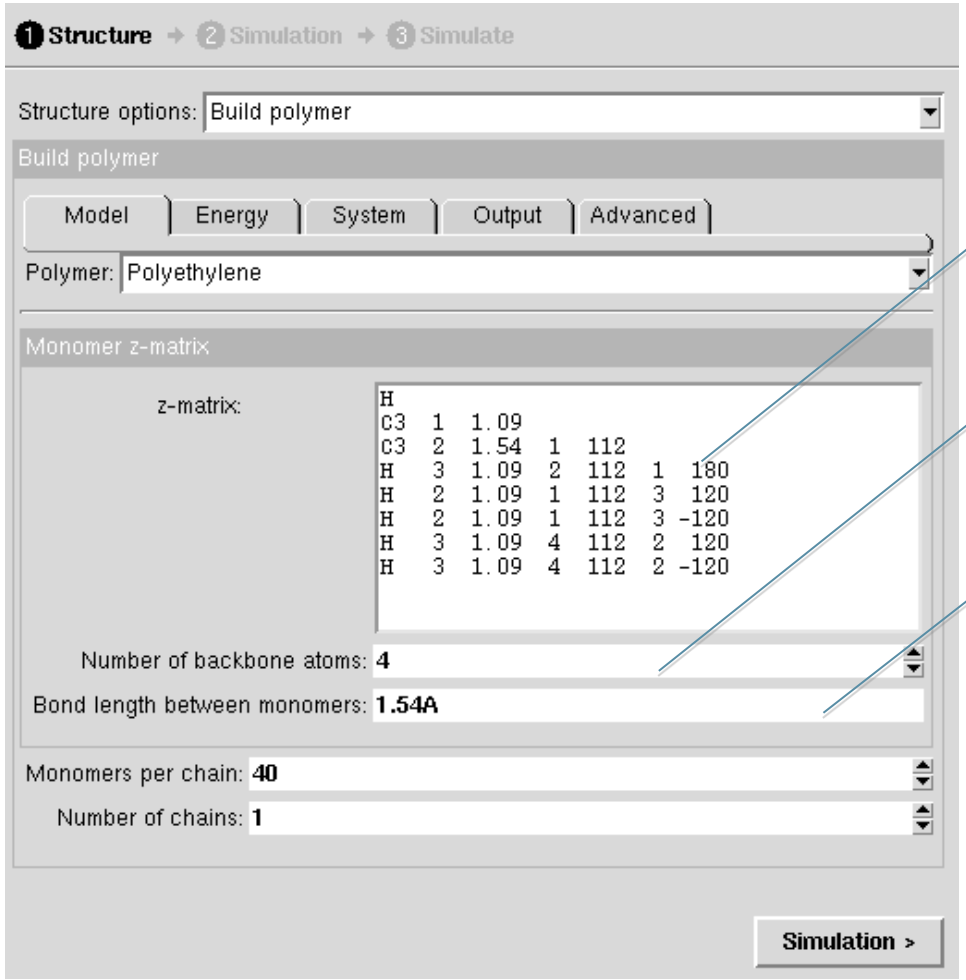
This panel appears after the simulation button, on the bottom right corner of the first panel, is pressed.

ADVANCED OPTIONS

Expert's Guide

Advanced Options

Steps to specify a new monomer



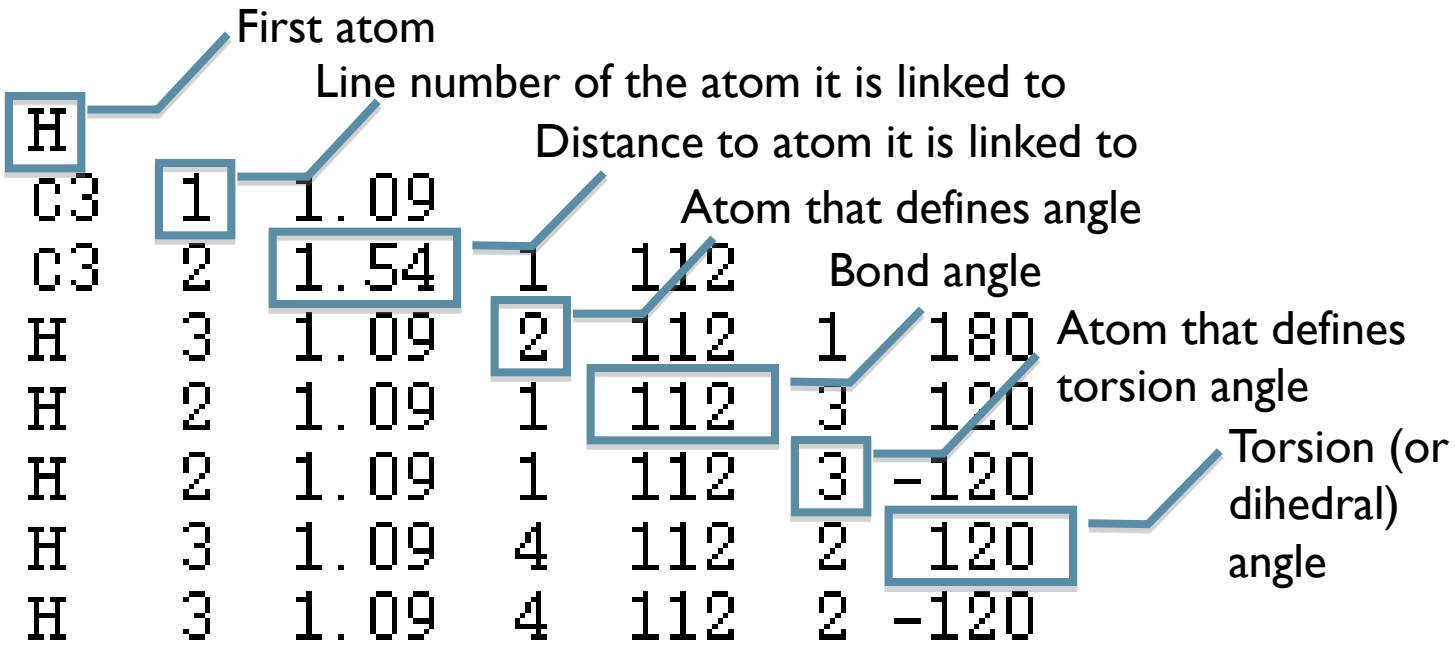
Step 1: Build the z-matrix

Step 2: Specify backbone atoms

Step 3: Specify bond length

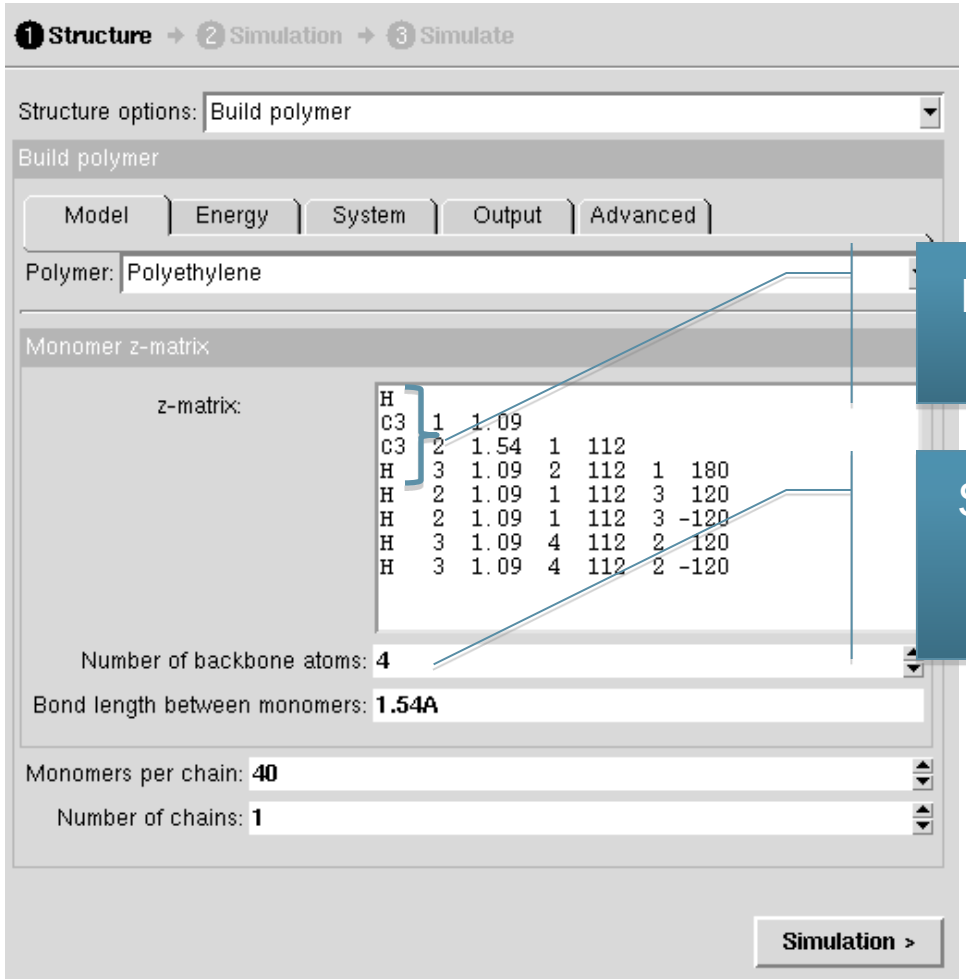
Advanced Options

Step 1: Building the z-matrix



Advanced Options

Step 2: Specifying the backbone atoms

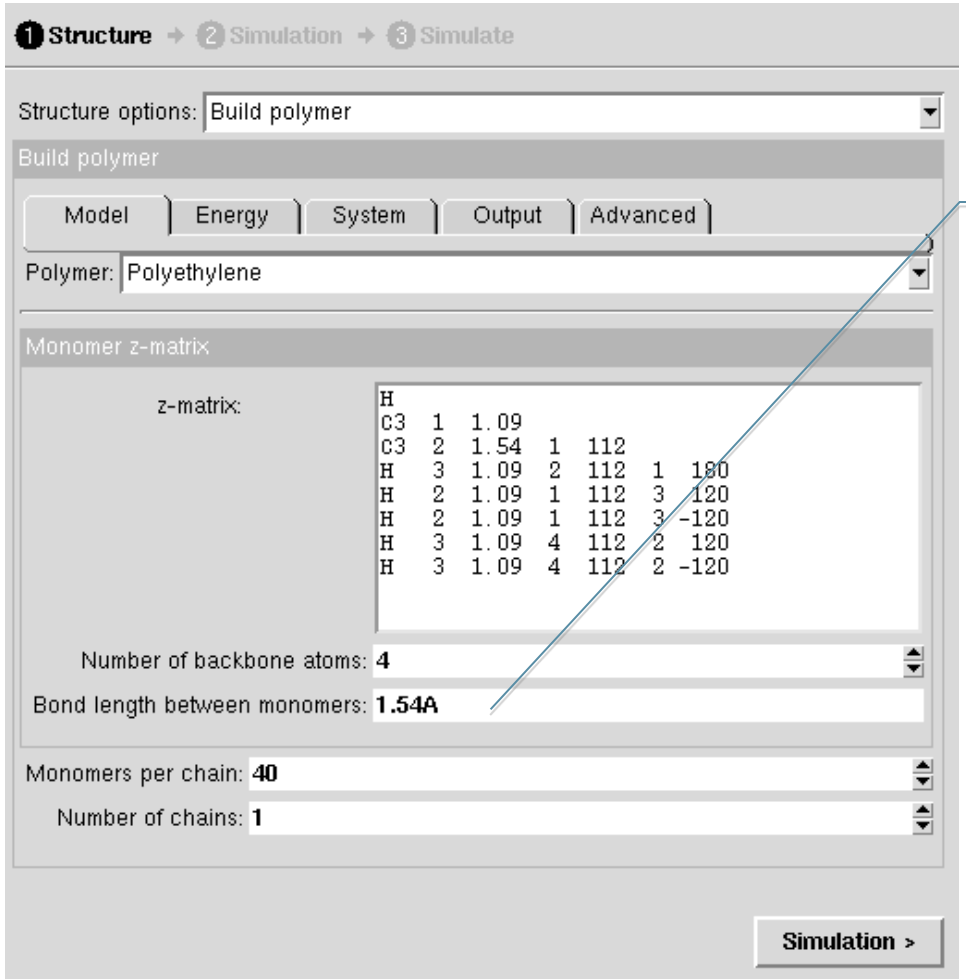


Backbone atoms MUST be listed first when creating the z-matrix

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

Advanced Options

Step 3: Specifying the bond length

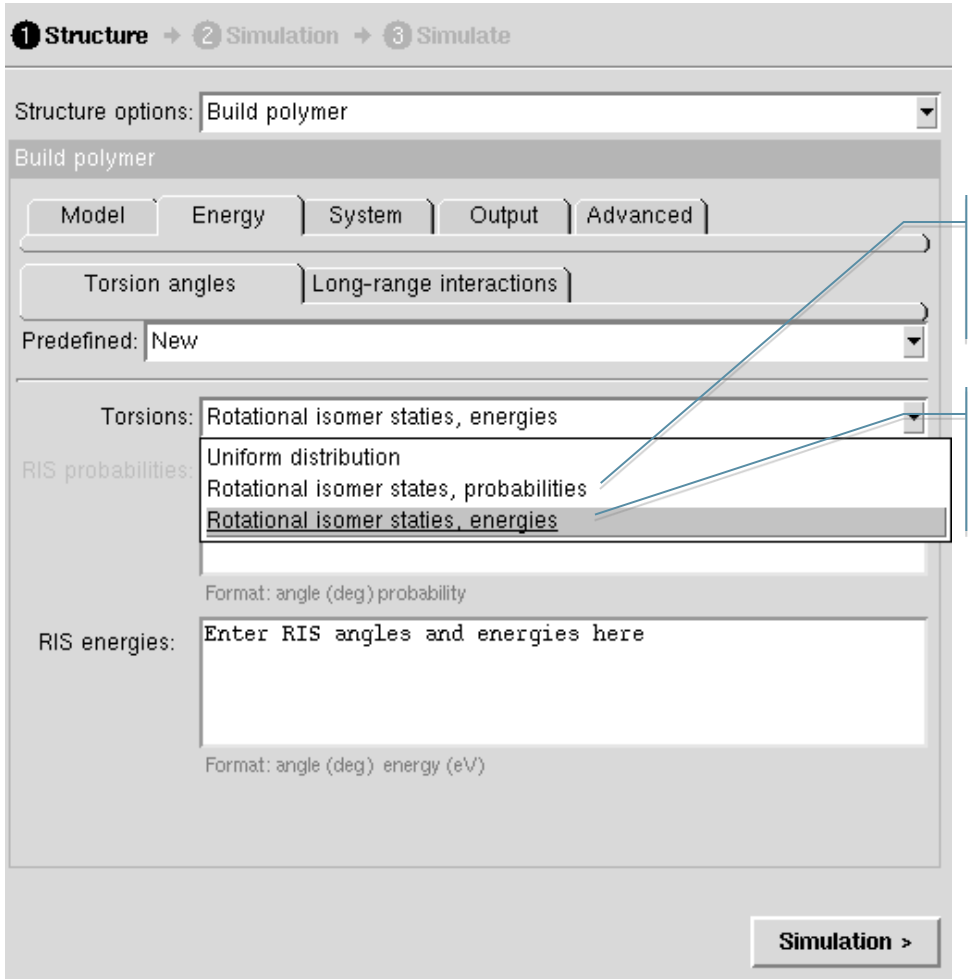


Specify the bond length between the monomers

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.

Advanced Options

Setting torsion angles



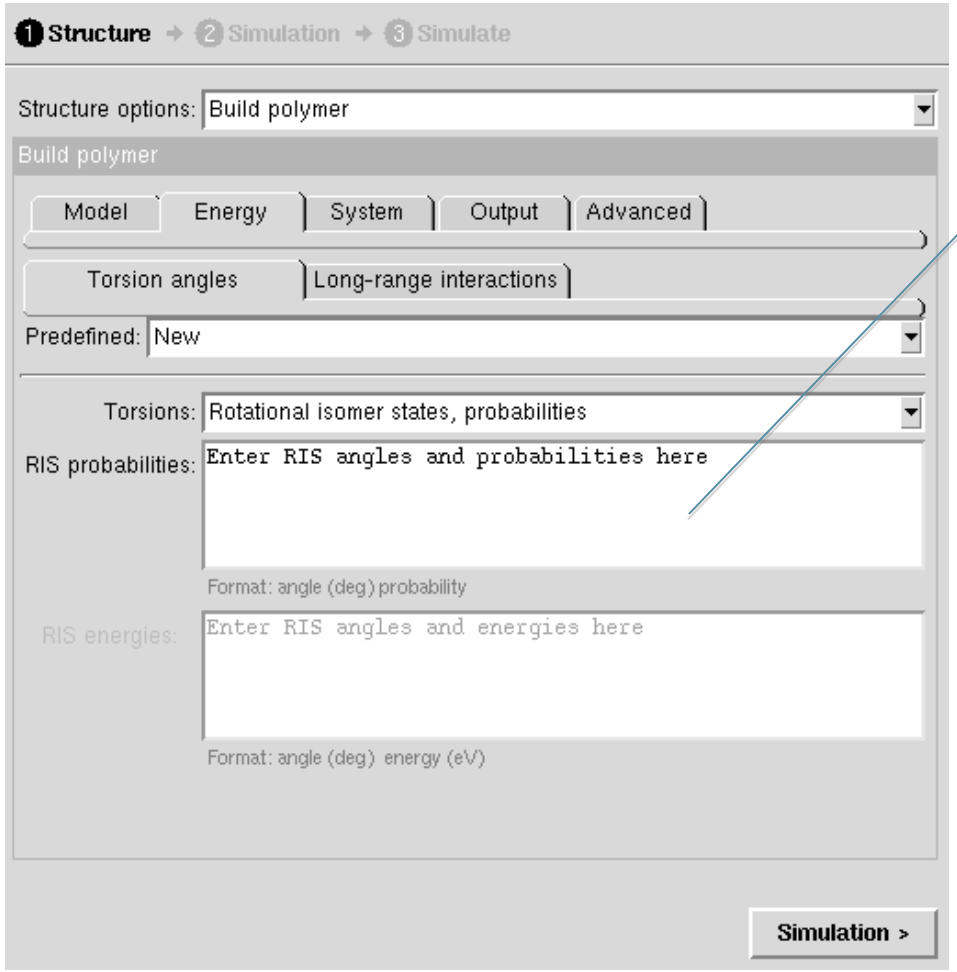
Define using probabilities

Define using energies

Specify which torsions angles are energetically favored

Advanced Options

Define torsion angles occurrence using probabilities

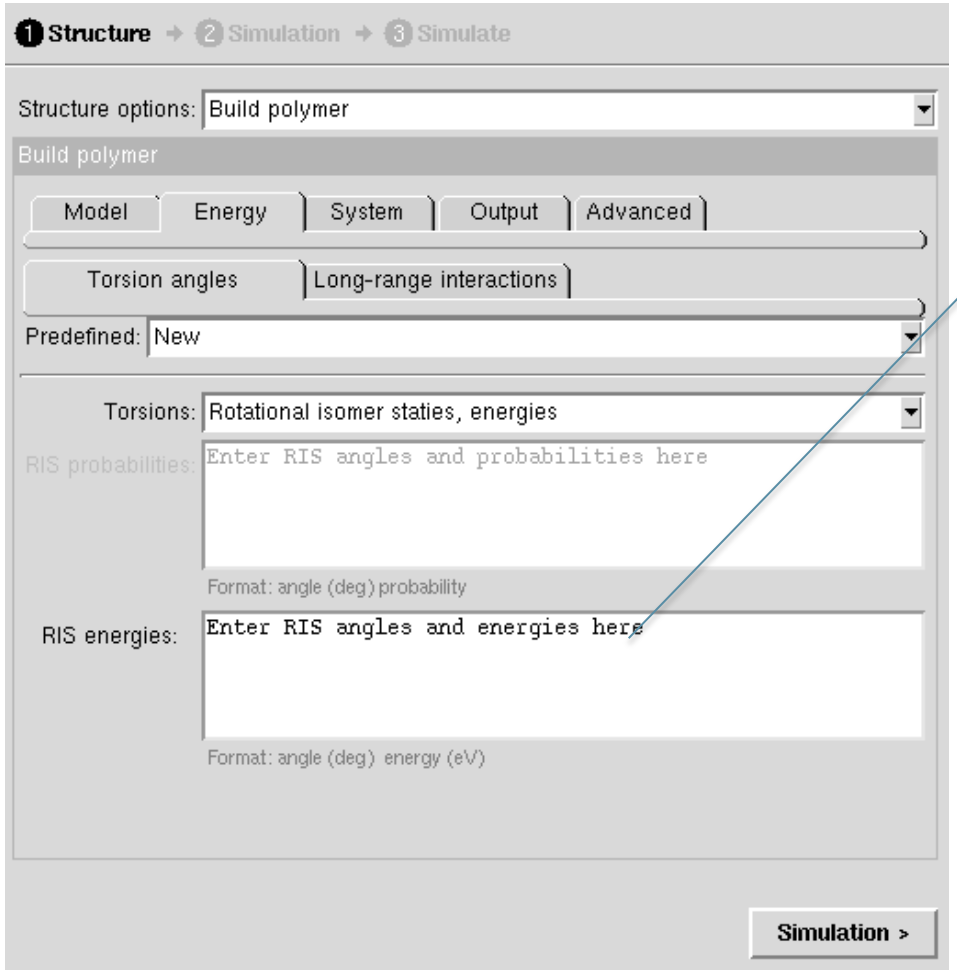


To specify torsion angles using probabilities, enter angle (in degrees) followed by probability, separated by a space

Note: Do NOT include units in input

Advanced Options

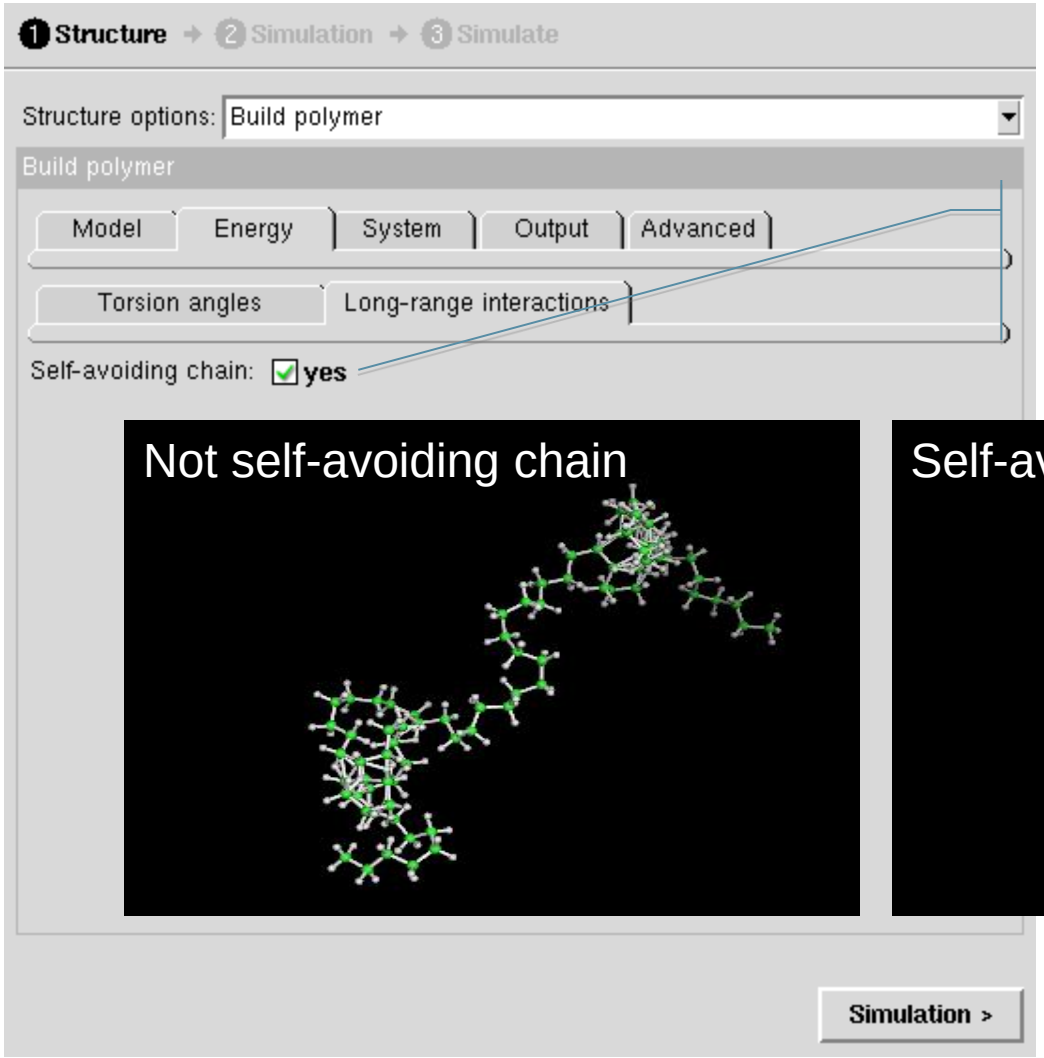
Define torsion angles occurrence using energies



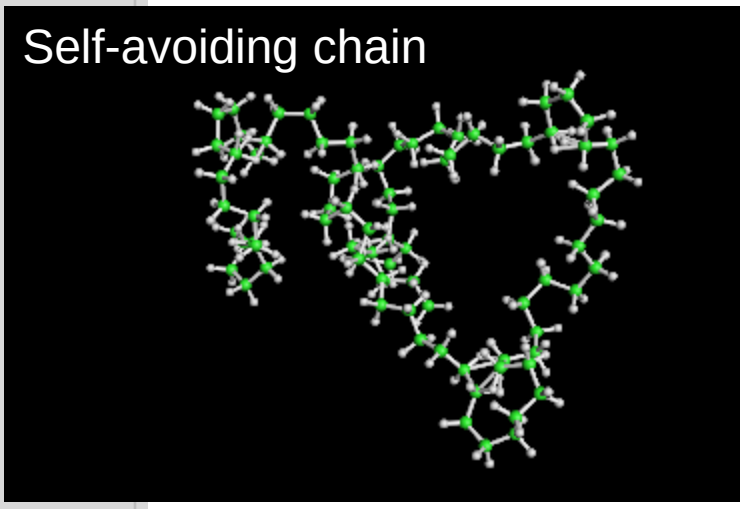
To specify torsion angles using energies, enter angle (in degrees) followed by its energy (in eV), separated by a space

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

Advanced Options

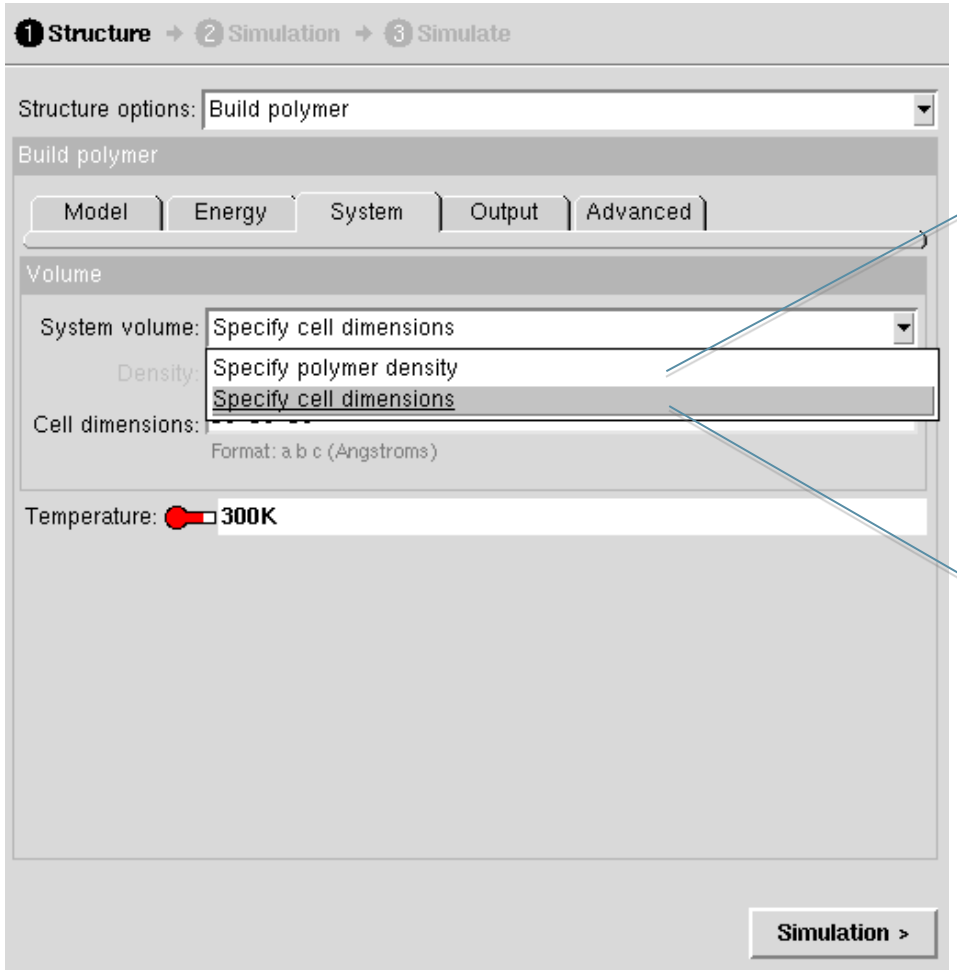


Prevents polymer chains from self intersecting



Advanced Options

Define the system volume



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

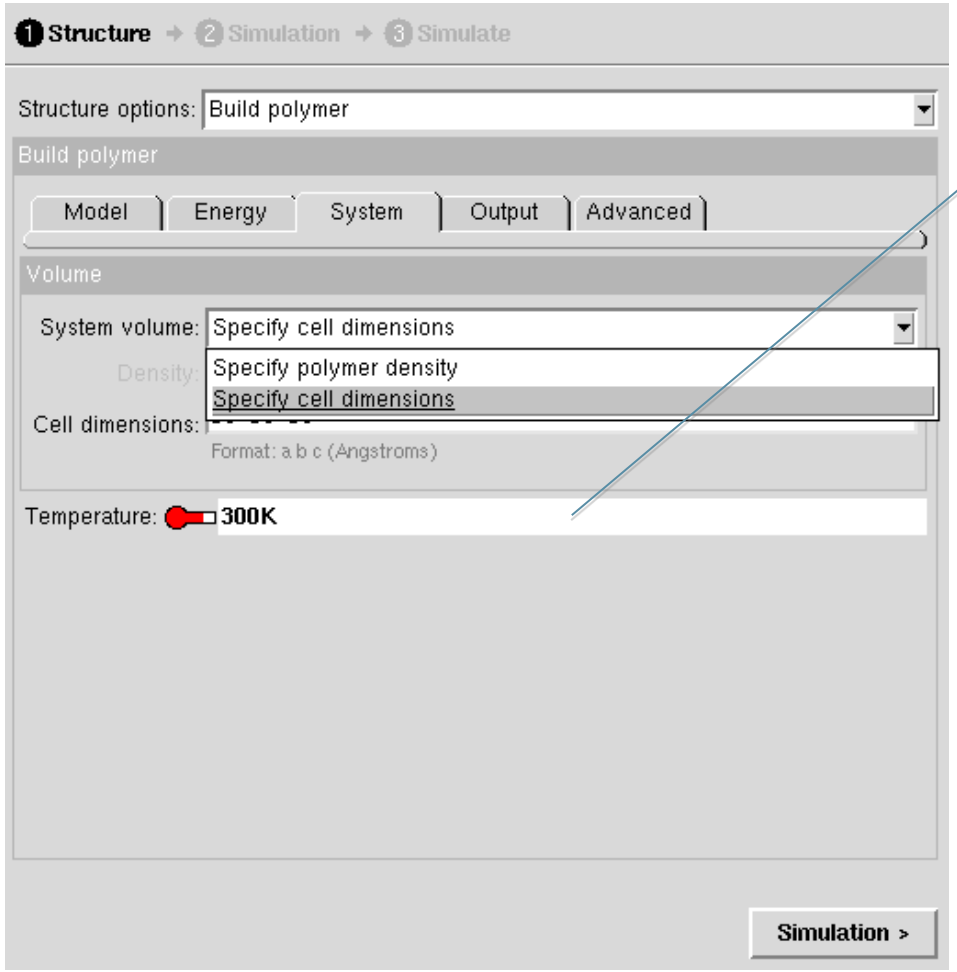
Express density in grams per cubic centimeter (g/cm^3)

Specify the cell dimensions of the system in Angstroms

Note: Do NOT include units in input

Advanced Options

Define the system temperature

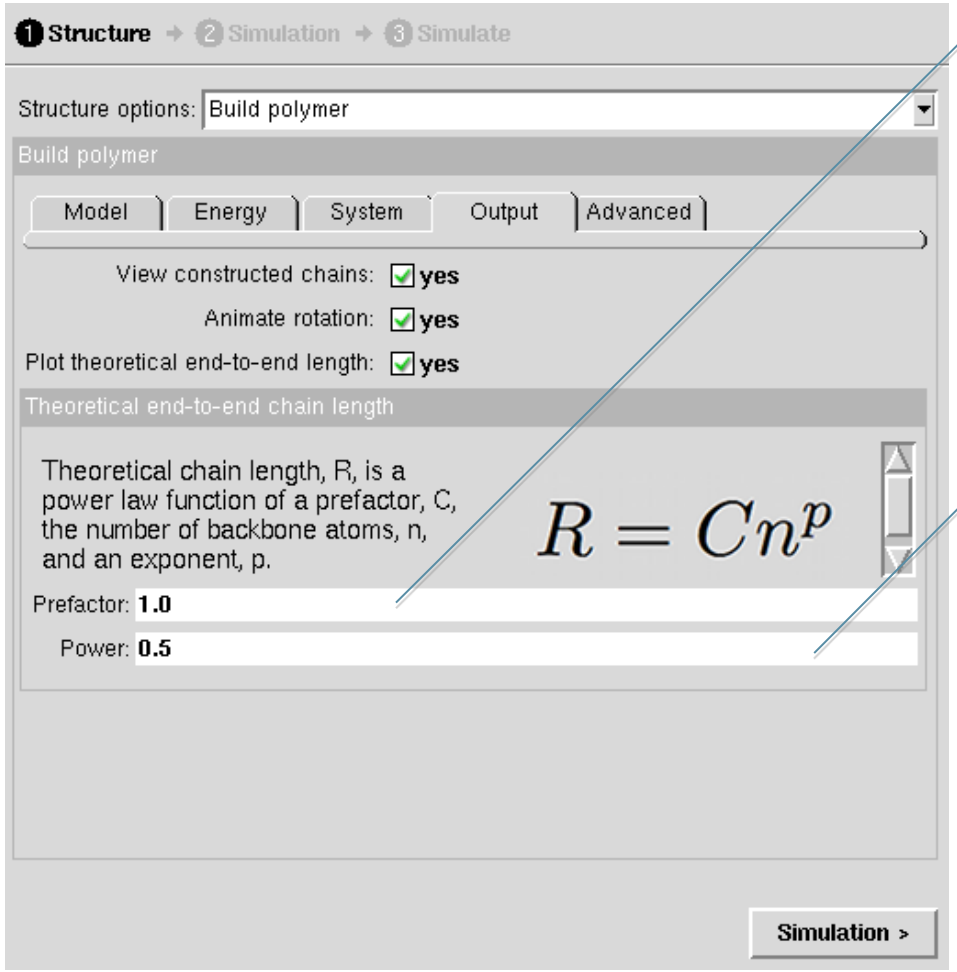


Specify the temperature of the system

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



The prefactor C depends of the polymer being built

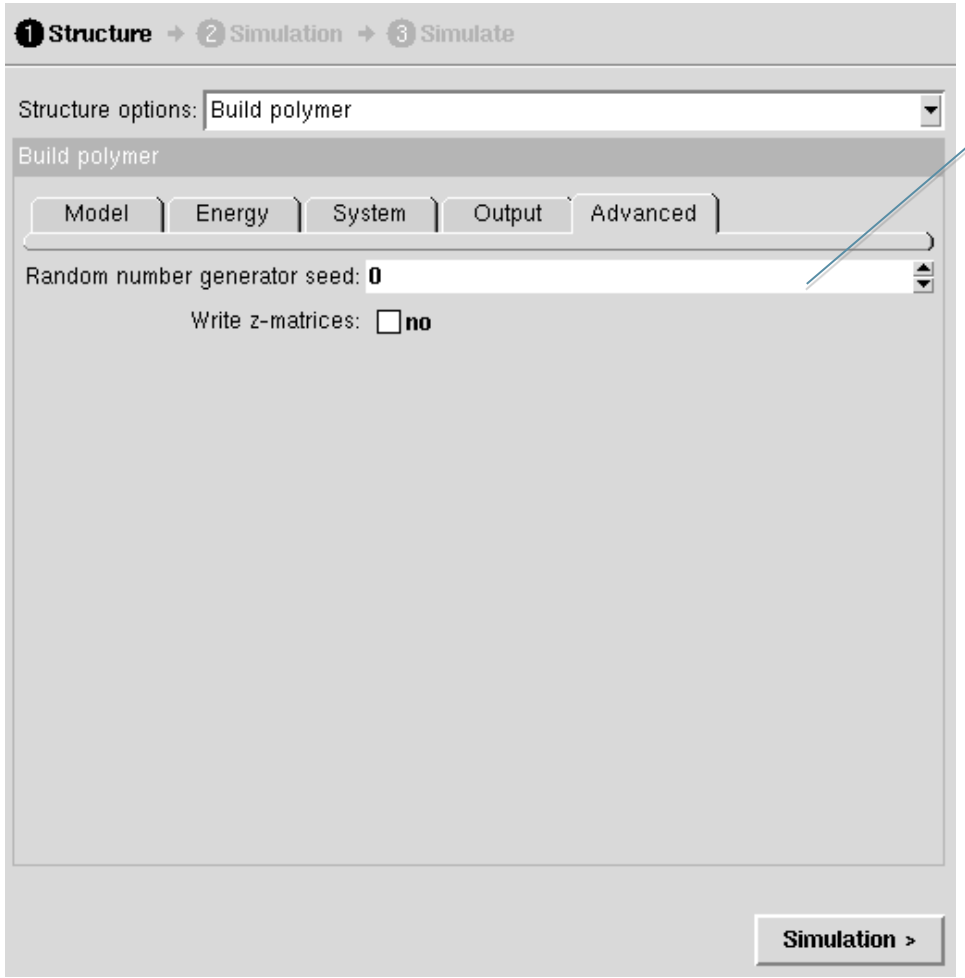
For polyethylene:
Rod-like chain C → 1.28,
Freely-rotating chain C → 2.28.

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

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

Advanced Options

Exploring other options



Assign a number generator seed to exactly reproduce results later

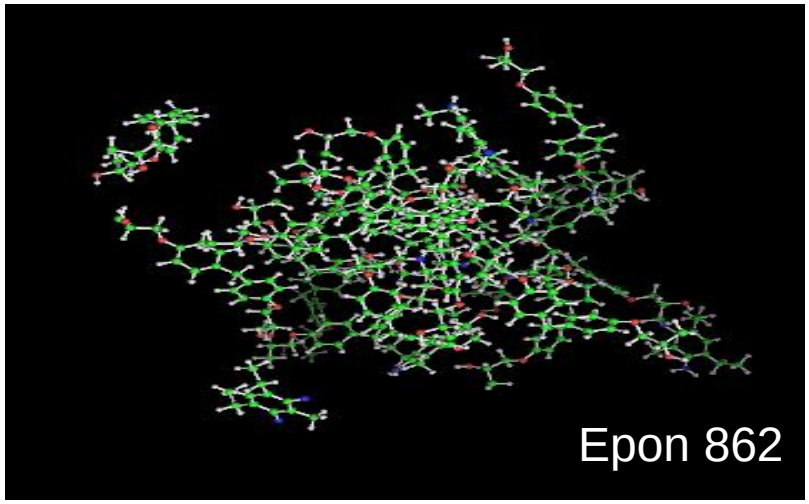
MOLECULAR DYNAMIC SIMULATIONS

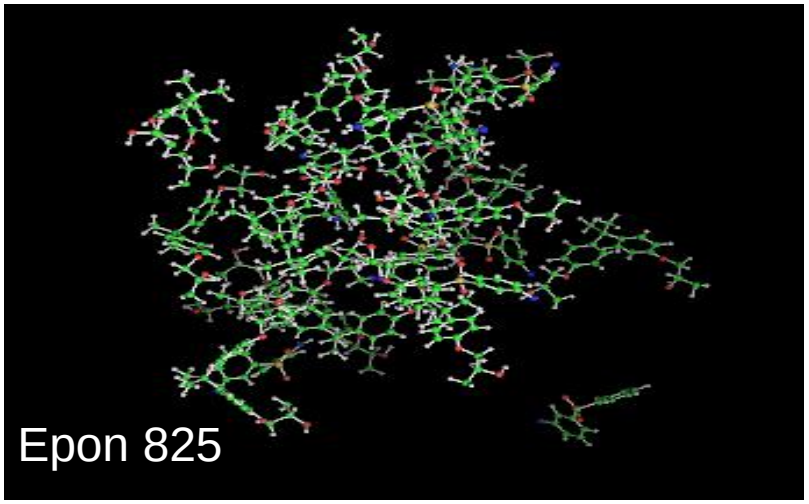
OUTLINE: Molecular Dynamic Simulations

- 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.

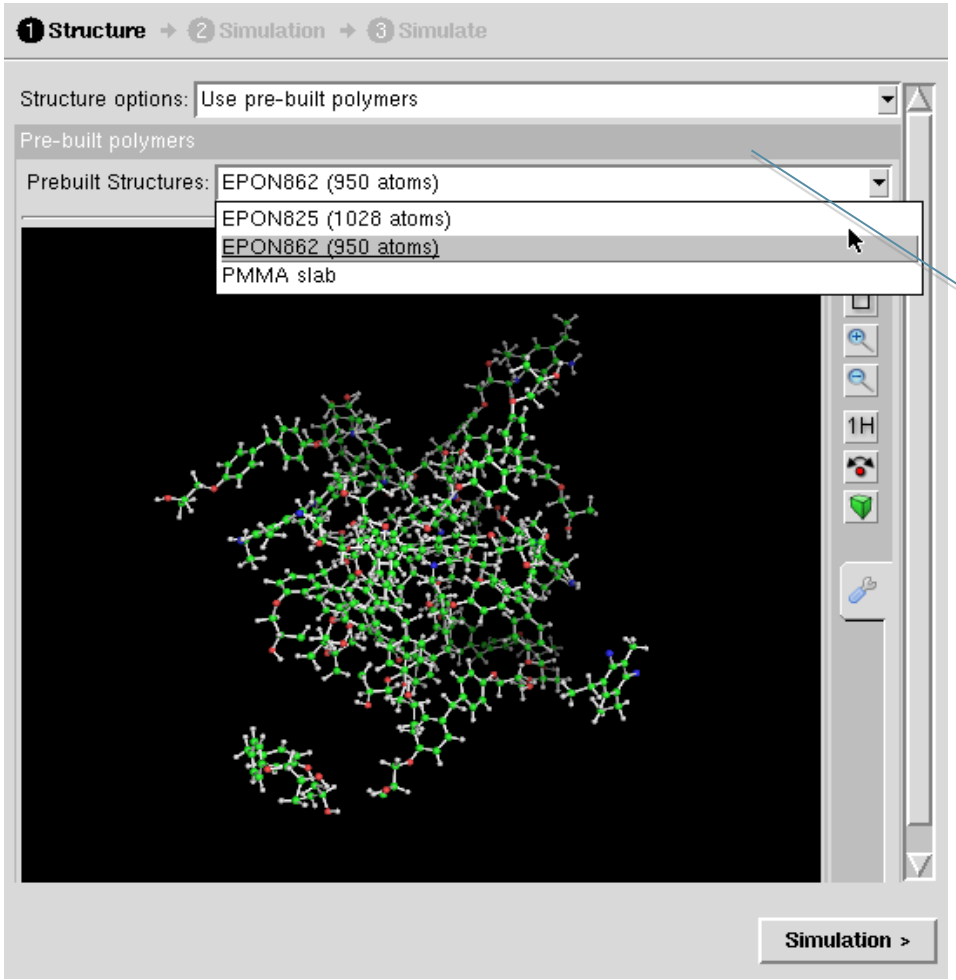




GETTING STARTED

Beginner's Guide

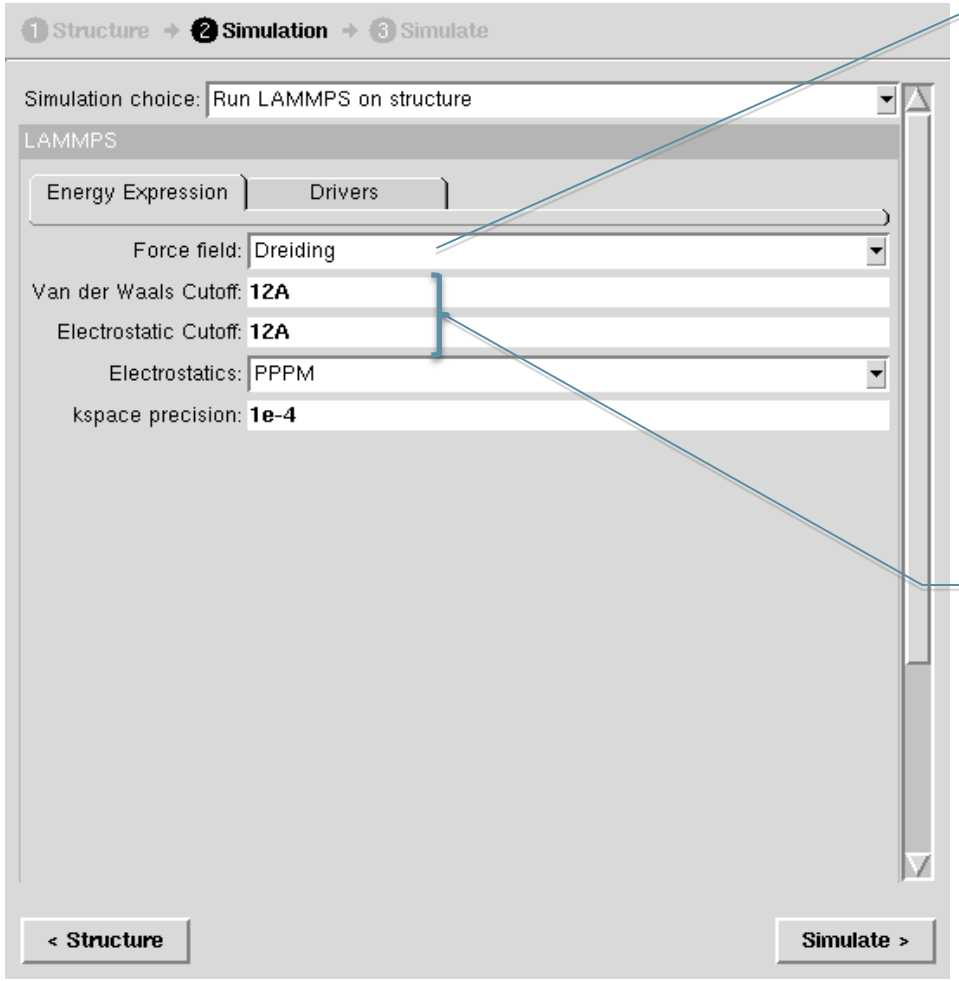
Using pre-built polymers



Select any of the polymer pre-built structures

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

Running LAMMPS on structure

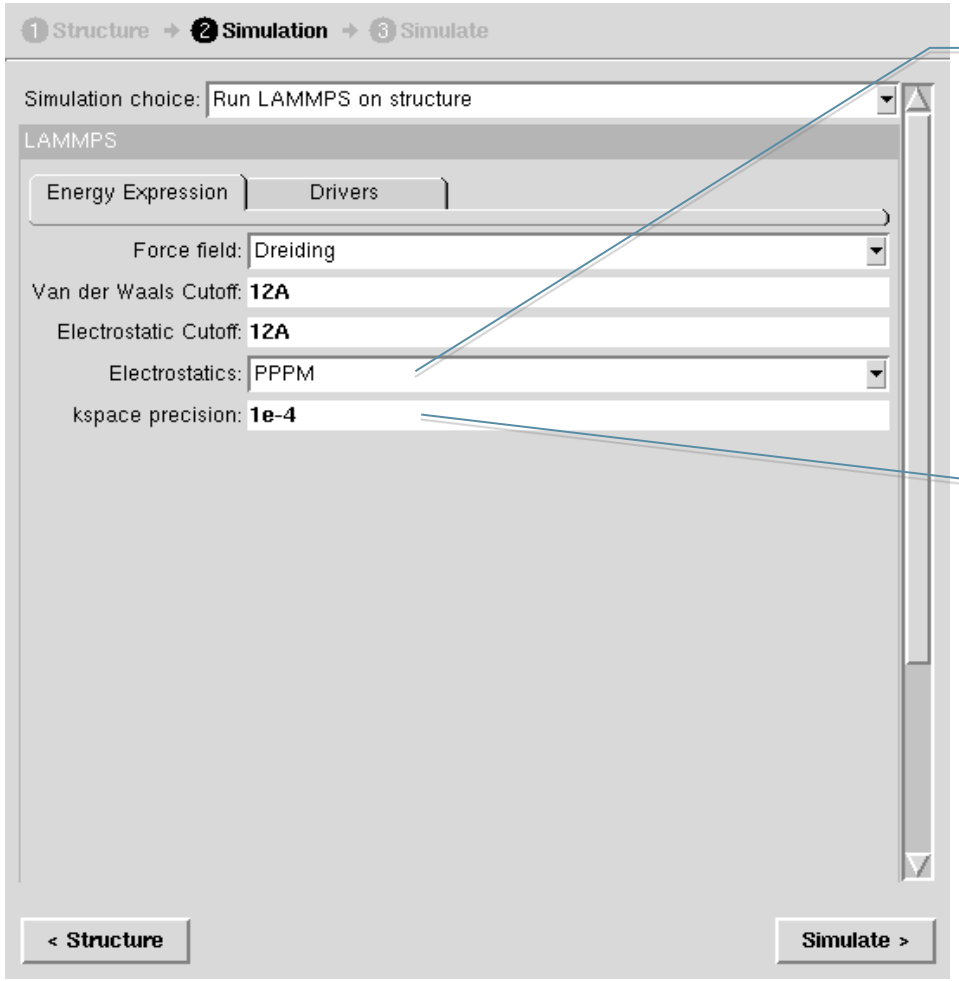


Force fields dictate how the forces between atoms are approximated.

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.

Running LAMMPS on structure



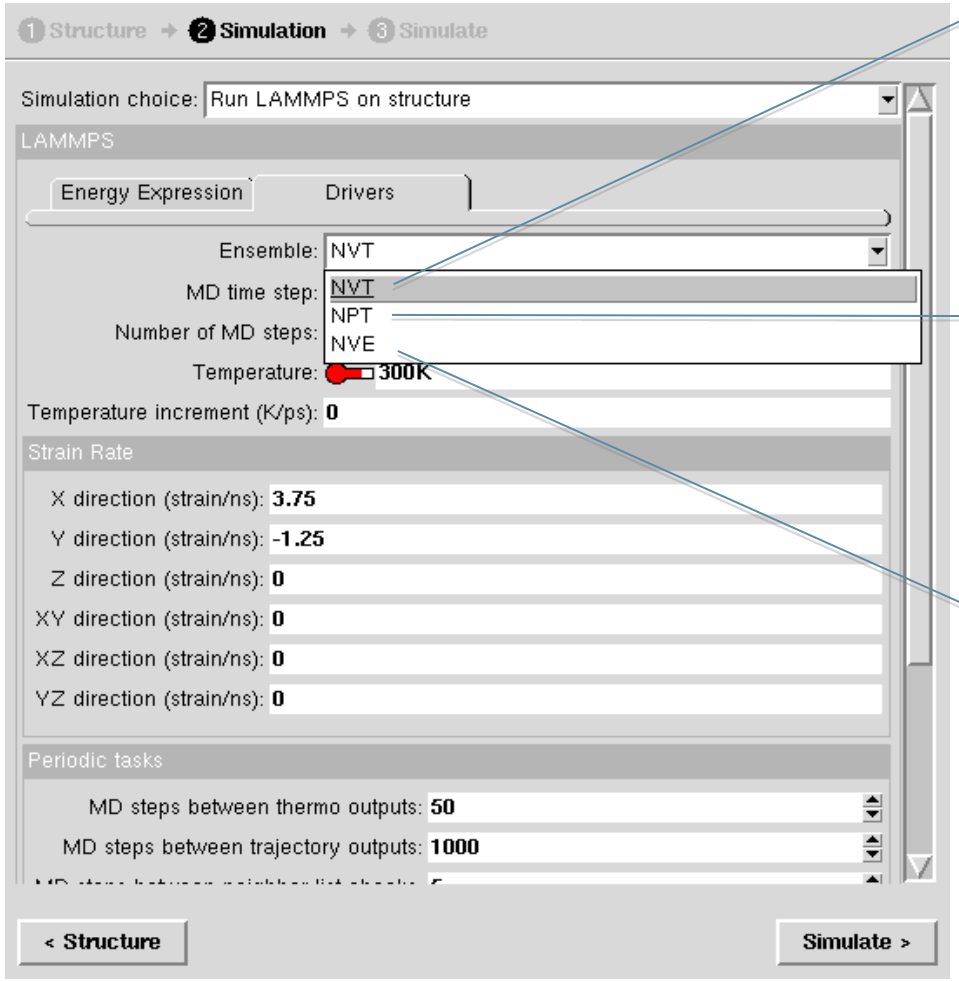
The PPPM and ewld options will calculate electrostatic interactions beyond the cutoff specified above

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

Setting the ensemble



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

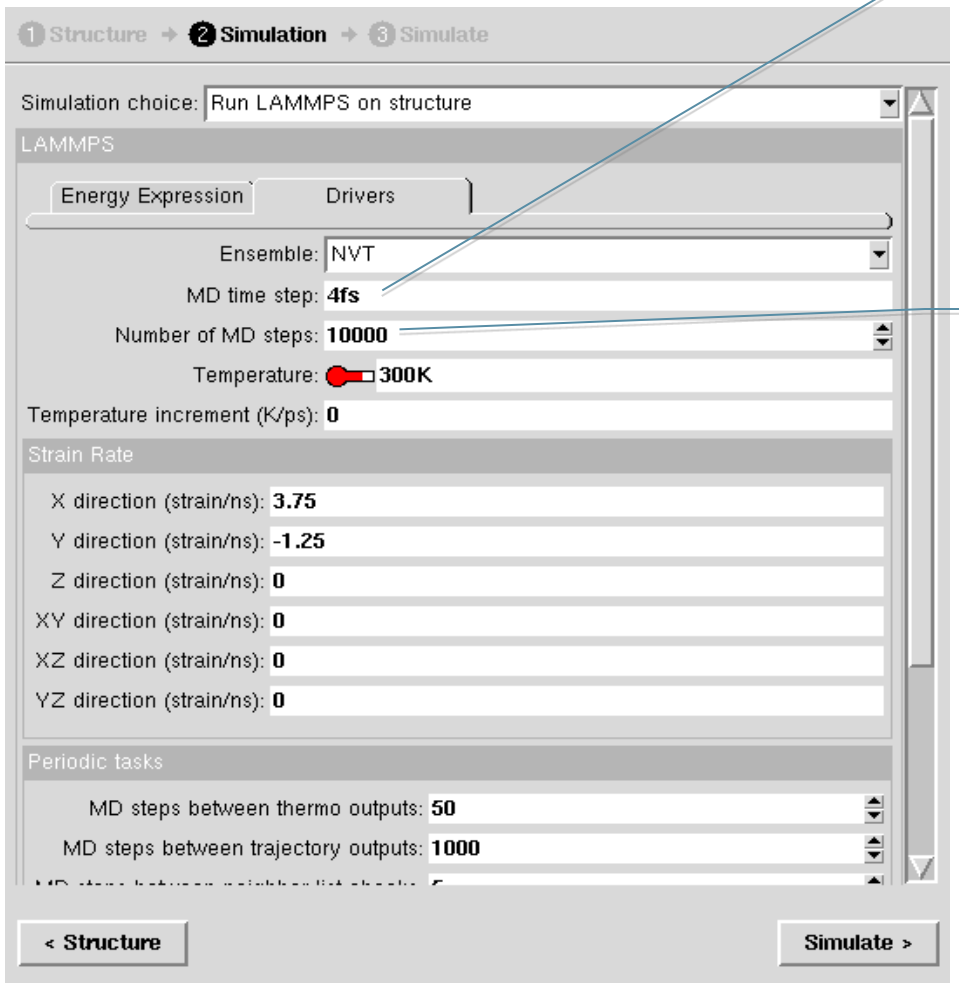
This ensemble controls the number of atoms, pressure, and temperature of the system.

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

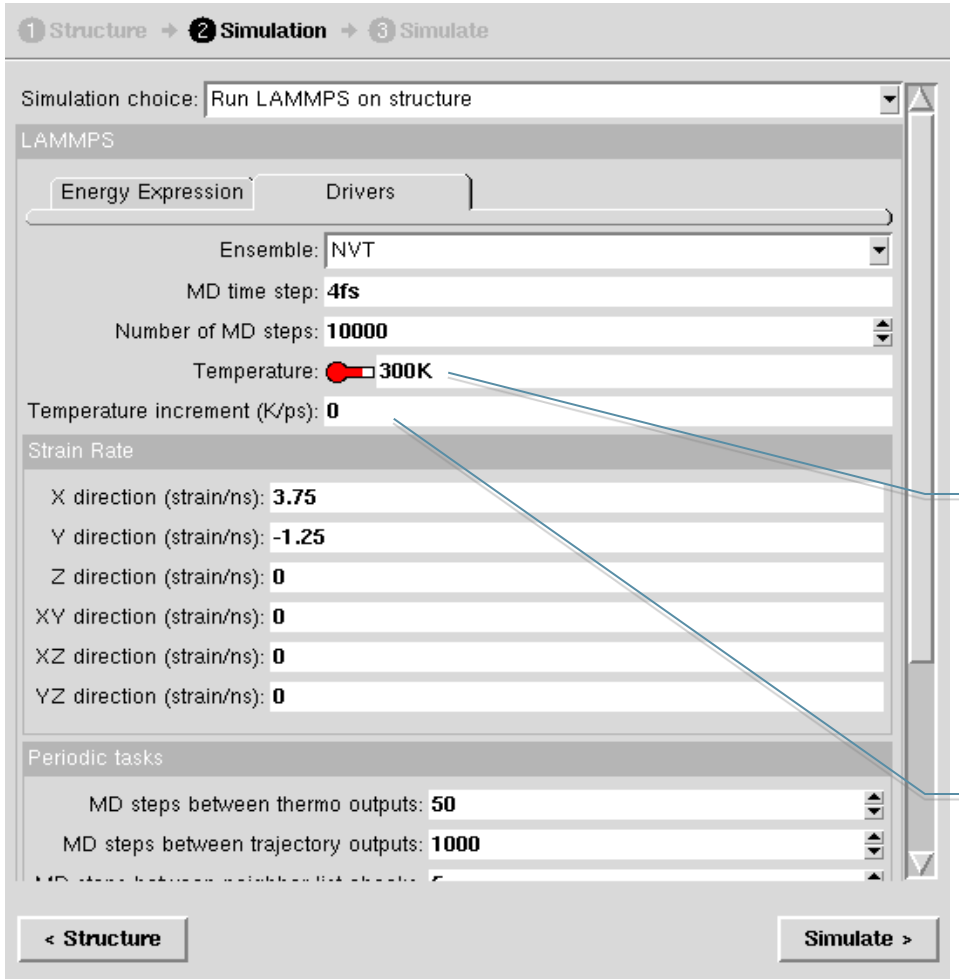


Length of time between MD steps.

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

Total number of time steps in the simulation.

Specify the different drivers

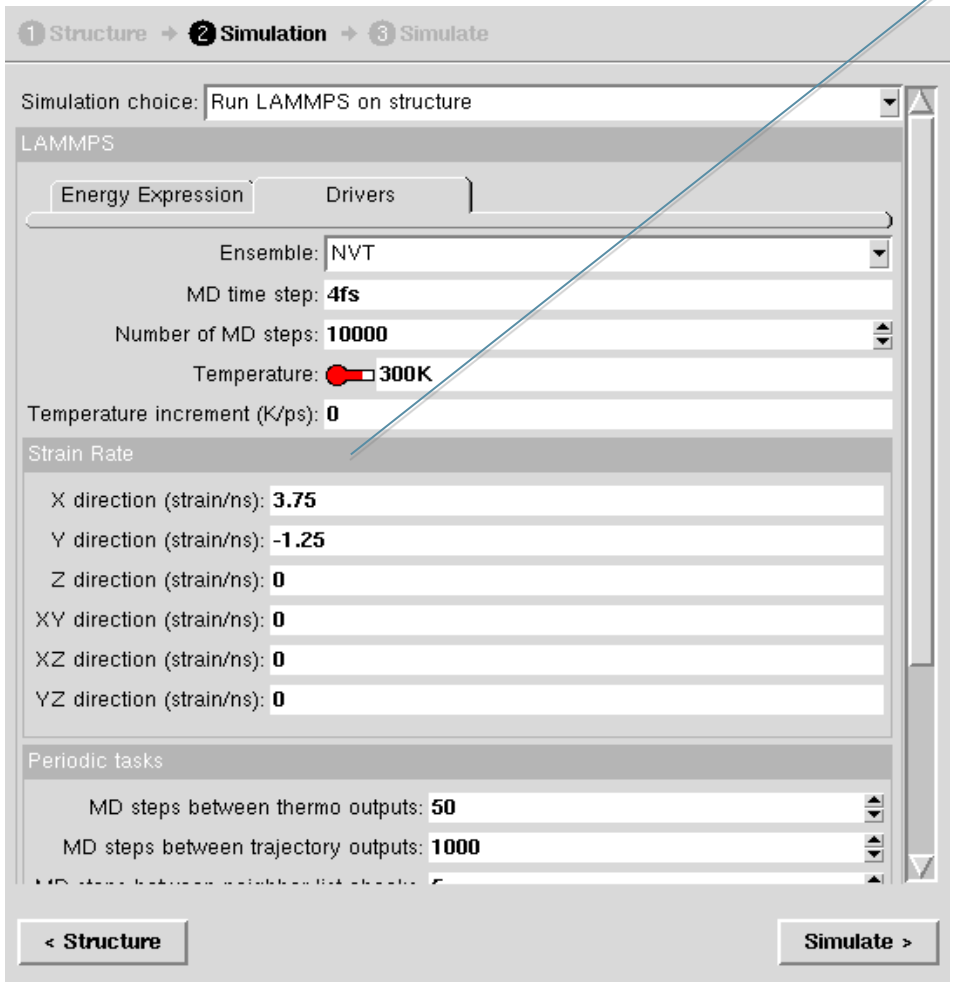


Sets the temperature of the system.

System temperature is regulated using a Nose/Hoover thermostat.

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

Set the strain rate for the different directions

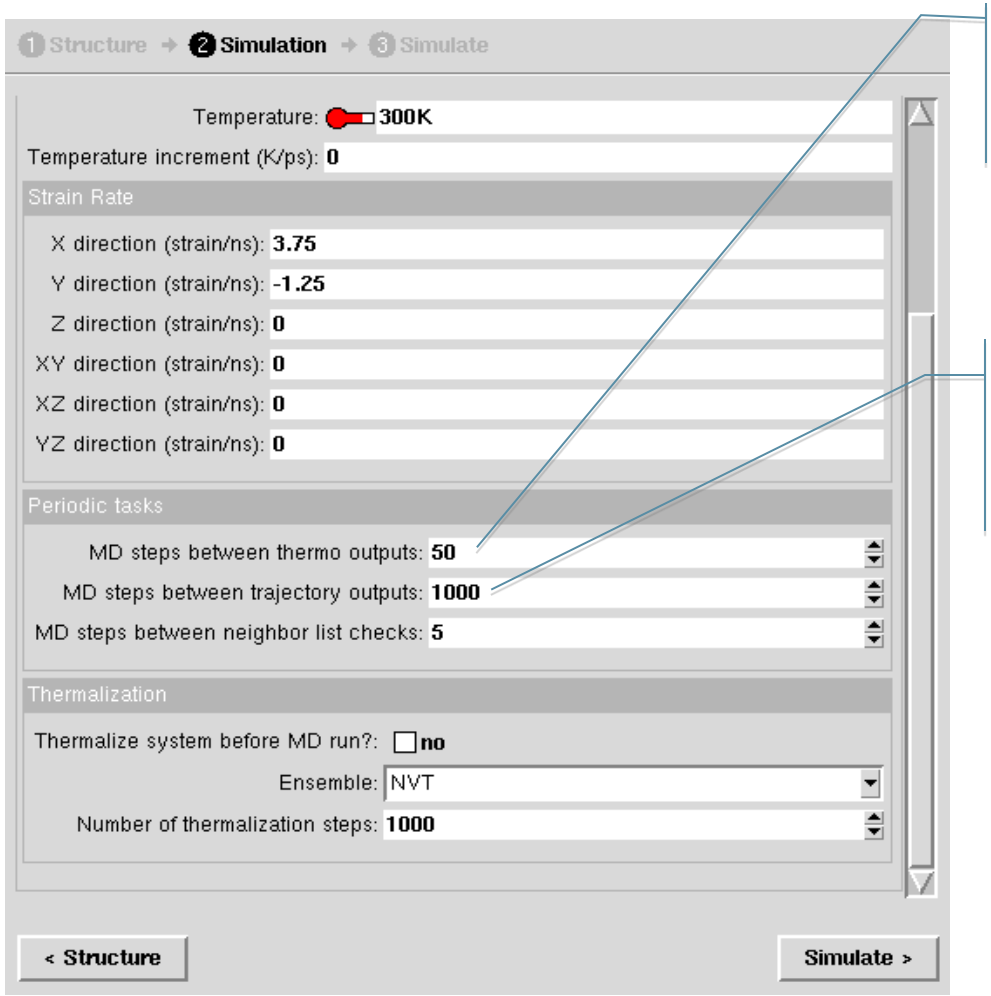


The strain rate controls the rate of deformation performed on the system. Deformation can be applied in any combination of the principle and shear directions.

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.

Periodic Tasks

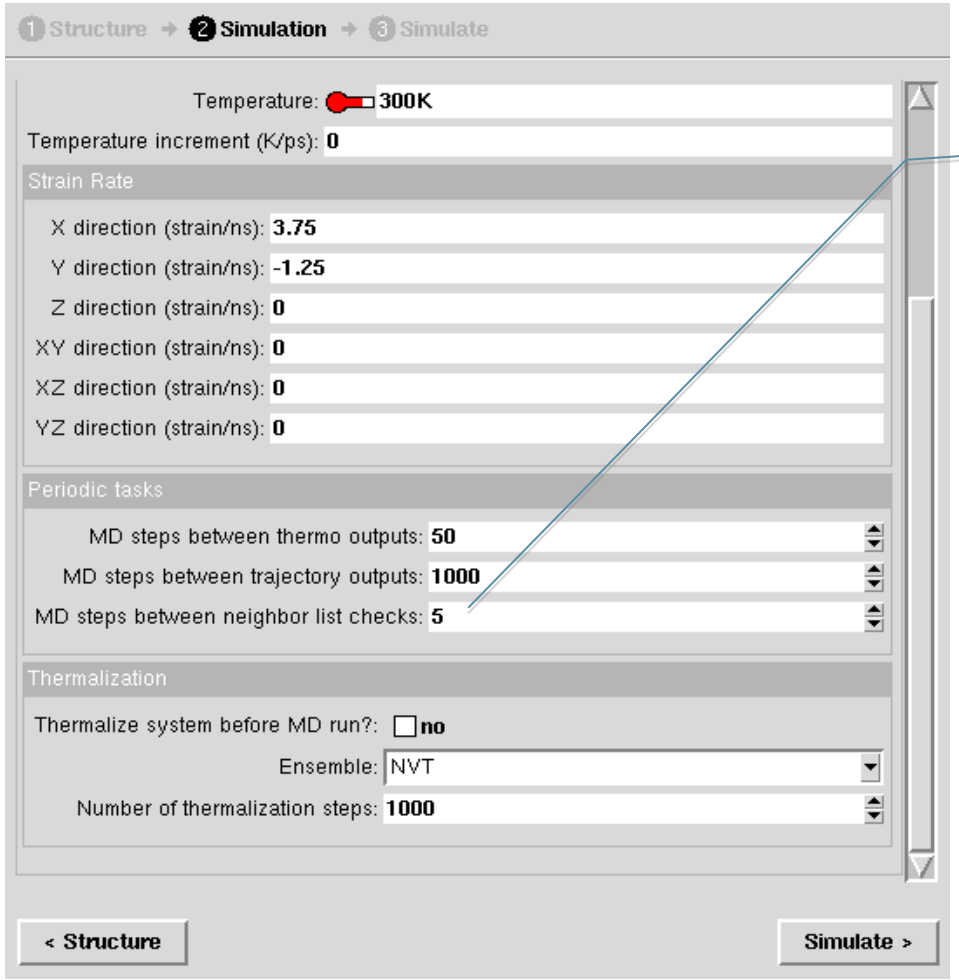


How many steps between output writings

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



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

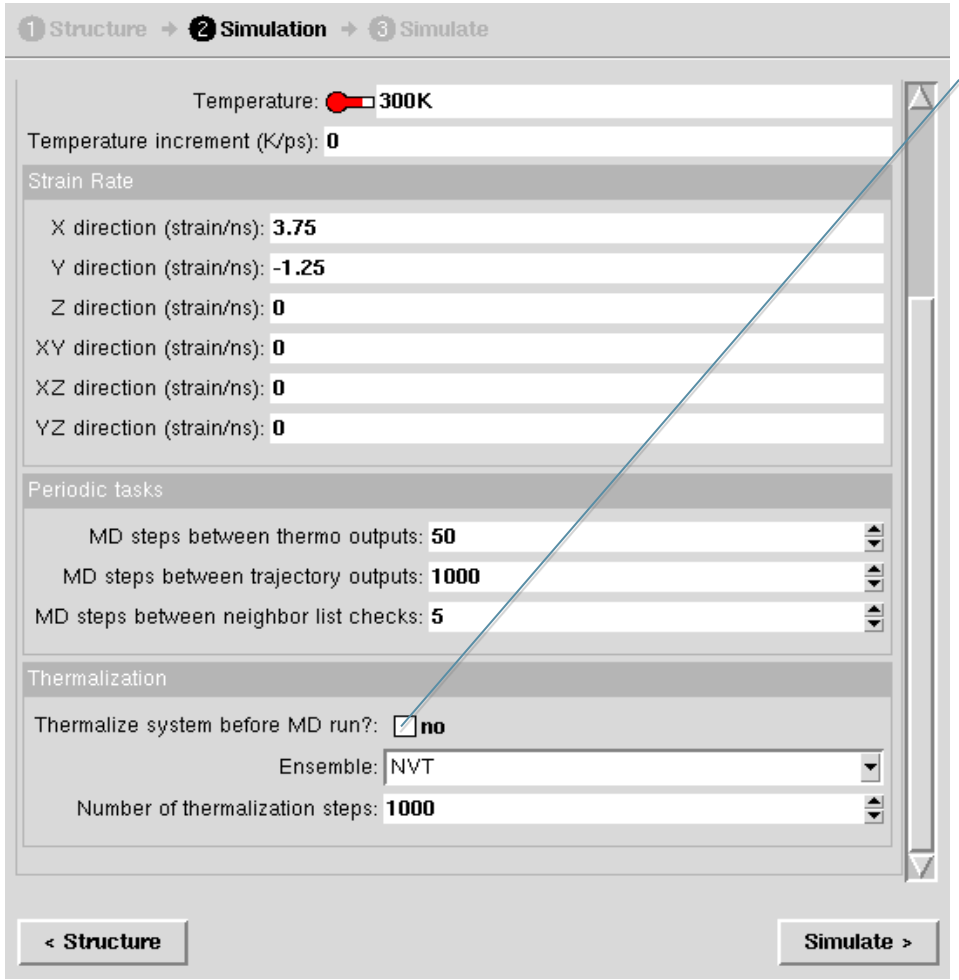
If an error stating an atom has been lost occurs, decreasing this number will create a new neighbor list more often. However, lower values increase computation time.

ADVANCED OPTIONS

Expert's Guide

Advanced Options

Check the box to thermalize system before running simulations



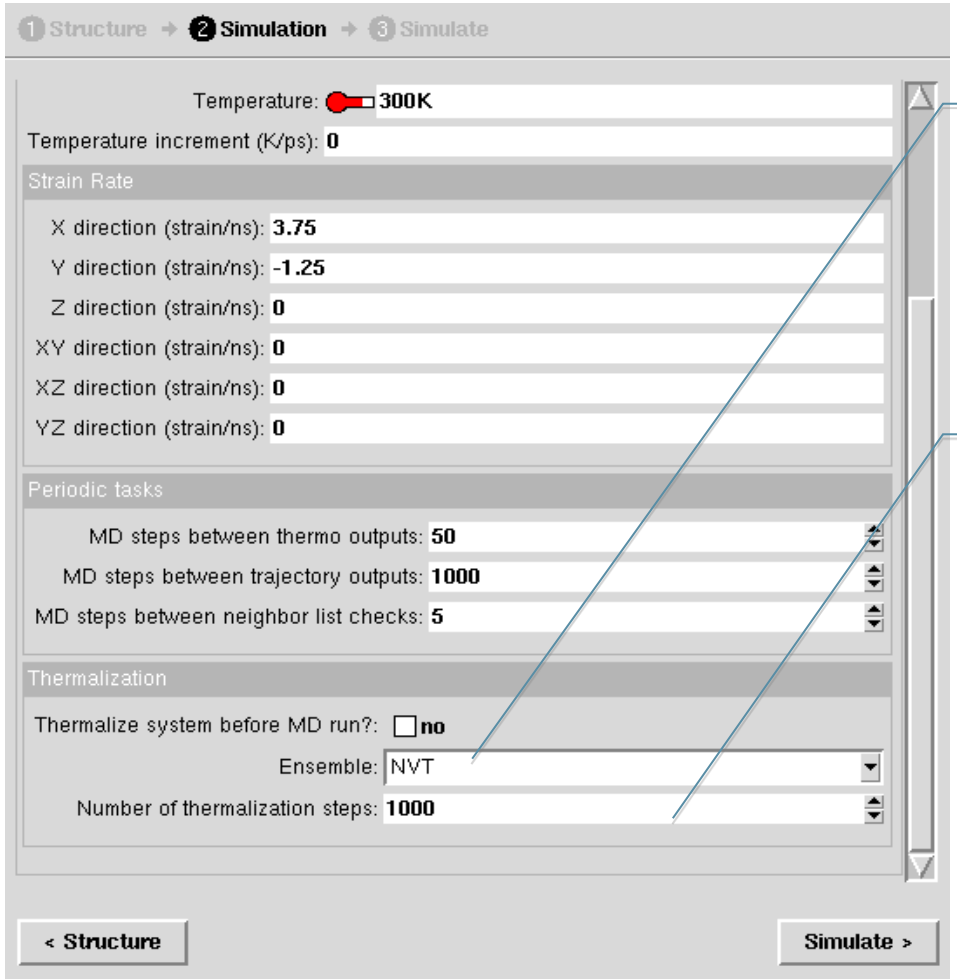
Heats the system to 600K for a period of time in order to allow atoms to shift positions and reach an overall lower energy configuration.

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



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.