

Materials Studio 5.0: Use Cases for Polymer Scientists

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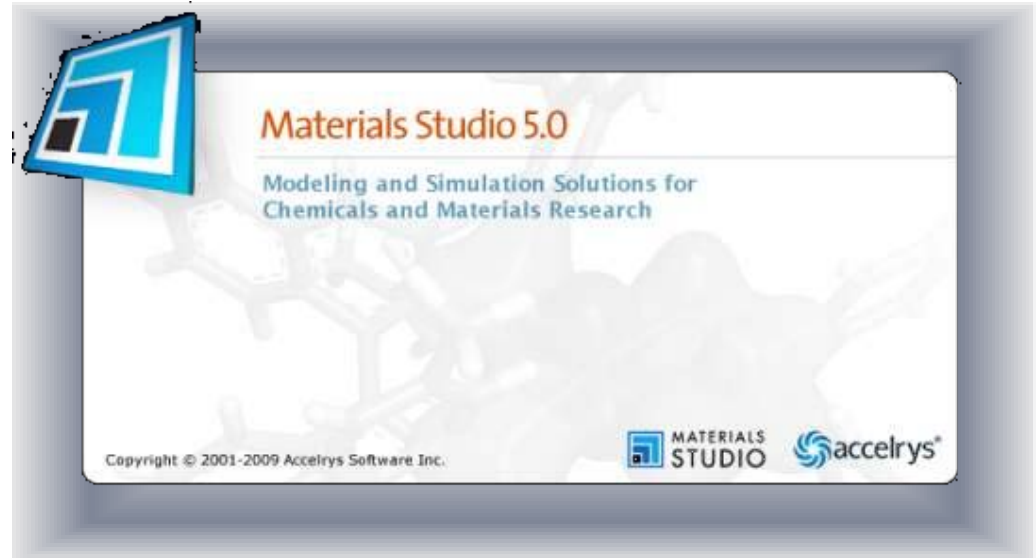
**Webinar Series: Materials Studio – What's new in 5.0?
Nov 18th 2009**

Amorphous Cell

- Construction algorithm
- Packing task

DPD

- New DPD Functionality
- Application Example



Three different tasks

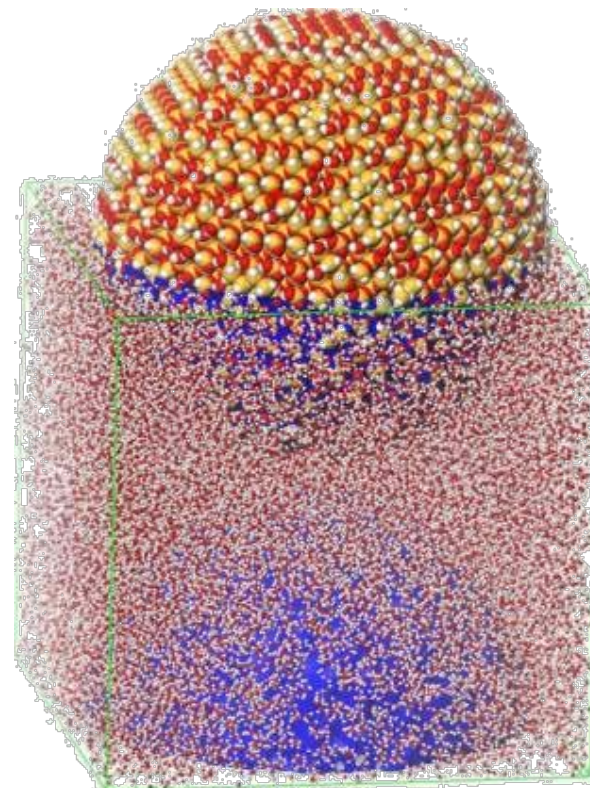
- Construction
- Packing
- Confined layer

User *and* scripting interface

- Automate workflows
- Pipelinable

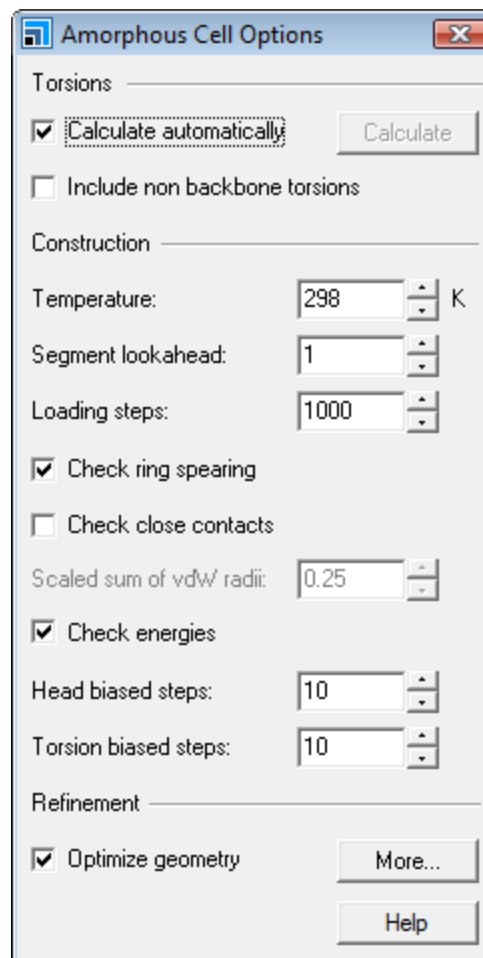
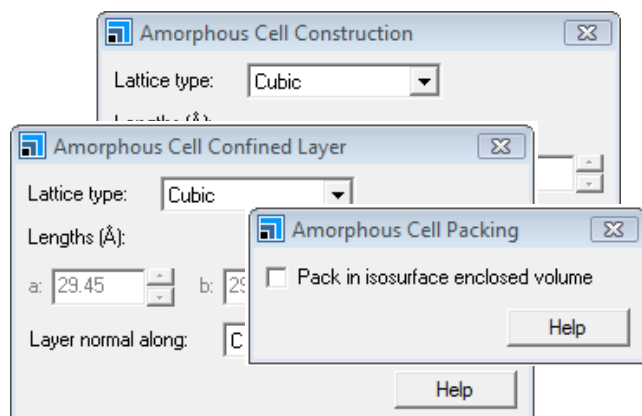
Improved forcefield support

Flexible torsion assignment



Same algorithm for all tasks

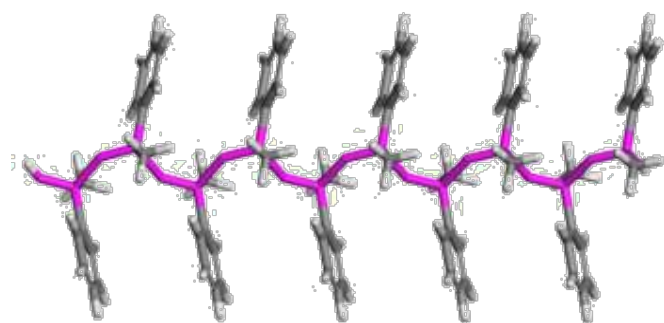
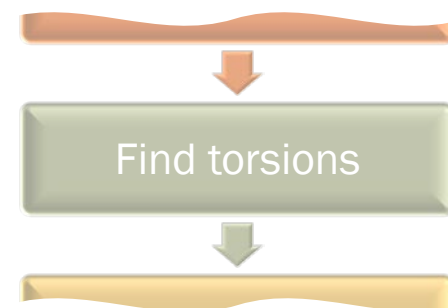
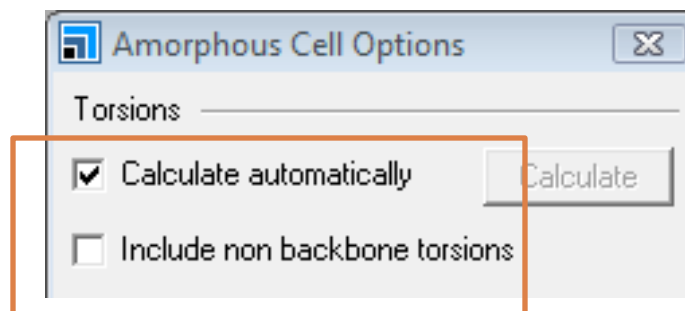
- Common controls on options dialog
- Individual controls on task dialogs



Algorithm: Find torsions

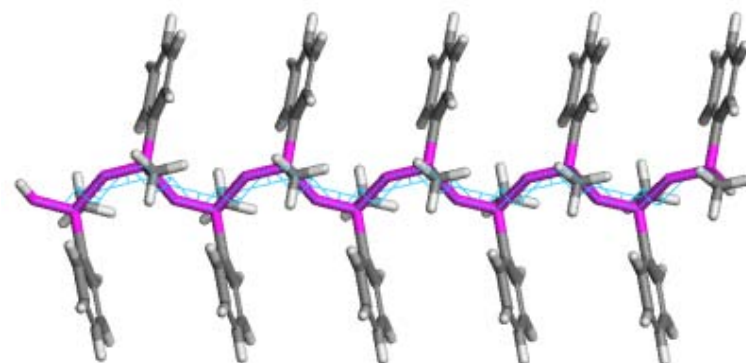
Automatic assignment

- Backbone torsions
- Side chain torsions

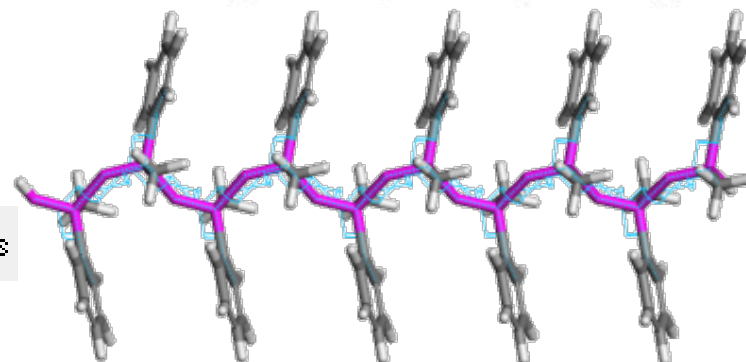


poly methyl phenyl siloxane

Include non backbone torsions

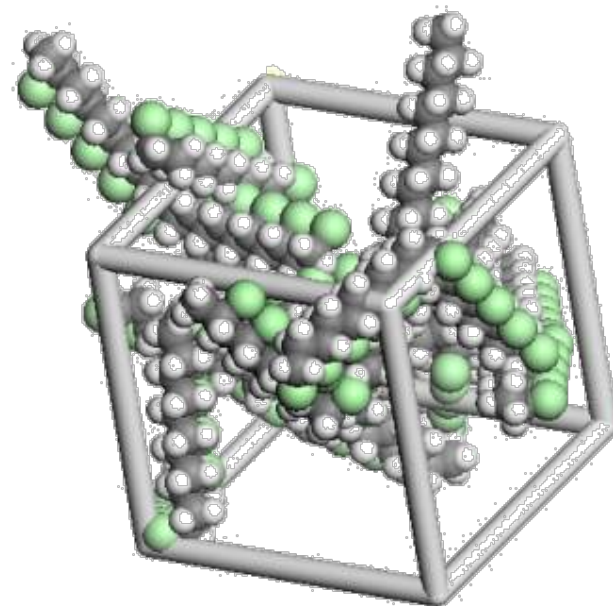
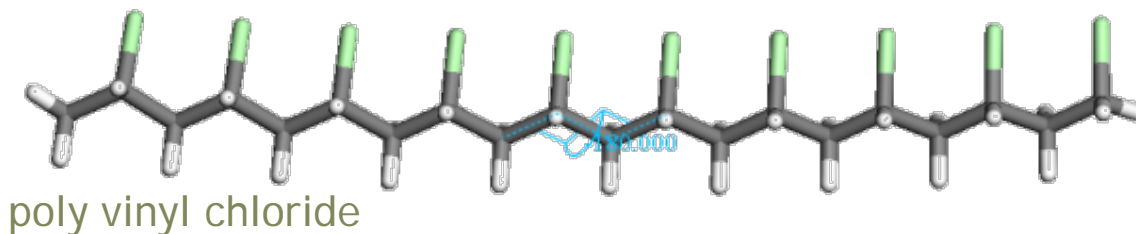
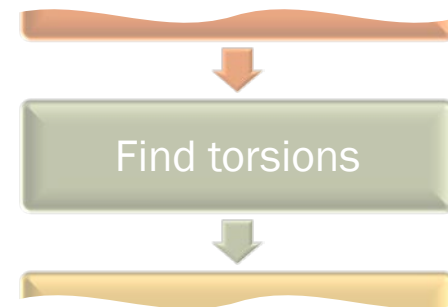
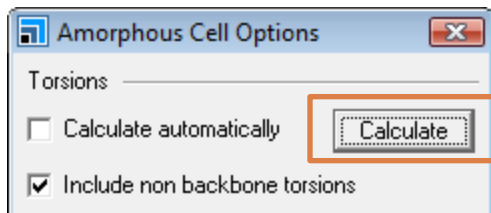


Include non backbone torsions



Manual assignment

- Verify automatic assignment
- Torsion monitors



Excluded torsions:

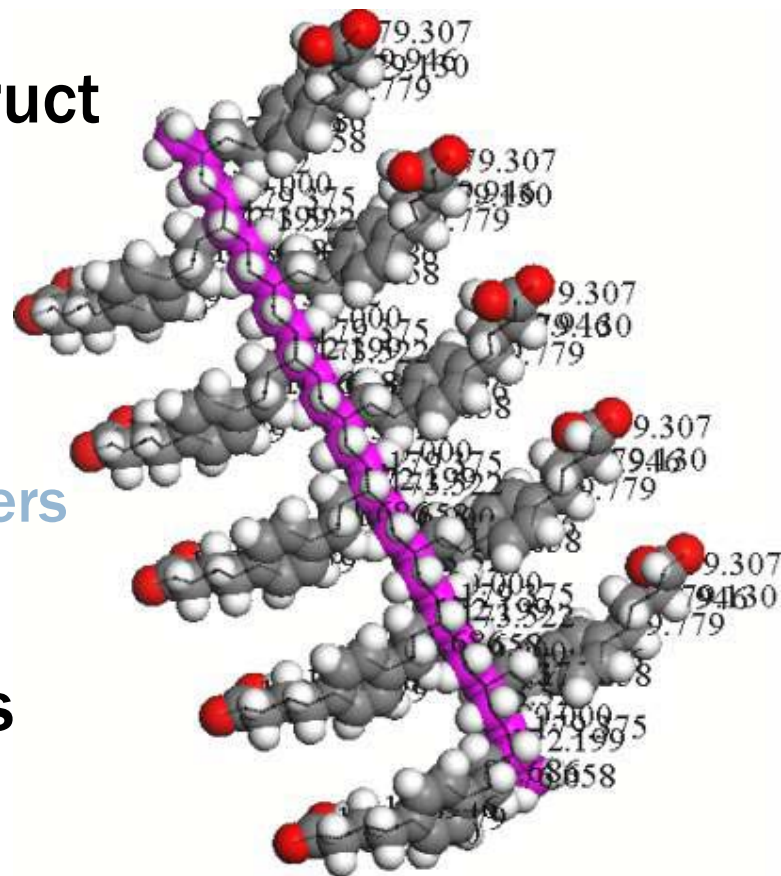
- bonds in rings
- double bonds
- constrained (symmetry/geometry)
- terminal hydrogens (can be assigned manually)

Long sidechains difficult to construct in legacy Amorphous Cell

- Construct at very low density and compress
- Ramp density
- Very hard to construct confined layers

Choose to rotate all flexible bonds

- Build at 1.2 g/cc
- Build at 1.6 g/cc

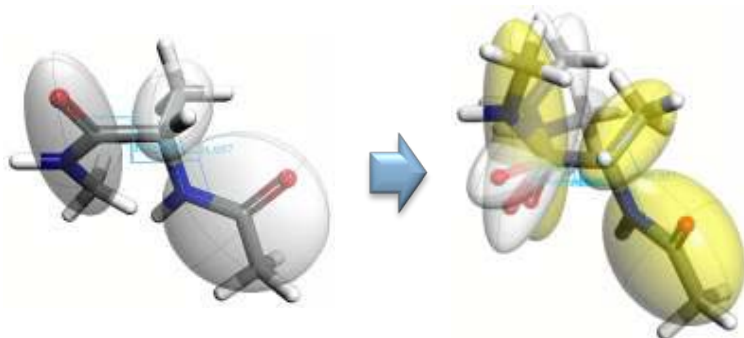


Loading Steps are also important!

Algorithm: torsion biased steps

Place 2nd, 3rd, ... segment

- Sample multiple torsions
- Boltzmann distributed



Construction _____

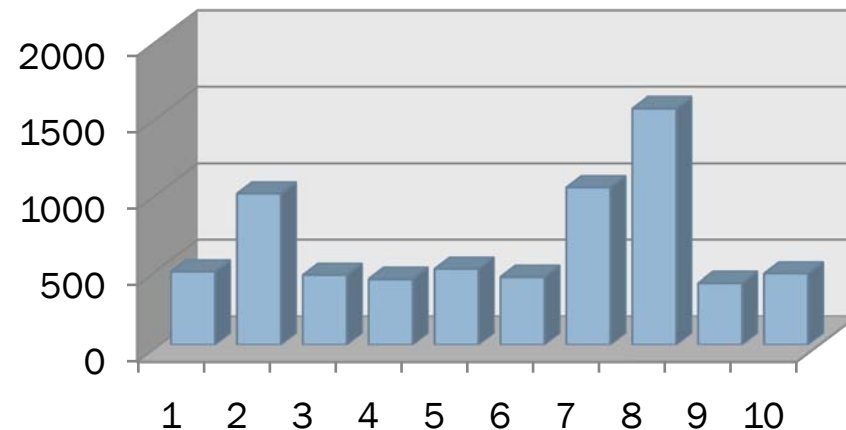
Temperature: K

Check energies

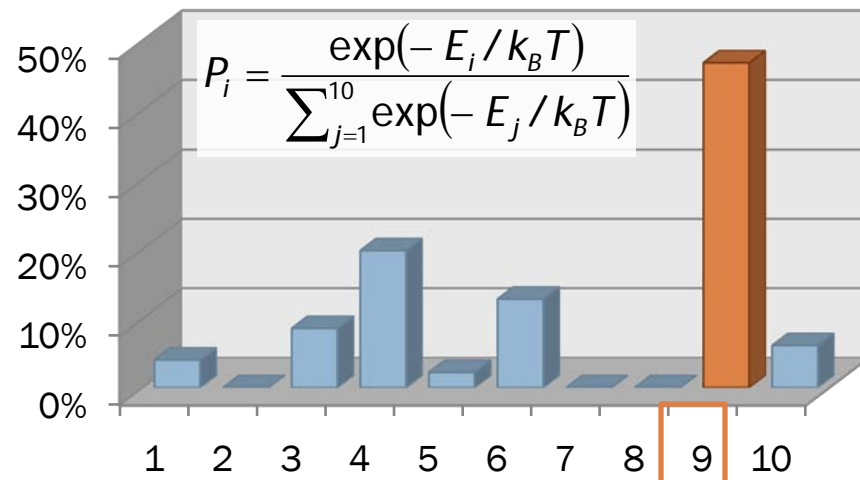
Head biased steps:

Torsion biased steps:

van der Waals energy



Probability



Algorithm: loading steps

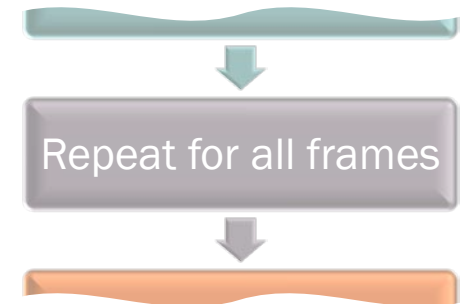
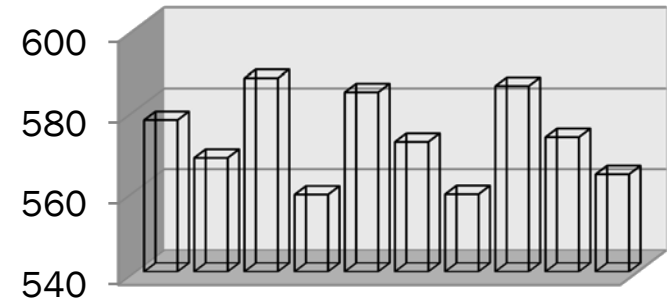
If all segment positions violate constraints:

1. Remove molecule
2. Continue with remaining segments
3. Reload molecule in next step

If maximum loading steps exceeded:

1. Store structure in studytable
2. Continue with remaining frames

van der Waals energy



Loading steps:

1000

Amorphous density is **1.37g/cc**

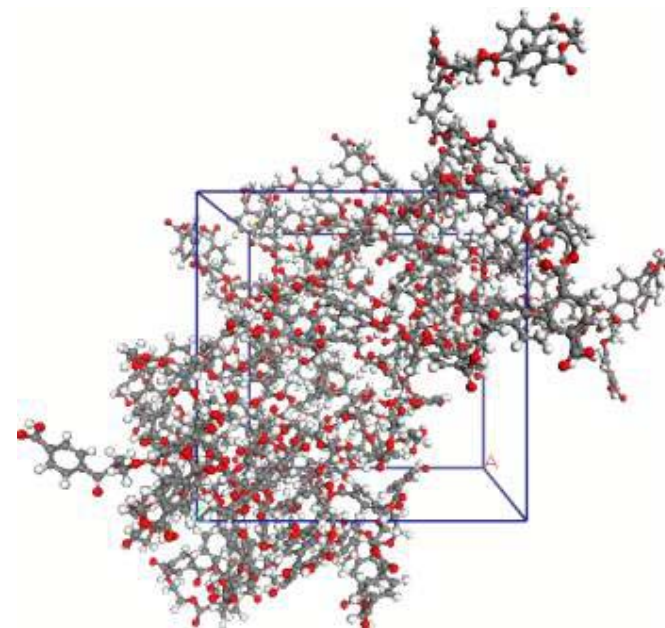
Rings in backbone!

Legacy Amorphous Cell

- Build at 0.6 - 0.7g/cc and compress

New Amorphous Cell builds at **experimental density** ✓

- Loading step flexibility
- Torsional sampling



Frame 1:	Loading steps	100
Frame 2:	Loading steps	169
Frame 3:	Loading steps	34
Frame 4:	Loading steps	71
Frame 5:	Loading steps	112

Close contact constraint

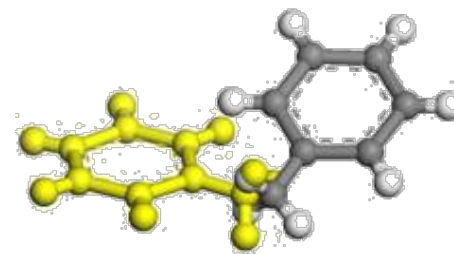
- Avoids energy calculation
- Useful for short chains

Undo energy calculation

- Athermal construction
- Very fast!

Check close contacts

Scaled sum of vdW radii:



Check close contacts

Scaled sum of vdW radii:

Check energies

Head biased steps:

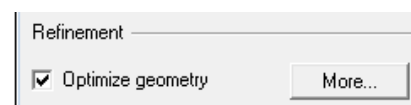
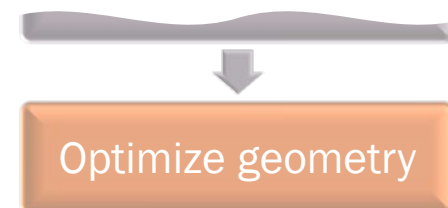
Torsion biased steps:

Optimize geometry of raw constructs

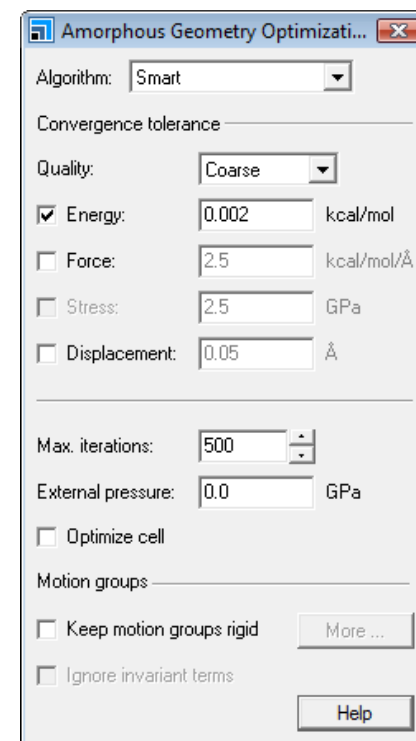
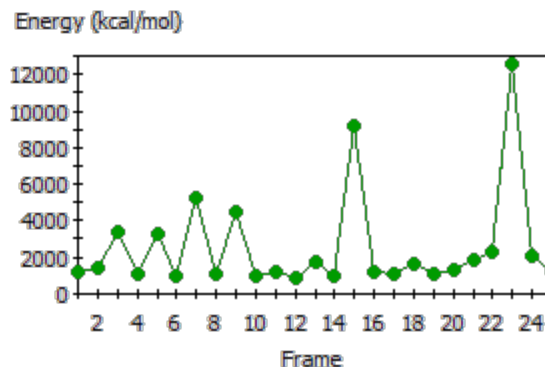
- To remove bad contacts
- Optional for construction & packing
- Not supported for confined layer
- Runs over all frames

Full control over optimization

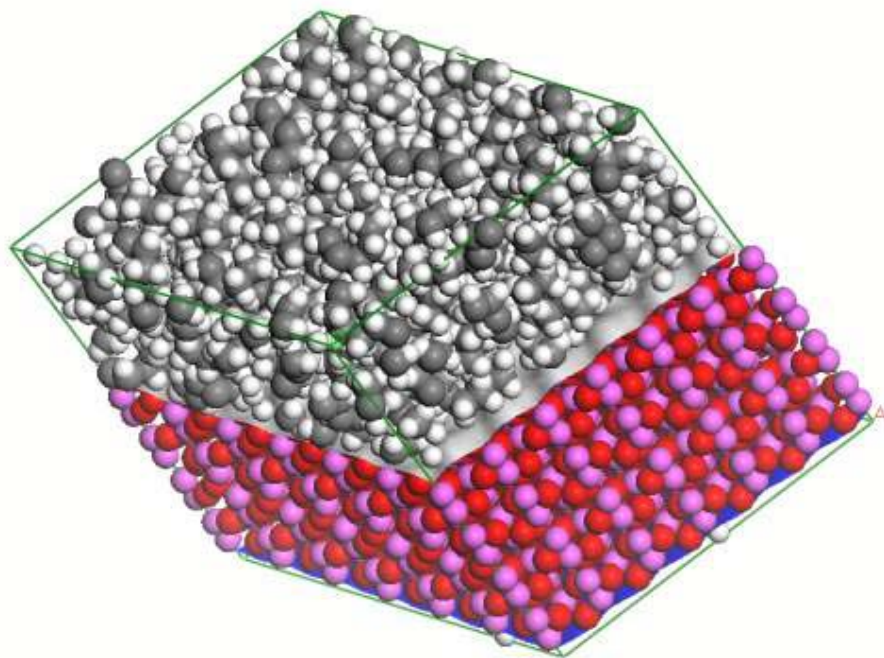
- Can be switched off
- Choice of algorithm
- Optimize cell parameters
- Keep motion groups fixed



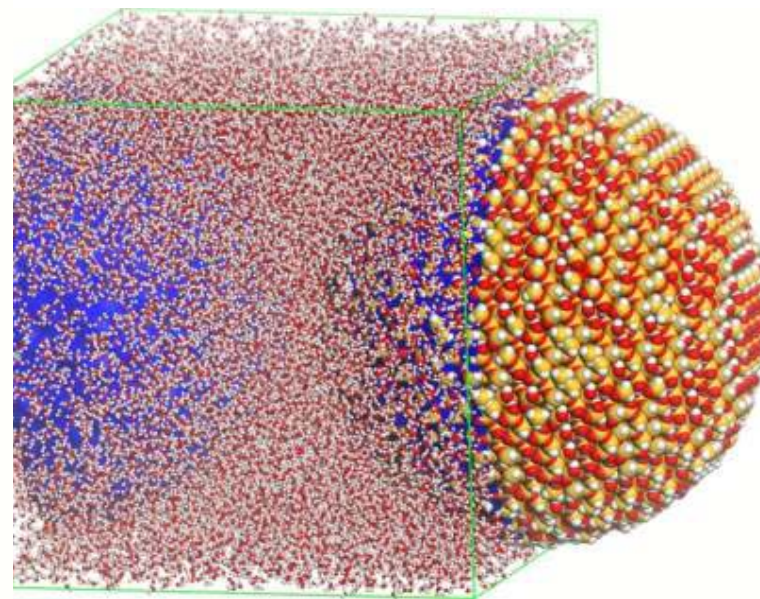
Geometry Optimization - Energy



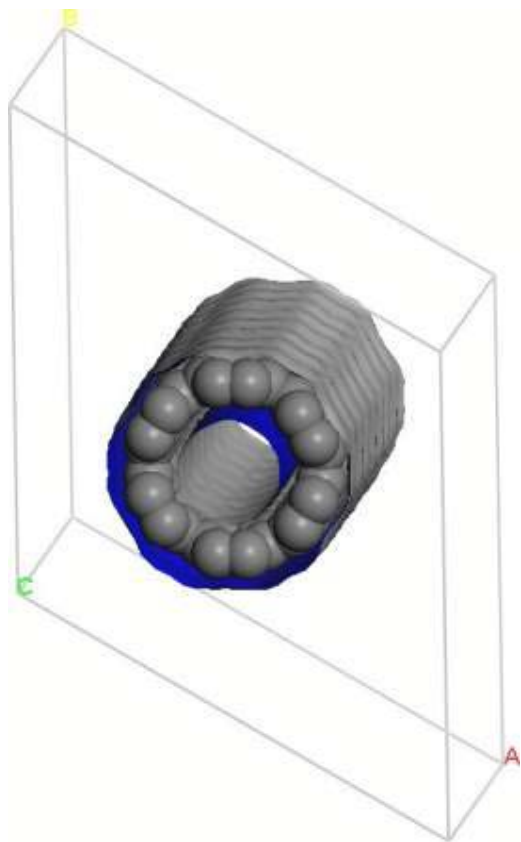
Pack molecules into an existing cell



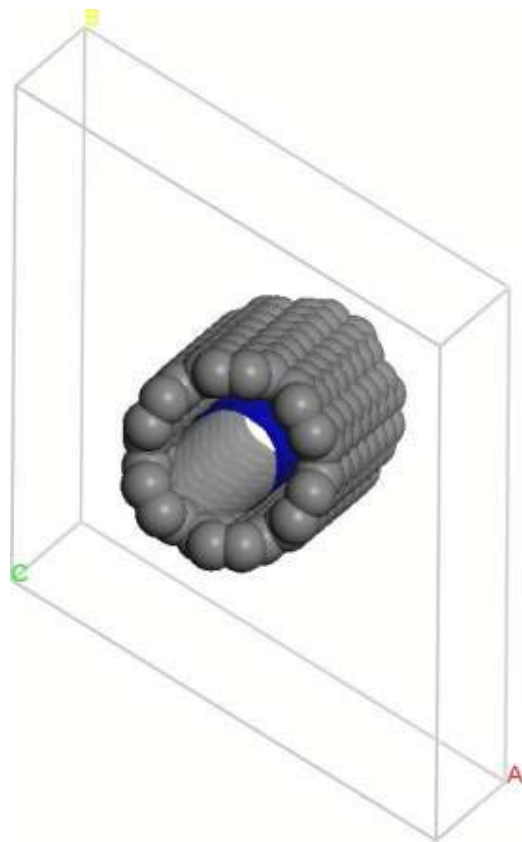
Build non-orthorhombic cells



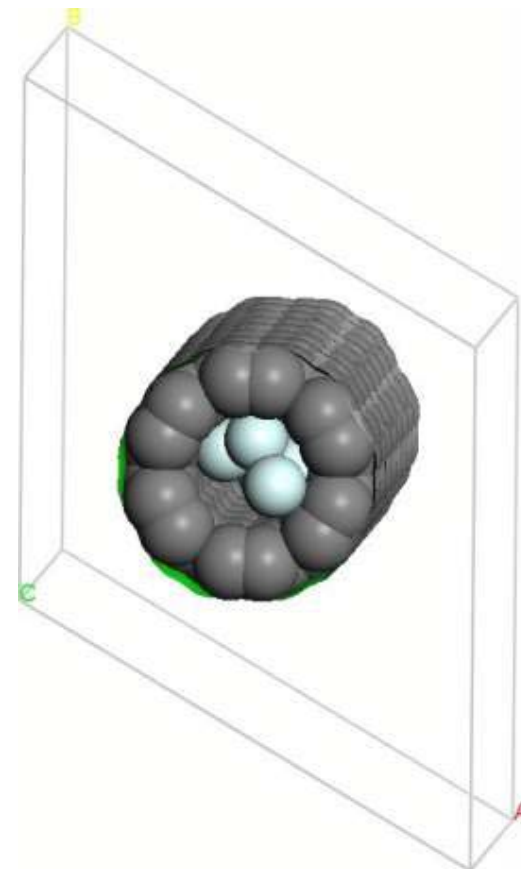
Soak a pre-existing structure



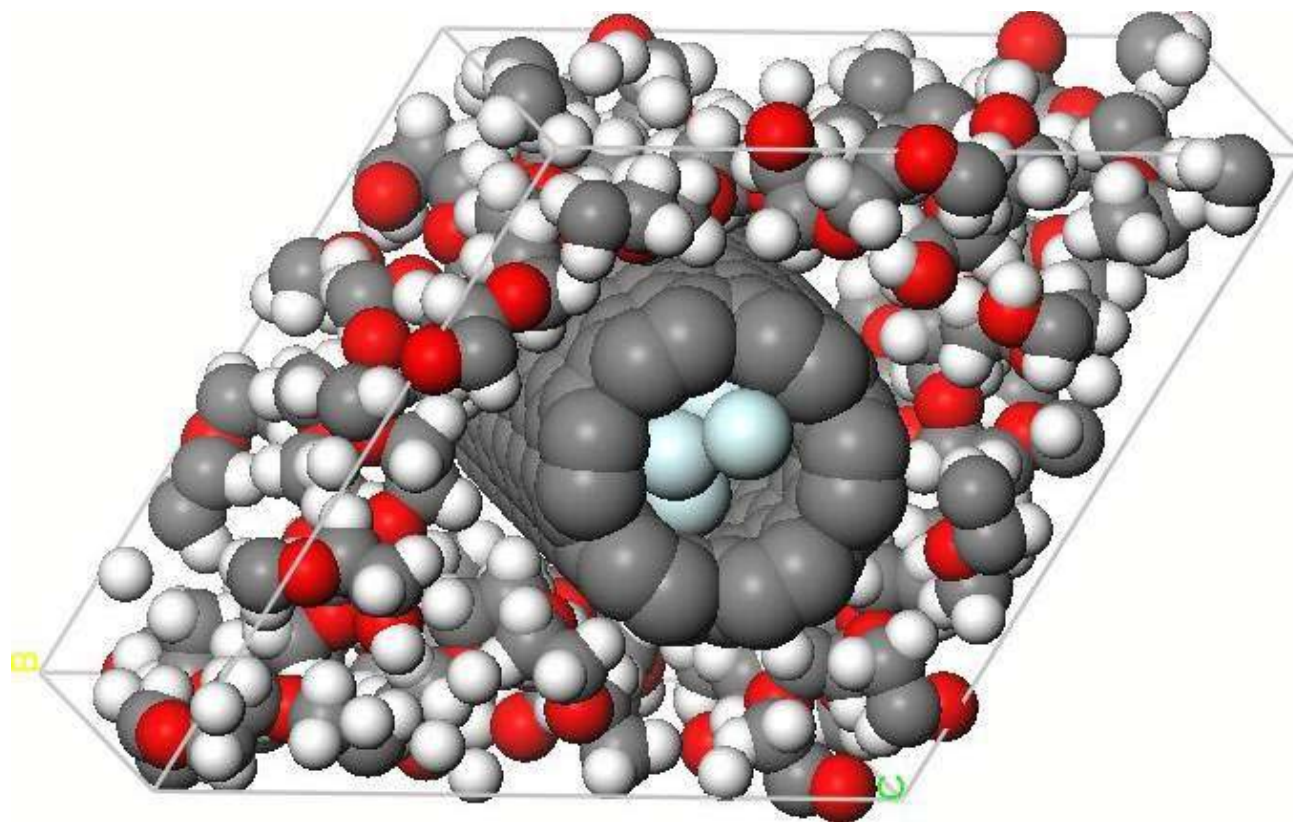
1. Add a Connolly field



2. Segregate the field



3. Pack gas into segregate



4. Pack polymer into segregate

LEGACY	Amorphous Cell 5.0
Optimization with COMPASS	Optimization with selected forcefield
Lookahead by exact enumeration/sampling	Lookahead by sampling
Confinement using restraints	Confinement using constraints
Confined layer optimized	Confined layer unoptimized
Terminal bonds allowed to spear	No spearing allowed
Always adds small molecule first to cell	Order is dependent on order in Components section
Atom and repeat unit names are not preserved	Atom and repeat unit names are preserved (great for labelling!)

Overview

- Parallelization
- Mesocite Analysis now available for DPD
- Provide support for physical units
- Scripting
- Flexibility

Legacy DPD is still available

- No shearing in Mesocite

Intended for mesoscale modelling of the dynamics of polymers, etc

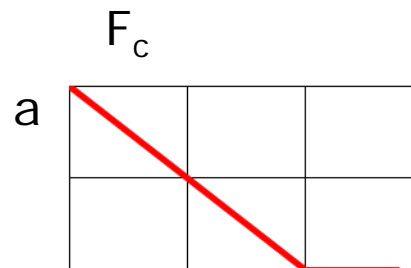
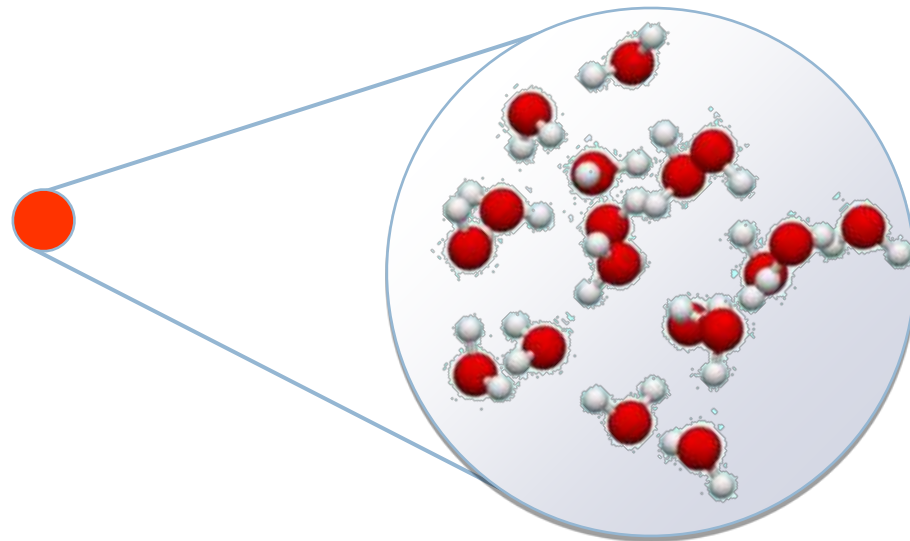
Highly coarse-grained representation

- Many atoms replaced by one bead

DPD models the dynamics of a system of beads, each representing a group of many atoms

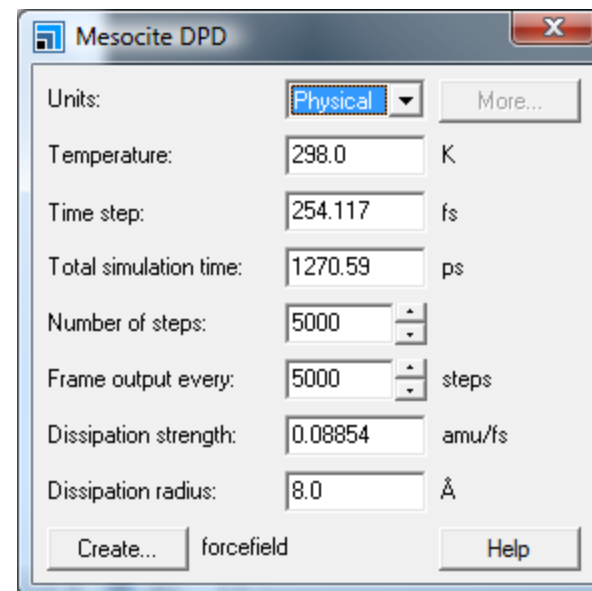
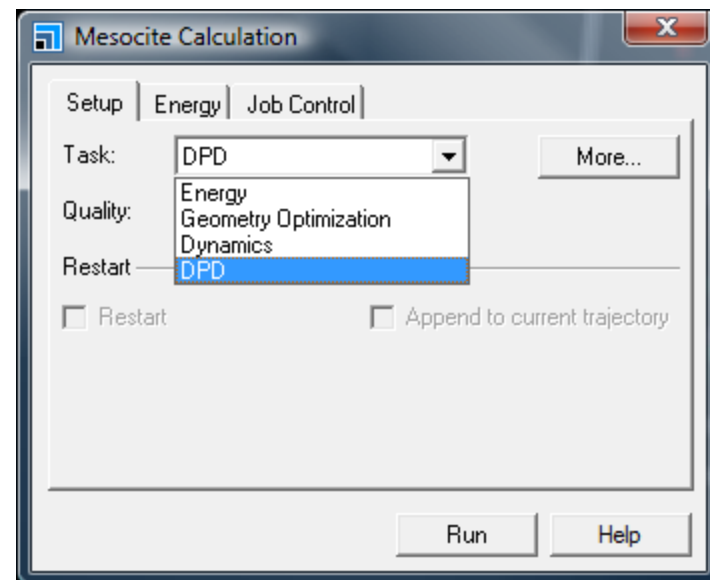
DPD beads interact with a Soft Harmonic potential (nonbond interaction)

- Each bead represents a group of atoms/molecules which can overlap, not a single atom



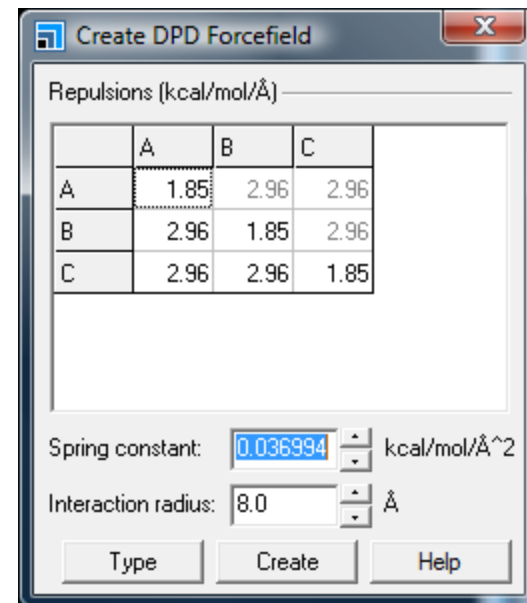
DPD is now another task in Mesocite

- Mesocite DPD has a dialog similar to Mesocite Dynamics
- Any forcefield can be used (select from the energy tab)
- Support is provided for soft harmonic potentials
- Input is a bead-based .xsd document (.xtd for restart)
- Output is a .xtd and can be analysed in the usual way
- NVT ensemble



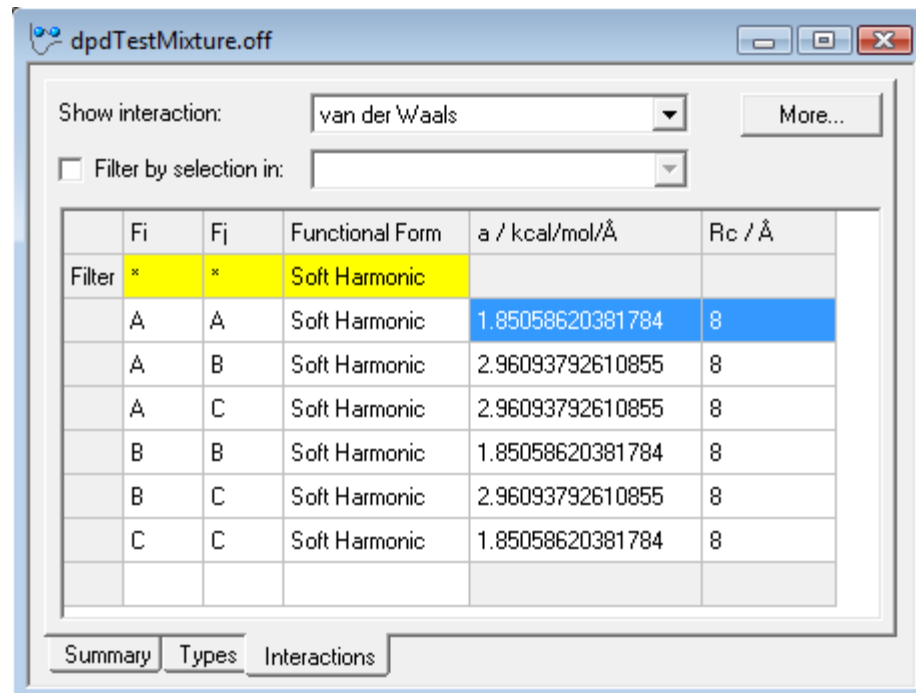
Create DPD Forcefield dialog

- Grid of repulsion parameters between all pairs of species (nonbonded interaction)
- Can be defined using physical or reduced units
- **Type button:**
 - Assigns forcefield types to beads in current structure document
 - Sets up rows and columns in grid
- **Create button:**
 - Makes a forcefield
 - Sets it into the Energy tab of Mesocite Calculation



DPD Forcefield

- Can be viewed and modified in the Forcefield viewer in the usual way
- Mesoscale non-bond interaction modeled as van der Waals
- 1-2 and 1-3 interactions are included
- Bonded interaction (Harmonic spring) has $R_0 = 0.1\text{\AA}$
 - Energy Server must have $R_0 > 0$
- Can be used for Mesocite Dynamics
 - Should give the same results as DPD for equilibrium thermodynamics in NVT
 - Kinetics and transport properties are different
- Easy to share!



dpdTestMixture.off

Show interaction: van der Waals More...

Filter by selection in:

	Fi	Fj	Functional Form	a / kcal/mol/Å	Rc / Å
Filter	*	*	Soft Harmonic		
	A	A	Soft Harmonic	1.85058620381784	8
	A	B	Soft Harmonic	2.96093792610855	8
	A	C	Soft Harmonic	2.96093792610855	8
	B	B	Soft Harmonic	1.85058620381784	8
	B	C	Soft Harmonic	2.96093792610855	8
	C	C	Soft Harmonic	1.85058620381784	8

Summary Types Interactions

Legacy DPD works in a 'reduced' system of units

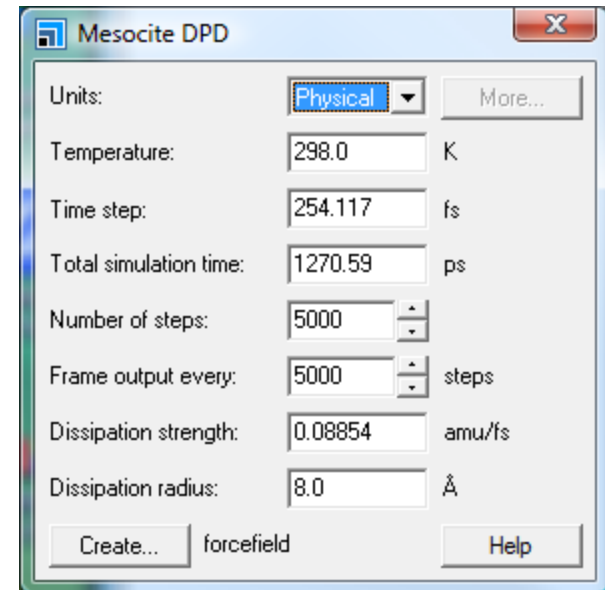
- Length: r_c (bead size); bead mass m ; energy: $k_B T$
- Derived units: time = $r_c \sqrt{(m/k_B T)}$

Mesocite uses 'physical' units

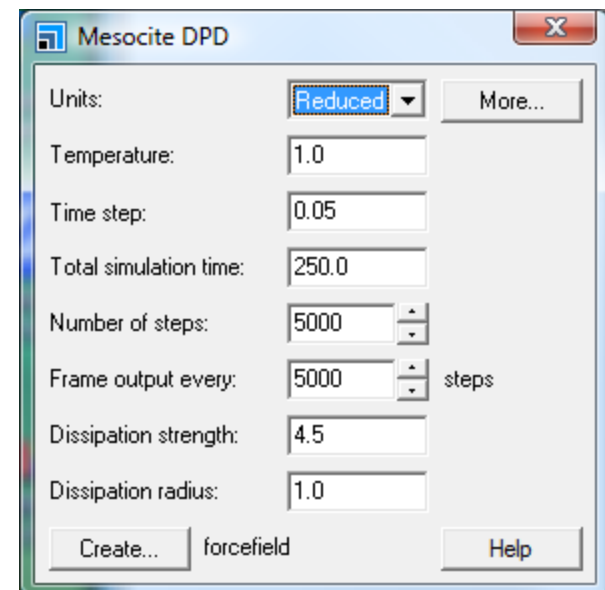
- Å, fs, amu, kcal/mol

Mesocite DPD can accept input parameters in either reduced or physical units

All Mesocite DPD output is in physical units



Mesocite DPD dialog box showing Physical units. The 'Units' dropdown is set to 'Physical'. Parameters include: Temperature: 298.0 K; Time step: 254.117 fs; Total simulation time: 1270.59 ps; Number of steps: 5000; Frame output every: 5000 steps; Dissipation strength: 0.08854 amu/fs; Dissipation radius: 8.0 Å. Buttons: Create... forcefield, Help.



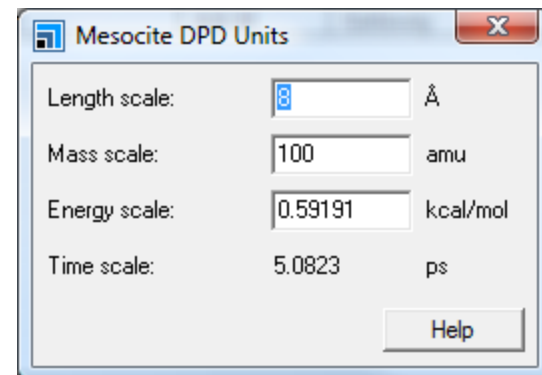
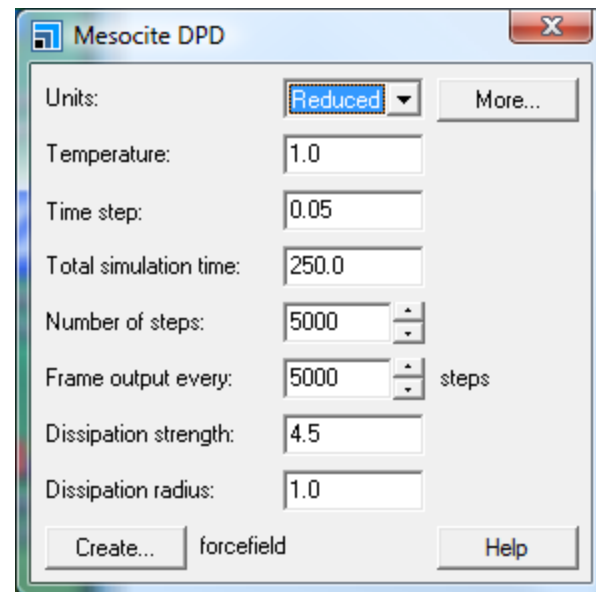
Mesocite DPD dialog box showing Reduced units. The 'Units' dropdown is set to 'Reduced'. Parameters include: Temperature: 1.0; Time step: 0.05; Total simulation time: 250.0; Number of steps: 5000; Frame output every: 5000 steps; Dissipation strength: 4.5; Dissipation radius: 1.0. Buttons: Create... forcefield, Help.

In 'reduced' mode, the length, mass and energy units can be specified

Defaults:

- Length = 8 Å
- Mass = 100 amu
- Energy = $k_B T$ at 298K
 - Given in units of kcal/mol
- Time unit is approx 5 ps
- Density is approx 1 g/cm³ if using 3 beads per r_c^3

Default values map to those in the mesostructure builders.



Effect of nonionic surfactants on cell membranes

Addition of disinfectants cause cell damage and death

Most common target is between cell membrane

- Consists of membrane lipids and membrane proteins

Nonionic surfactants can inhibit bacterial growth

- e.g. Detergent alcohol ethoxylates

How do the nonionic surfactants inhibit bacterial growth?

- Study interaction of nonionic surfactants with lipid membrane using DPD
- Create structures with varying concentrations of lipid and surfactant
- DPD accesses the correct time and length scales to study breakdown of cell walls



(1) Groot, R. D.; Rabone, K. L. *Biophysical Journal*. 2001, 81, 725.

System Definition - Mesomolecules

Built using Mesomolecule Builder

Surfactant: E06C12

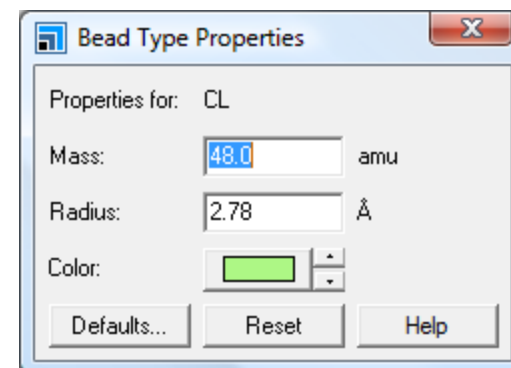
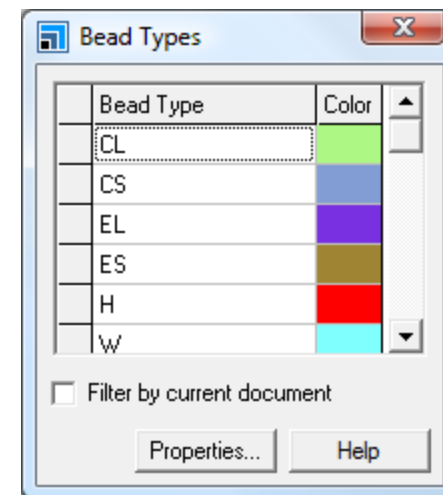


Lipid: phosphatidylethanolamine



All beads have same Mass and Radius

Only four different interaction types, C, E, H and W

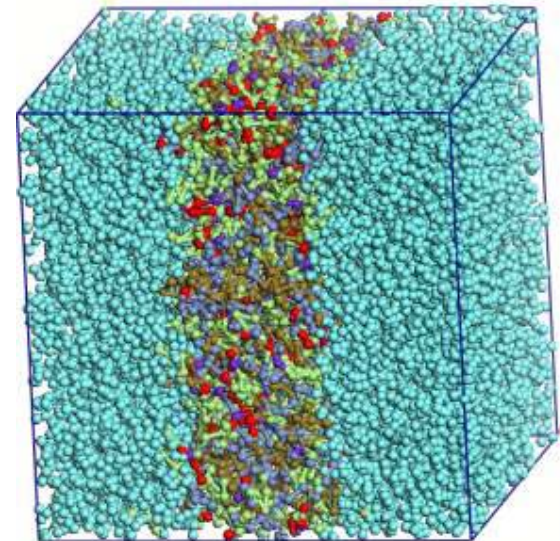
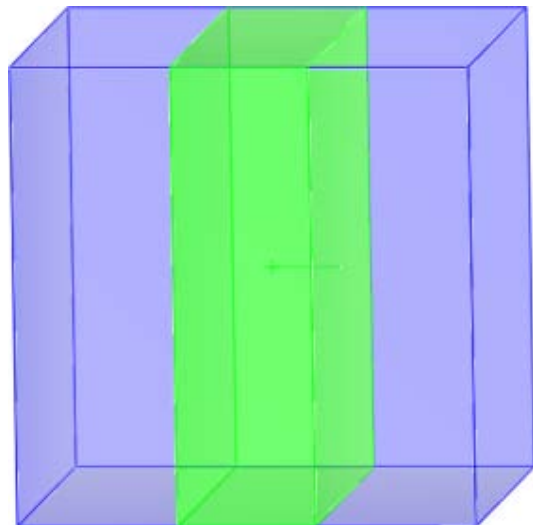
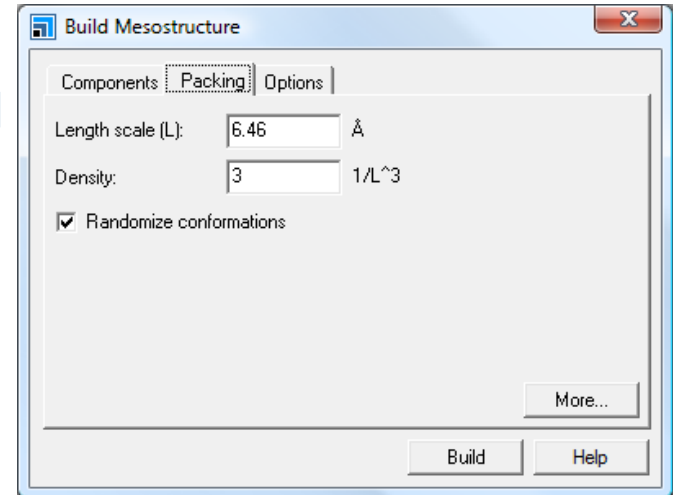


Use a volume packed mesostructure

- Create a slab to pack the surfactant and lipid – easy to set different ratios!

Build at correct length scale and density

- Length scale: 6.46Å
- Density: 3 beads/unit density
- Vary concentration of lipid and surfactant



Calculation settings defined in reduced units:

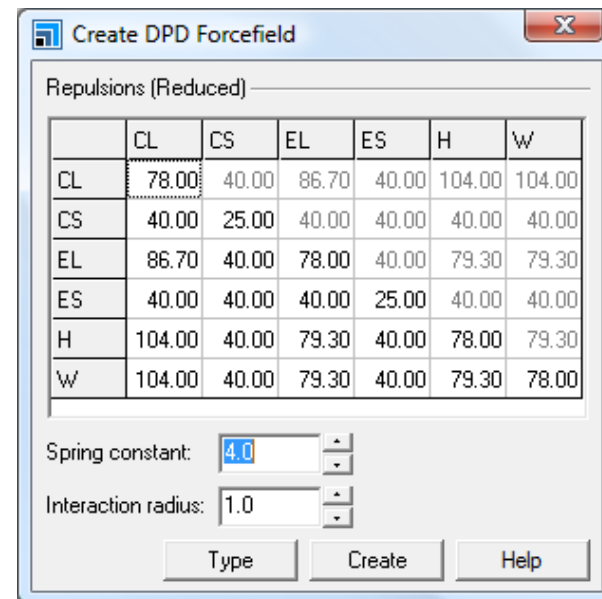
- Use mass, length scale to convert to physical
- Energy scale defines temperature

Interaction parameters taken from Groot and Rabone

Should set Summation method to bead based

- Cutoff should equal length scale
- Ewald summation is likely to give odd results with DPD

Structures should be “optimized” before dynamics



Create DPD Forcefield

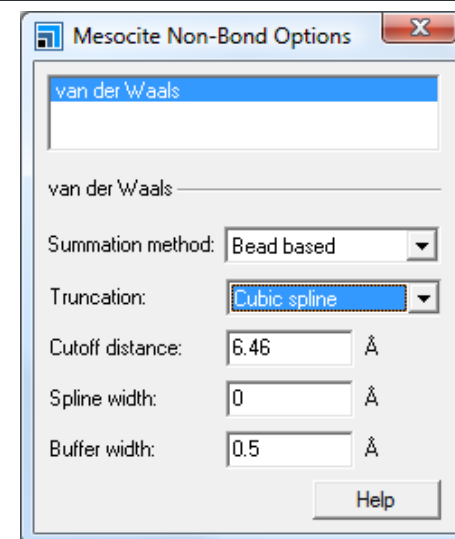
Repulsions (Reduced)

	CL	CS	EL	ES	H	W
CL	78.00	40.00	86.70	40.00	104.00	104.00
CS	40.00	25.00	40.00	40.00	40.00	40.00
EL	86.70	40.00	78.00	40.00	79.30	79.30
ES	40.00	40.00	40.00	25.00	40.00	40.00
H	104.00	40.00	79.30	40.00	78.00	79.30
W	104.00	40.00	79.30	40.00	79.30	78.00

Spring constant: 4.0

Interaction radius: 1.0

Type Create Help



Mesocite Non-Bond Options

van der Waals

van der Waals

Summation method: Bead based

Truncation: Cubic spline

Cutoff distance: 6.46 Å

Spline width: 0 Å

Buffer width: 0.5 Å

Help

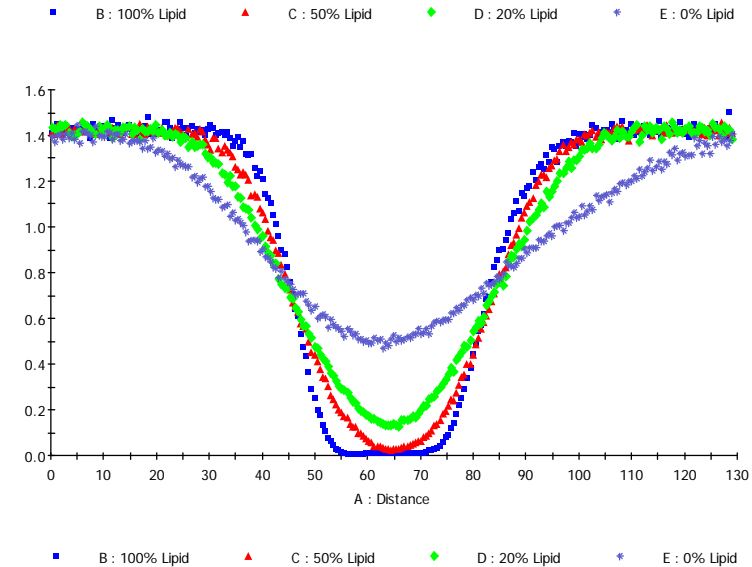
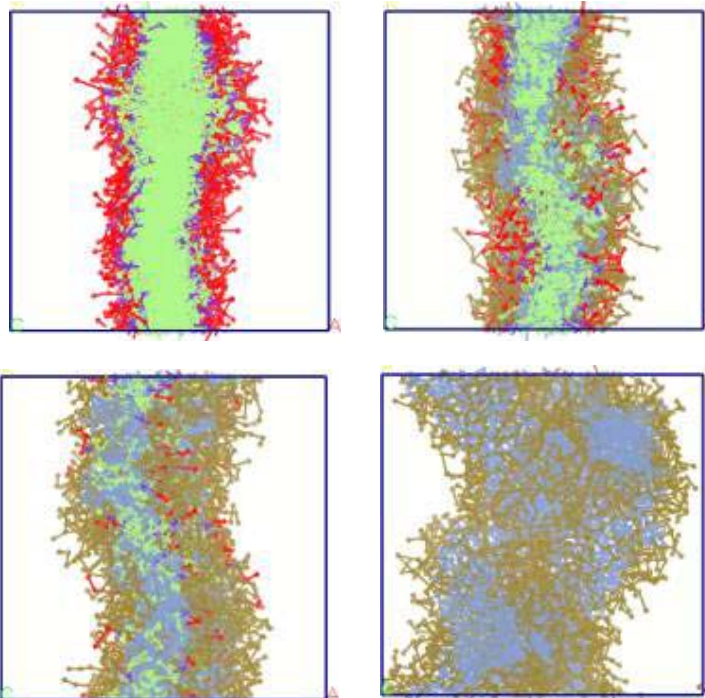
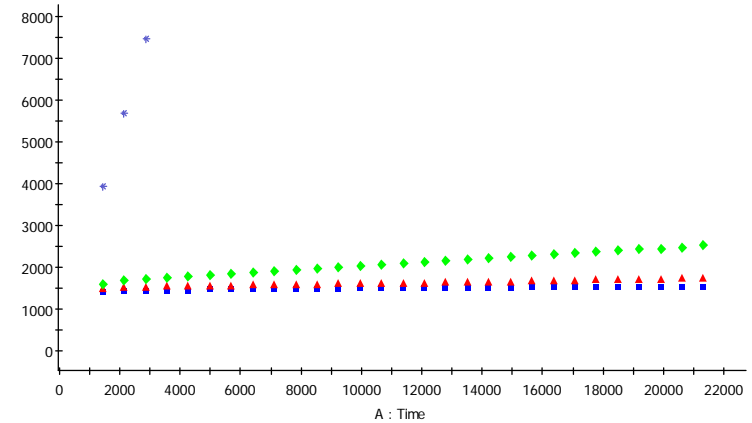
Increasing Surfactant Concentration

Increased diffusivity of solvent through membrane

- Analyse XX component of MSD

Decreases stability of lipid membrane

- Analyse concentration profile of water



Effect of Strain on Surface Tension

Strain the membrane

Equilibrate with MD

Calculate Surface Tension

```
my $stressXX = $stress->Eij(1,1) ;  
my $stressYY = $stress->Eij(2,2) ;  
my $stressZZ = $stress->Eij(3,3) ;  
  
my $surfaceTension = ($stressXX - 0.5*($stressYY + $stressZZ)) * $lengthX;
```

% Lipid	Area/Original Area
90% Lipid	1.54
50% Lipid	1.20
20% Lipid	1.06

Script is available here:

<http://tinyurl.com/yh8fe7e>

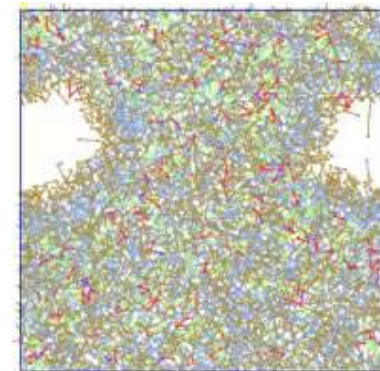
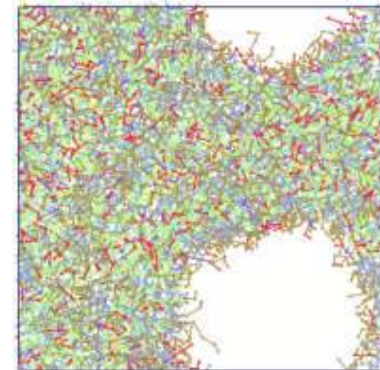
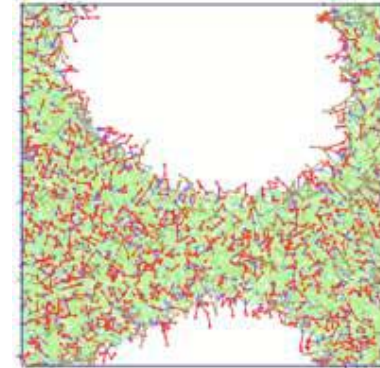
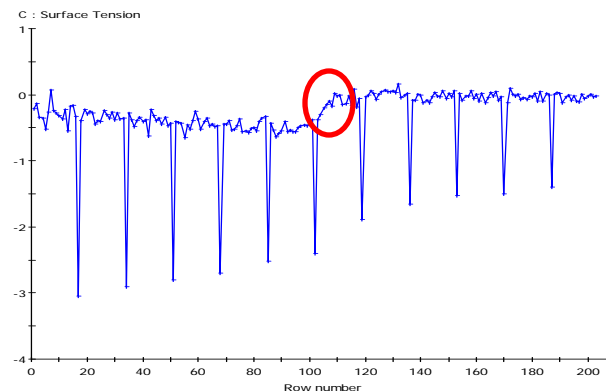
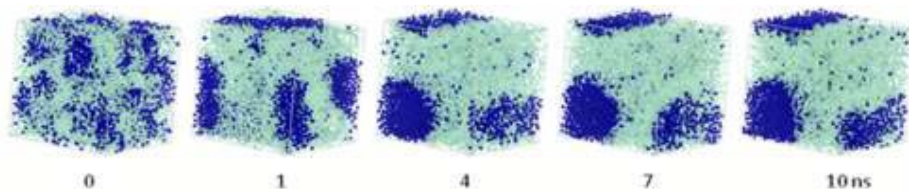


Table 1. Segment name and definition.

Name	All-atom
W	(H ₂ O) ₃
CT	CH ₃ CH ₂ CH ₂ -
CM	-CH ₂ CH ₂ CH ₂ -
CT2	CH ₃ CH ₂ -
EOT	CH ₃ -O-CH ₂ -
EO	-CH ₂ -O-CH ₂ -
OA	HOCH ₂ -



W. Shinoda, R. Devane, M.L. Klein, Multi-property fitting and parameterization of a coarse grained model for aqueous surfactants, *Mol. Sim.*, **33**:27-36, 2007

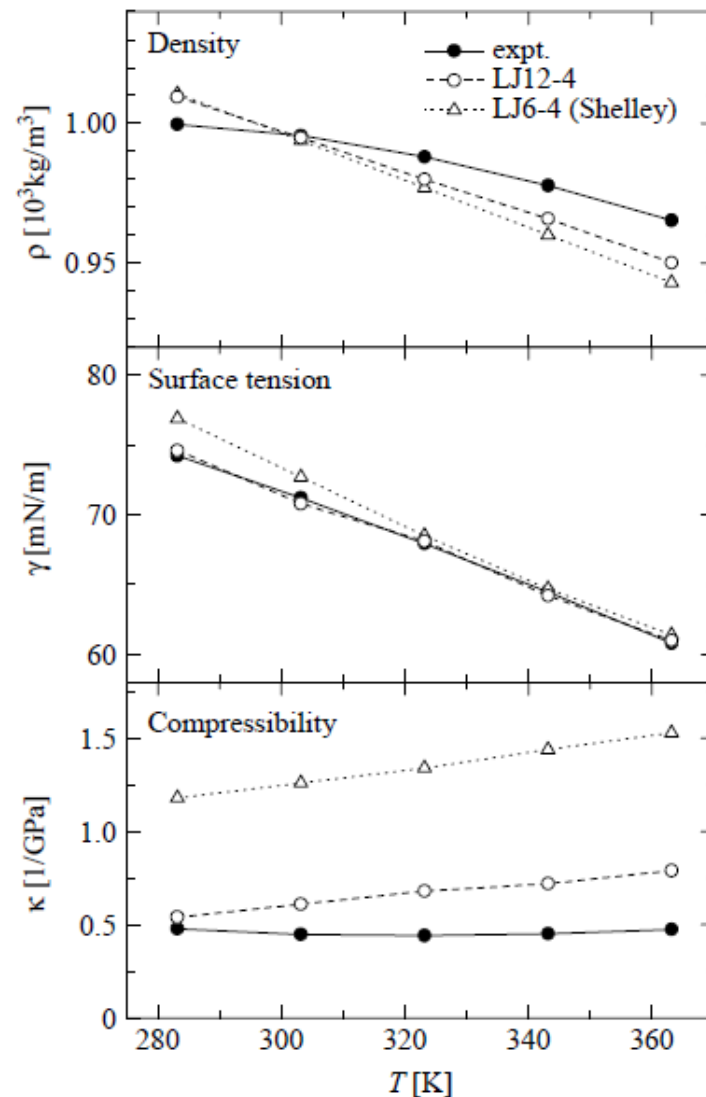


Figure 4. Temperature dependence of thermodynamic properties of CG models. Experimental data are taken from Ref. [33].

Much improved flexibility

- Create amorphous cells at experimental densities
- Build a range of different amorphous cells
- New “Packing” task enables wide range of functionality
- Physical units and a parallel DPD

Improved automation and integration

- Exposed through MaterialsScript for automation
- Perform new simulations such as straining mesoscale systems

New Amorphous Cell and DPD in Mesocite extend your capability to solve your polymer challenges

Join us for future webinars in the Materials Studio 5.0 series:

- Dec 2: Materials Studio 5.0: Spectroscopy methods in CASTEP
- Jan 13: Exploring New Fuel Cell Materials: High Throughput Calculations and Data Analysis with Materials Studio 5.0 and Pipeline Pilot

To learn more and register visit:

<http://accelrys.com/events/webinars/materials-studio-50/>

Visit us at upcoming events:

- Dec 1-3: MRS (Materials Research Society), Boston, MA
- May 4-6: Accelrys User Group Meeting, Boston, MA

To see all events we'll be attending visit: <http://accelrys.com/events>