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8 - Building complex molecular systems

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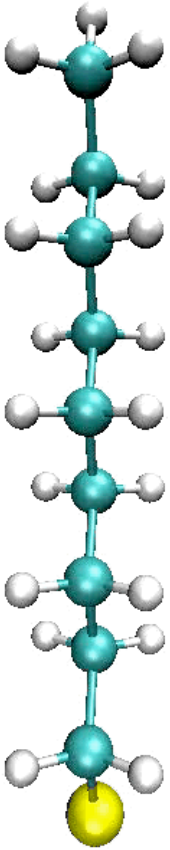
Overview

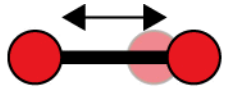
1. **Aspects of an atomistic data file**
2. **General approaches to building complex systems**
3. **System building tools**
4. **Example systems and builders**
   - Water solvent
   - Decane solvent
   - Self-assembled monolayer
   - Water in nano-confinement
   - Coated nanoparticle
   - Nanoparticle in solution

Aspects of many Molecular Models



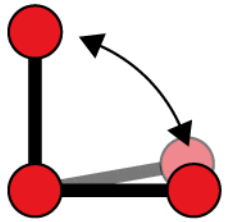
LAMMPS classical MD (multiple ensemble)

- SPC/E, TIP3P, TIP4P, etc. water models
- OPLS, CHARMM, Smith potentials



Harmonic bonded interactions

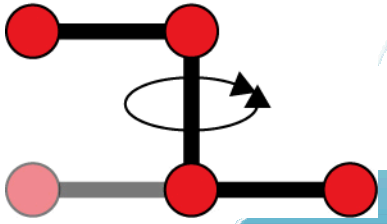
- Bond
- Angle
- Dihedral



Long-range coulomb interaction

Non-bonded Lennard-Jones interaction

Each interaction must be enumerated in a LAMMPS data file



carbon

Silicon or sulfur

hydrogen

oxygen

Components of LAMMPS data files

LAMMPS data files have several required and optional sections which can be complex for complex systems. Some information can be included either in the input script or the data file.

- Required: # of atoms, bonds, angles, dihedrals, etc.
- Required: # of types of atoms, bonds, angles, dihedrals, etc.
- Required: System dimensions
- Optional: Mass and coefficients for each type
- Required: Position for each atom
- Required: Connectivity for bond, angle, dihedral, etc.
- Optional: Velocity for each atom

General approach to building complex systems

Complex systems are often constructed from simpler systems either within the LAMMPS framework or with external tools.

1. Build a component molecule (Outside LAMMPS)
2. Equilibrate (LAMMPS)
3. Modify the system (LAMMPS or outside)

   Cut, resize, replicate, deform, enlarge, equilibrate, indent, etc.
4. Merge system components (Outside)
5. Build a hierarchy of complexity

System building tools

Pizza.py

molTemplate

Input data converters

Custom scripting languages like perl and python

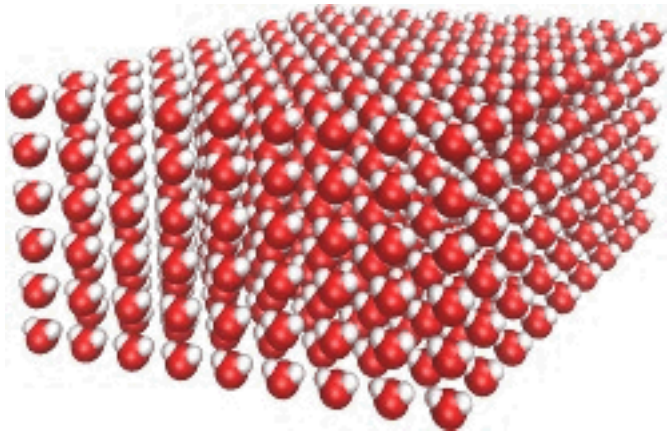
- Toolbox approach to facilitate builder scripts
- Simple tools
  - » read_data, read_dump
  - » output_data, output_xyz
  - » Rebuild (remove deleted atoms/bonds/etc. and compress)
  - » simple_merge (append and shift ids)

Example systems and builders

Builders and example data files for published research:

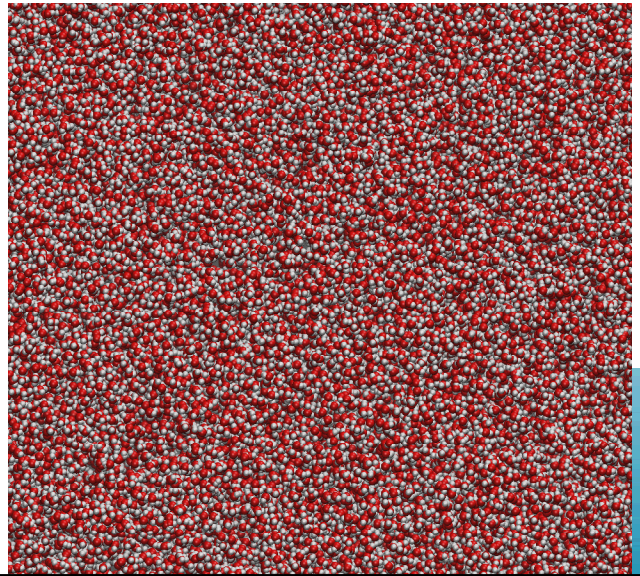
- Water solvent
- Decane solvent
- Self-assembled monolayer
- Water in nano-confinement
- Coated nanoparticle
- Nanoparticle in solution

Water slab example



Create grid of Oxygen positions
Add hydrogen atoms displaced to produce appropriate angles
Add bonds between O and H (2 per molecule)
Add angle between H O H (1 per molecule)

Create simple water box
Use LAMMPS to:
- Replicate to enlarge system
- Equilibrate at temperature and pressure



Water slab external code

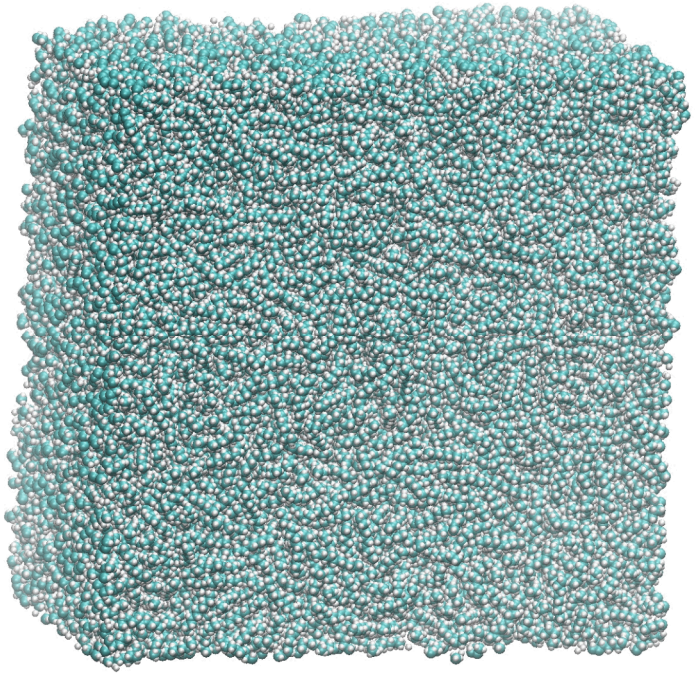
See accompanying files
Water.data
Water.in
Water.pl

Decane solvent example

Add first carbon position
Add three hydrogen atoms displaced to produce appropriate angles
Add three bonds between C and H
Add three angles between H-C-H

Add second carbon position of backbone
Add C-C bond
Add two hydrogen atoms as above
Add bonds 2 more C H bonds
Add all the C-C-H angles
Add the H-C-H bond

Add third carbon position of backbone
Add C-C bond
Add C-C-C angle
Add H-C-C-C Dihedrals



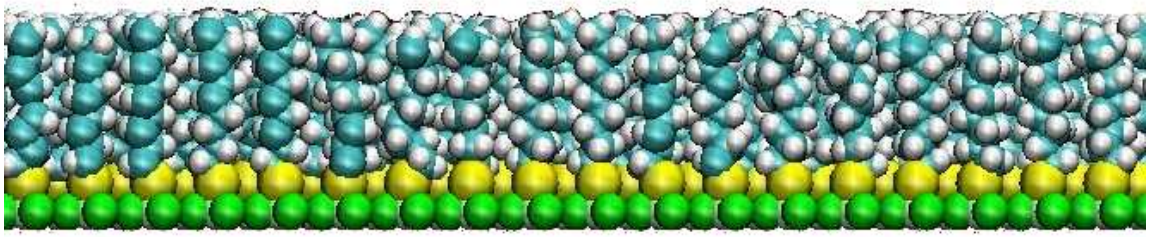
Create simple decane box
Use LAMMPS to:
- Replicate to enlarge system
- Equilibrate at elevated temperature and pressure

Decane slab external code

See accompanying files
Decane.data
Decane.in
Decane.pl

Self-assembled monolayer example

Use a process very similar to decane to produce chains but terminate one end with sulfur.



Replication won't work in this case to produce a regularly ordered array of chains, so each chain is built and individually placed with the builder.

In this case, the surfur atoms are held, either with a muffin tin potential or by rigidly holding the atoms in place. The chains can then be equilibrated using LAMMPS.

Self-assembled monolayer external code

See accompanying files
Thiol_slab.data
Thiol_slab.in
Thiol_slab.pl

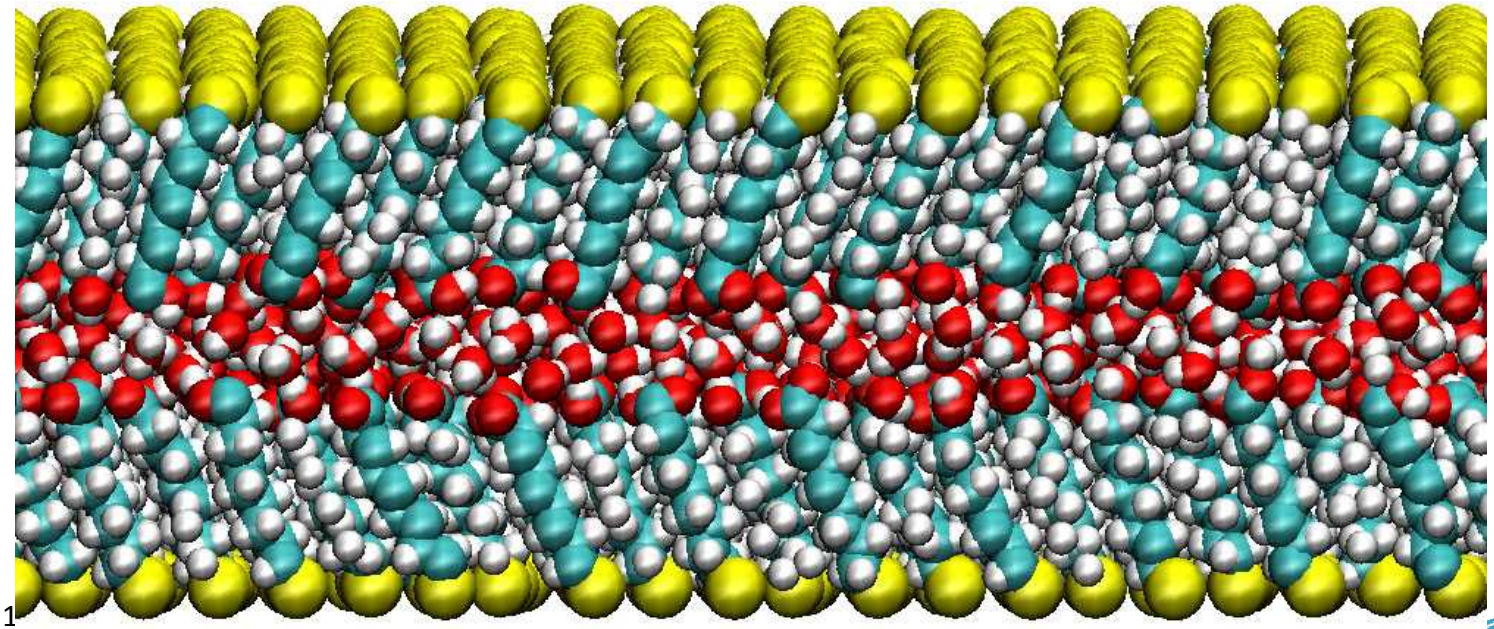
Nano-confined water between SAM layers

System characteristics

- Two opposing SAMs
- Periodic in plane
- Extremely large systems for statistics of thin layer

Alkanethiol SAMs details

- $r30\sqrt{3}$ on Au (111) substrate
- 250 Å x 260 Å grid 4.6 chains/nm^2
- 6000 S-$(CH_2)_8$-x chains
- x = COOH / CH_3 head groups
- Approximate tilt agreement w/ exp.



Confinement procedure

1. Start with raw materials: bulk water and single SAM layer

2. Duplicate and rotate SAM, crop water and merge

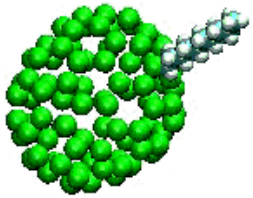
3. Use LAMMPS to compress water to chosen uniaxial pressure

Self-assembled monolayer external code

See accompanying files
Thiol_sandwich.data
Thiol_sandwich.in
Thiol_sandwich.pl

Constructing simple model nanoparticles

1. Use simple fullerene structure for bonding sites
2. Functionalize with ground-state chains oriented radially from particle center



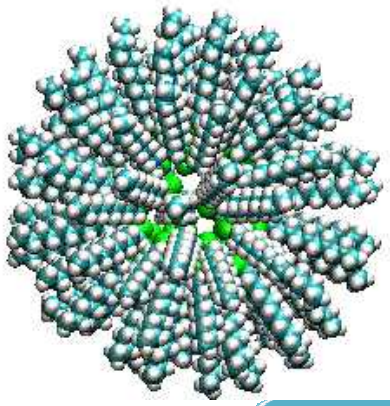
Fact sheet:

S-$(CH2)_8$-CH_3 chains

2.4 nm diameter core – approx 225 Au implicit

86 chains bonding sites from fullerene structure

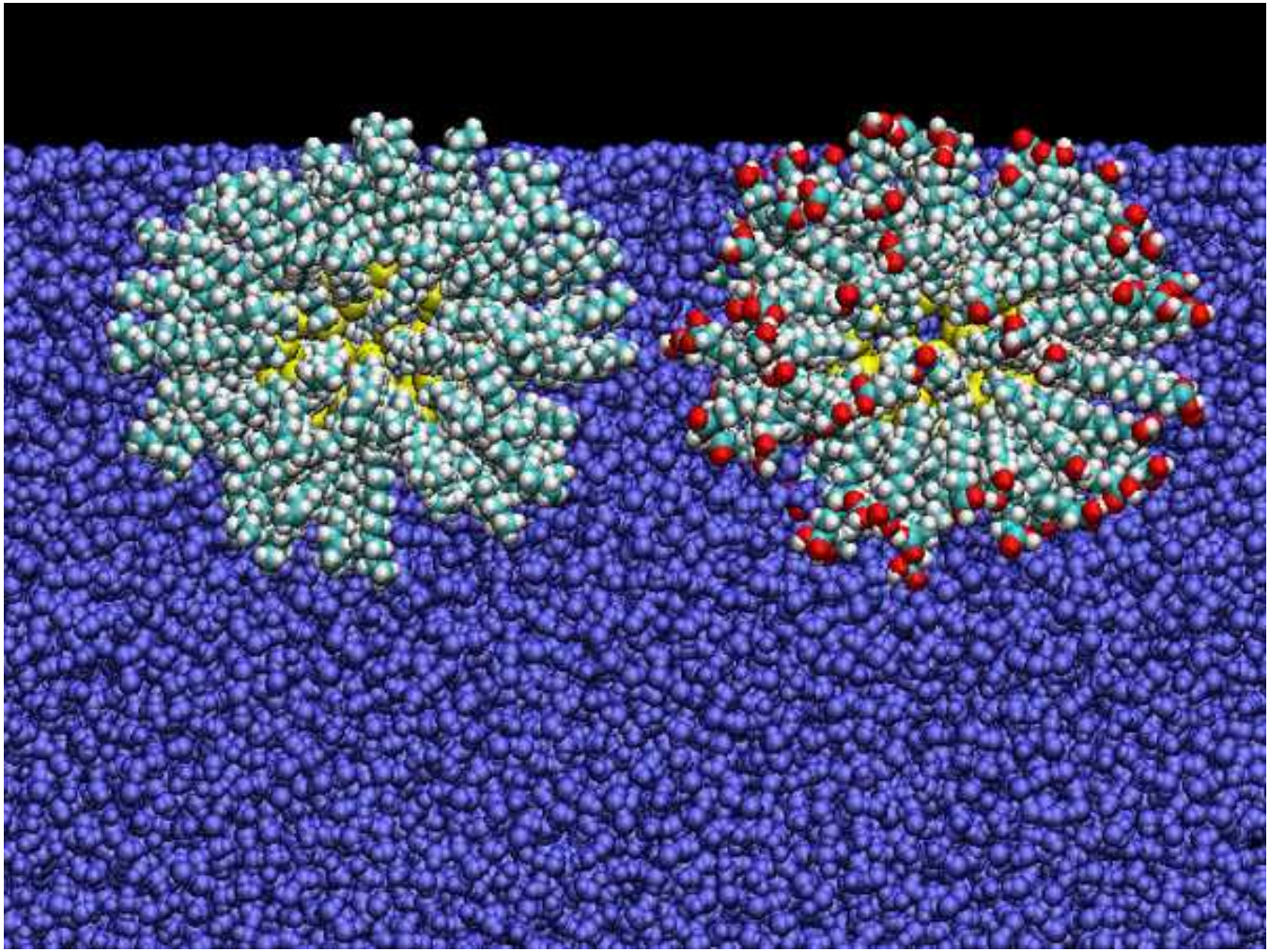
Coverage density of 21 $Å^2$ per chain



Coated nanoparticle external code

See accompanying files
NP5.data
NP5.in
NP5.pl

Building systems of particles and solvents



Solvent
- water
- decane

Interfaces/bulk

Functional group
- Termination
  - COOH or CH3
- Chain length
- Family
  - Alkanethiols
  - protein groups

Particle size/shape

Nanoparticle in solution external code

See accompanying files
NP5_water.data
NP5.in
Merge_NP5_water.pl