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Computational Rheology via LAMMPS, Octo

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5: Atomistic Applications with LAMMPS

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National Nuclear Security Administration

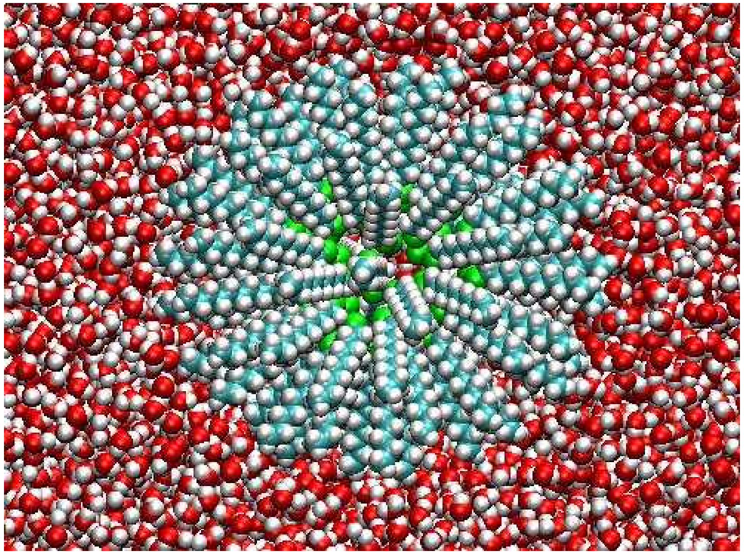
Example research studies using LAMMPS

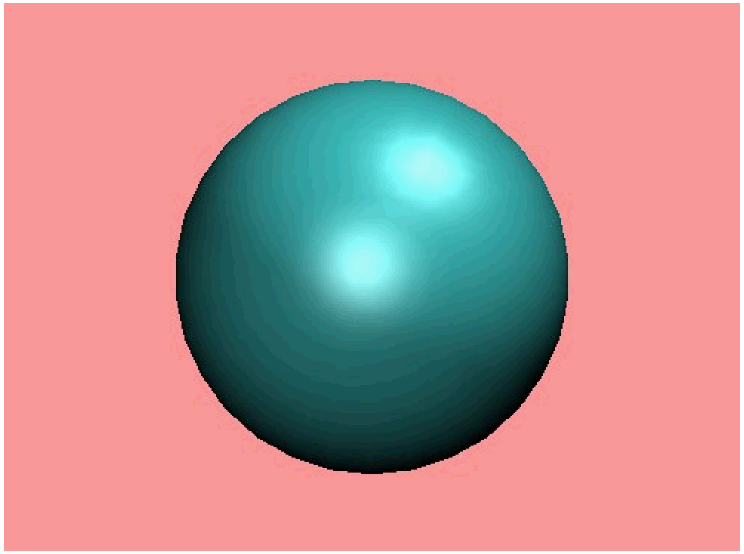
Sorts of problems which can be addressed using atomistic systems in LAMMPS

- Water interaction w/ self-assembled monolayers
- Ionomer morphologies
- Nanoparticle coating structures
- Self-assembly of lipid surfaces
- Soft material rheology
- Wetting and surface properties of complex fluids

Go to lammps.sandia.gov for many more examples.

Motivation: atomistic nanoparticles





Advantages:

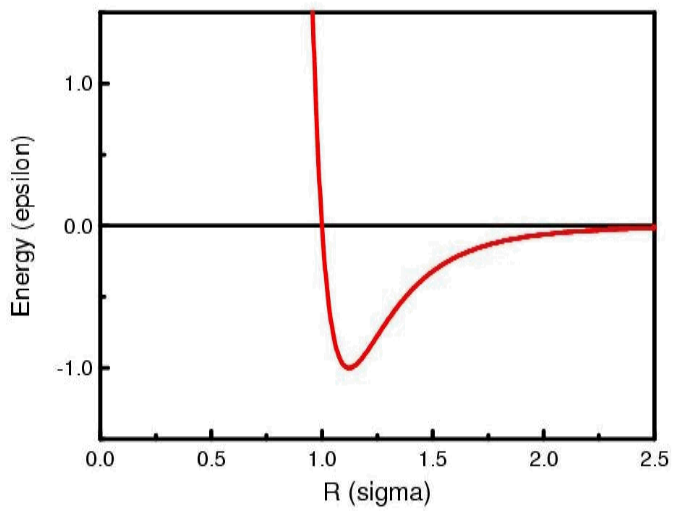
- Well-defined building blocks
- Well-defined interatomic potentials
  - Capture mesoscale effective forces as emergent phenomena

Disadvantages:

- Computationally intensive (limits simulation size & duration)
- Difficult to construct

Classical MD Basics (review)

- Each of N particles is a point mass
  - atom
  - group of atoms (united atom)
  - macro- or meso- particle
- Particles interact via empirical force laws
  - all physics in energy potential → force
  - pair-wise forces (LJ, Coulombic)
  - many-body forces (EAM, Tersoff, REBO)
  - molecular forces (springs, torsions)
  - long-range forces (Ewald)
- Integrate Newton's equations of motion
  - F = ma
  - set of N, coupled ODEs
  - advance as far in time as possible
- Properties via time-averaging ensemble snapshots (vs MC sampling)



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Timescale in Classical MD (review)

- **Timescale of simulation is most serious bottleneck in MD**

- **Timestep size limited by atomic oscillations:**
  - C-H bond = 10 fmsec → ½ to 1 fmsec timestep
  - Debye frequency = 10^{13} → 2 fmsec timestep

- **Reality is often on a much longer timescale:**
  - protein folding (msec to seconds)
  - polymer entanglement (msec and up)
  - glass relaxation (seconds to decades)
  - nanoparticle rheology (milliseconds to seconds)

- **Even smaller timestep in tight-binding or quantum-MD**

Overview

1. **Atom styles**
2. **Potentials**
3. **Ensembles, thermostats and barostats**
4. **Modeling solvents explicitly**
5. **Useful fixes**
6. **Useful computes**
7. **Rheology examples**
    1. Water viscosity
    2. Diffusion in nano-confinement
    3. Nanoparticle interaction forces
    4. High-rate (shock) compression on hydrocarbon polymers

Atom styles

Molecular

Charge

Full

Atom styles are often determined by the potential being used.

Potentials or Force Fields

A significant advantage to LAMMPS is the availability of many standard interatomic interaction potentials

- LAMMPS features
  - Hybrid potentials
  - Standard library potentials (e.g. KIM)
  - Advanced potentials (e.g. COMB, eFF, GAP/SNAP)
  - Comparison between potentials is easy!
- Molecular constraints
  - bonds, angles and dihedral interactions
  - – create and break on the fly
  - SHAKE algorithm for specific bonds and angles
  - Rigid structures

LAMMPS potentials

none	hybrid	hybrid/overlay	adp
airebo	born	born/coul/long	buck
buck/coul/cut	buck/coul/long	colloid	comb
coul/cut	coul/debye	coul/long	dipole/cut
dpd	dpd/tstat	dsmc	eam
eam/alloy	eam/fs	eim	gauss
gayberne	gran/hertz/history	gran/hooke	gran/hooke/history
hbond/dreiding/lj	hbond/dreiding/morse	lj/charmm/coul/charmm	lj/charmm/coul/charmm/implicit
lj/charmm/coul/long	lj/class2	lj/class2/coul/cut	lj/class2/coul/long
lj/cut	lj/cut/coul/cut	lj/cut/coul/debye	lj/cut/coul/long
lj/cut/coul/long/tip4p	lj/expand	lj/gromacs	lj/gromacs/coul/gromacs
lj/smooth	lj96/cut	lubricate	meam
morse	peri/lps	peri/pmb	reax
rebo	resquared	soft	sw
table	tersoff	tersoff/zbl	yukawa
yukawa/colloid			

LAMMPS potentials

Lennard-Jones type interactions

none	hybrid	hybrid/overlay	adp
airebo	born	born/coul/long	buck
buck/coul/cut	buck/coul/long	colloid	comb
coul/cut	coul/debye	coul/long	dipole/cut
dpd	dpd/tstat	dsmc	eam
eam/alloy	eam/fs	eim	gauss
gayberne	gran/hertz/history	gran/hooke	gran/hooke/history
hbond/dreiding/lj	hbond/dreiding/morse	lj/charmm/coul/charmm	lj/charmm/coul/charmm/implicit
lj/charmm/coul/long	lj/class2	lj/class2/coul/cut	lj/class2/coul/long
lj/cut	lj/cut/coul/cut	lj/cut/coul/debye	lj/cut/coul/long
lj/cut/coul/long/tip4p	lj/expand	lj/gromacs	lj/gromacs/coul/gromacs
lj/smooth	lj96/cut	lubricate	meam
morse	peri/lps	peri/pmb	reax
rebo	resquared	soft	sw
table	tersoff	tersoff/zbl	yukawa
yukawa/colloid			

LAMMPS potentials

Atomic interactions

none	hybrid	hybrid/overlay	adp
airebo	born	born/coul/long	buck
buck/coul/cut	buck/coul/long	colloid	comb
coul/cut	coul/debye	coul/long	dipole/cut
dpd	dpd/tstat	dsmc	eam
eam/alloy	eam/fs	eim	gauss
gayberne	gran/hertz/history	gran/hooke	gran/hooke/history
hbond/dreiding/lj	hbond/dreiding/morse	lj/charmm/coul/charmm	lj/charmm/coul/charmm/implicit
lj/charmm/coul/long	lj/class2	lj/class2/coul/cut	lj/class2/coul/long
lj/cut	lj/cut/coul/cut	lj/cut/coul/debye	lj/cut/coul/long
lj/cut/coul/long/tip4p	lj/expand	lj/gromacs	lj/gromacs/coul/gromacs
lj/smooth	lj96/cut	lubricate	meam
morse	peri/lps	peri/pmb	reax
rebo	resquared	soft	sw
table	tersoff	tersoff/zbl	yukawa
yukawa/colloid			

LAMMPS potentials

Coarse-grain interactions

none	hybrid	hybrid/overlay	adp
airebo	born	born/coul/long	buck
buck/coul/cut	buck/coul/long	colloid	comb
coul/cut	coul/debye	coul/long	dipole/cut
dpd	dpd/tstat	dsmc	eam
eam/alloy	eam/fs	eim	gauss
gayberne	gran/hertz/history	gran/hooke	gran/hooke/history
hbond/dreiding/lj	hbond/dreiding/morse	lj/charmm/coul/charmm	lj/charmm/coul/charmm/implicit
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lj/cut	lj/cut/coul/cut	lj/cut/coul/debye	lj/cut/coul/long
lj/cut/coul/long/tip4p	lj/expand	lj/gromacs	lj/gromacs/coul/gromacs
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morse	peri/lps	peri/pmb	reax
rebo	resquared	soft	sw
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LAMMPS potentials

Toy interactions

none	hybrid	hybrid/overlay	adp
airebo	born	born/coul/long	buck
buck/coul/cut	buck/coul/long	colloid	comb
coul/cut	coul/debye	coul/long	dipole/cut
dpd	dpd/tstat	dsmc	eam
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morse	peri/lps	peri/pmb	reax
rebo	resquared	soft	sw
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LAMMPS potentials

Meta interactions

none	hybrid	hybrid/overlay	adp
airebo	born	born/coul/long	buck
buck/coul/cut	buck/coul/long	colloid	comb
coul/cut	coul/debye	coul/long	dipole/cut
dpd	dpd/tstat	dsmc	eam
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lj/cut	lj/cut/coul/cut	lj/cut/coul/debye	lj/cut/coul/long
lj/cut/coul/long/tip4p	lj/expand	lj/gromacs	lj/gromacs/coul/gromacs
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lj/charmm/coul/long	lj/class2	lj/class2/coul/cut	lj/class2/coul/long
lj/cut	lj/cut/coul/cut	lj/cut/coul/debye	lj/cut/coul/long
lj/cut/coul/long/tip4p	lj/expand	lj/gromacs	lj/gromacs/coul/gromacs
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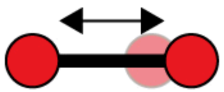
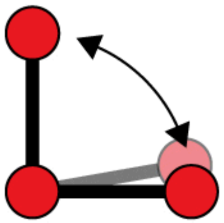
Selected LAMMPS soft matter potentials

Bonded type interactions

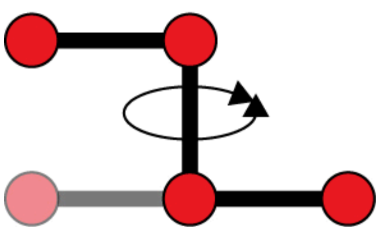


LAMMPS allows for more complex interactions
- SPC/E and TIP3P water models
- OPLS force field for SAMs
- CHARMM, AMBER, COMPASS (class 2), etc.



Non-bonded Lennard-Jones interaction

Harmonic bonded interactions
- Bond
- Angle
- Dihedral



Long-range coulomb interaction with Ewald and PPPM

Ensembles, thermostats and barostats

Definition of atomic temperature

- **size and neighborhood dependent from velocity distr.**

Major thermostats

- **Langevin (damping and kicking)**
- **Nose-Hoover (velocity scaling)**

Freedom to redefine to specific dimensions or regions

- **Example of thermostat in shear**
- **Example of temperature bath**

Ensembles, thermostats and barostats

Definition of atomic pressure

Major barostats

Pressure/stress measurements

virial and per-atom

Again, freedom to redefine to specific dimensions or regions

Modeling solvents explicitly

Explicit modeling of solvents raises significant issues with computational expense, system size and equilibration times. Consider the following before attempting a large-scale explicit solvent simulation:

- System building
- System equilibration
- System size effects
- Implicit modeling

Useful fixes

Boundaries

boundary **vs** fix_walls

Constraints

fix_shake, fix_rigid, fix_freeze

Deformations

fix_deform

Adding/removing atoms and/or bonds

Useful computes for rheology

Mean-square-displacement

Radial distribution function (i.e. g(r))

Atoms-to-Continuum User package

Per-atom stress tensor stress/atom

Center-of-mass and Radius of gyration

Rheology examples with input scripts

1. **Viscosity of water**

2. **Diffusion in nano-constrained fluid layer**

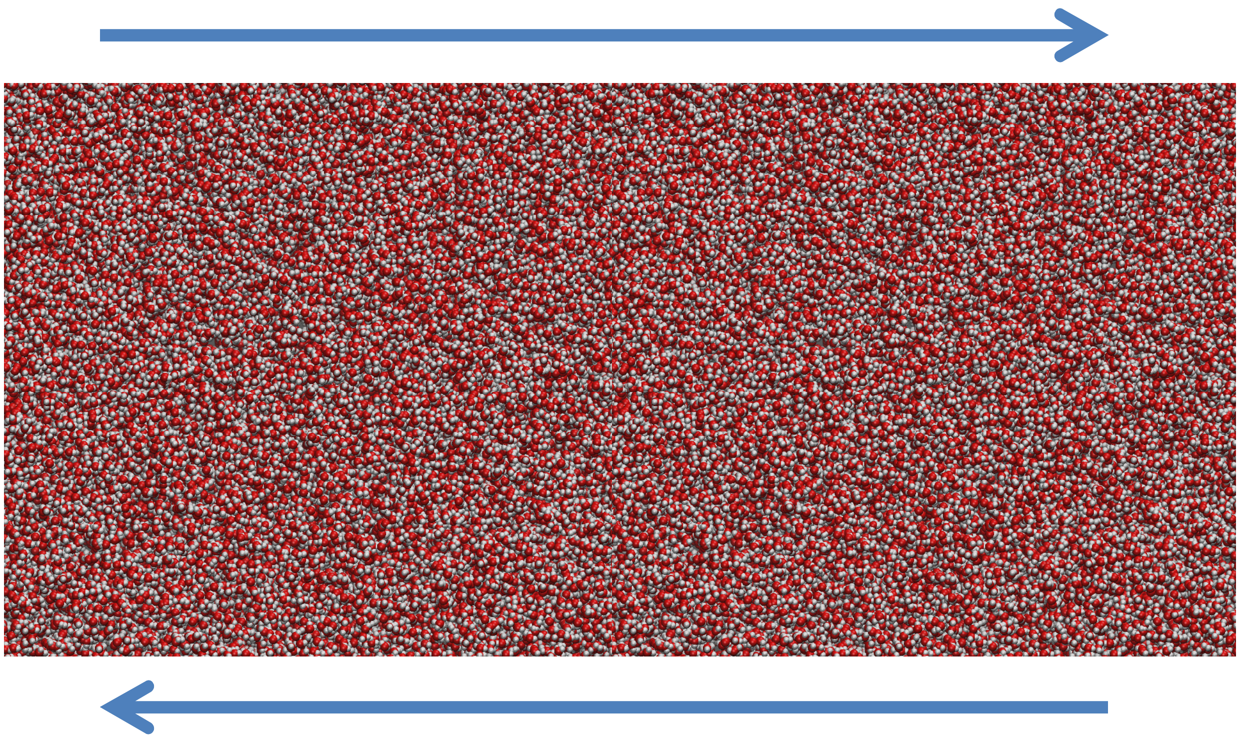
3. **Nanoparticle drag and interaction forces**

4. **High-rate compression response**

Sample Research: Viscosity of water

Objective: Measure the shear viscosity of liquid water at various temperatures and pressures

Procedure: Apply the NEMD (Mueller-Plathe) method for momentum transfer



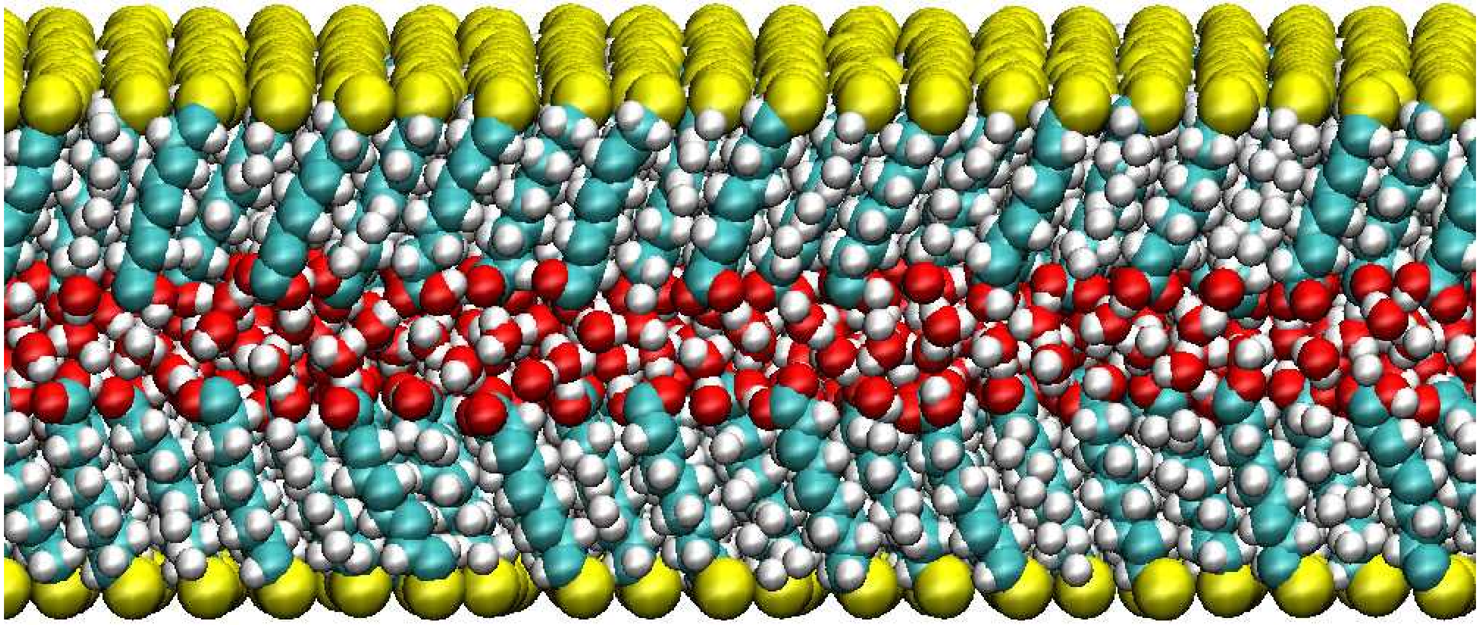
Sample Research: Viscosity of water

See accompanying files
water_viscosity.data
water_viscosity.in

Sample Research: Diffusion in nano-constrained fluid layer

Objective: Measure the diffusion coefficient in a thin layer of water confined between two hydrophobic self-assembled monolayers

Procedure: Measure 2D mean-square displacement and calculate diffusion



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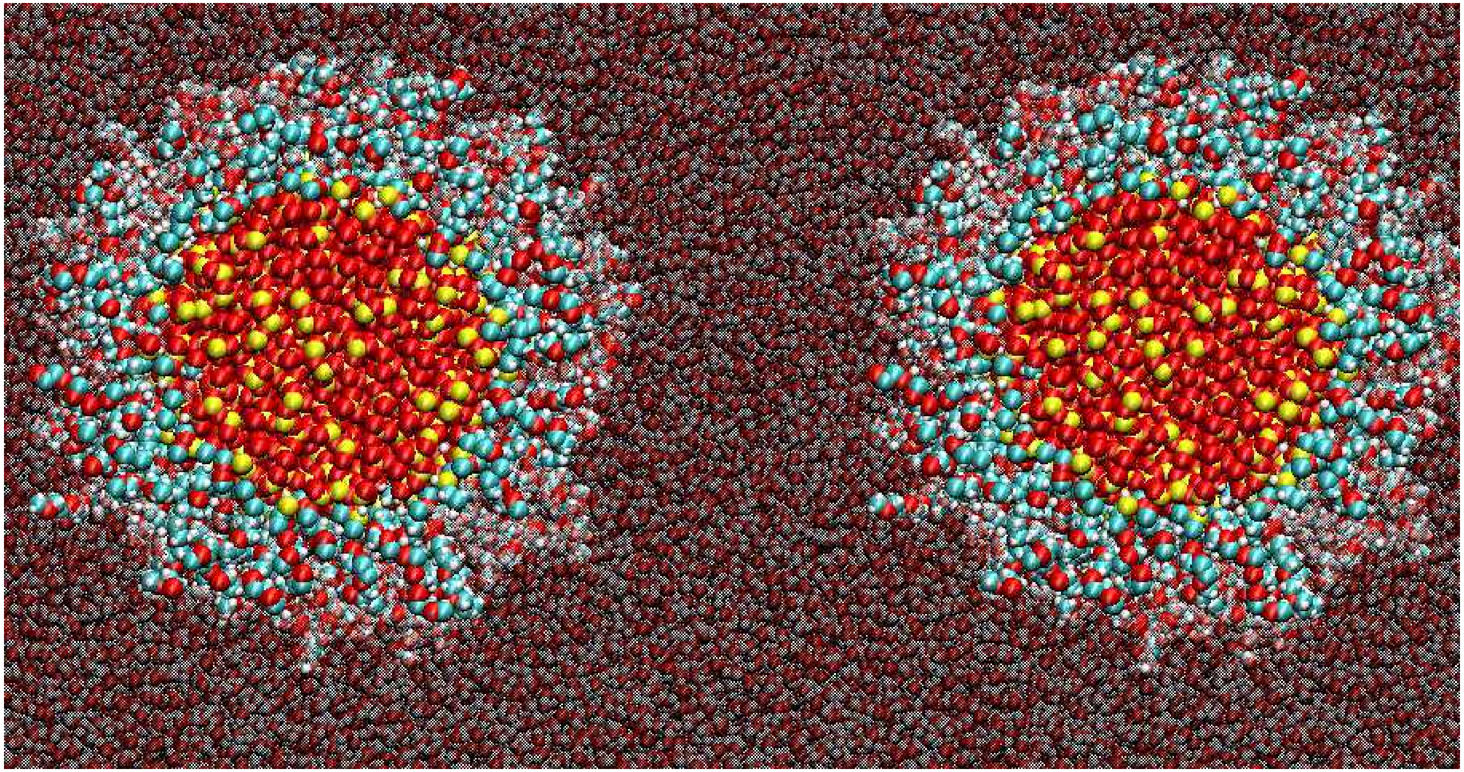
Sample Research: Diffusion in nano-constrained fluid layer

See accompanying files
water_SAM_diffusion.data
water_SAM_diffusion.in

Sample Research: Forces Between Nanoparticles

Objective: Measure the forces between two PEO coated silica nanoparticles in an explicit water solvent

Procedure: Move particles through the solvent at constant velocity and measure the aggregated force which acts back on the nanoparticle



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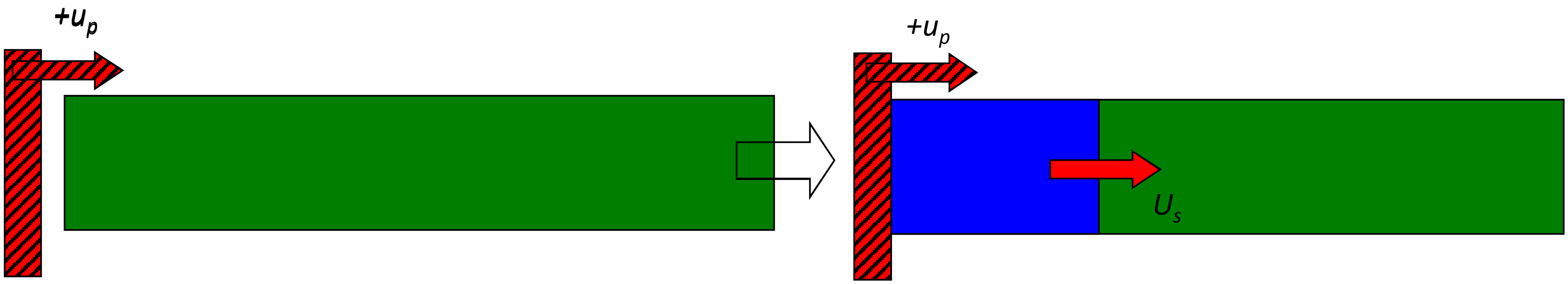
Sample Research: Forces Between Nanoparticles

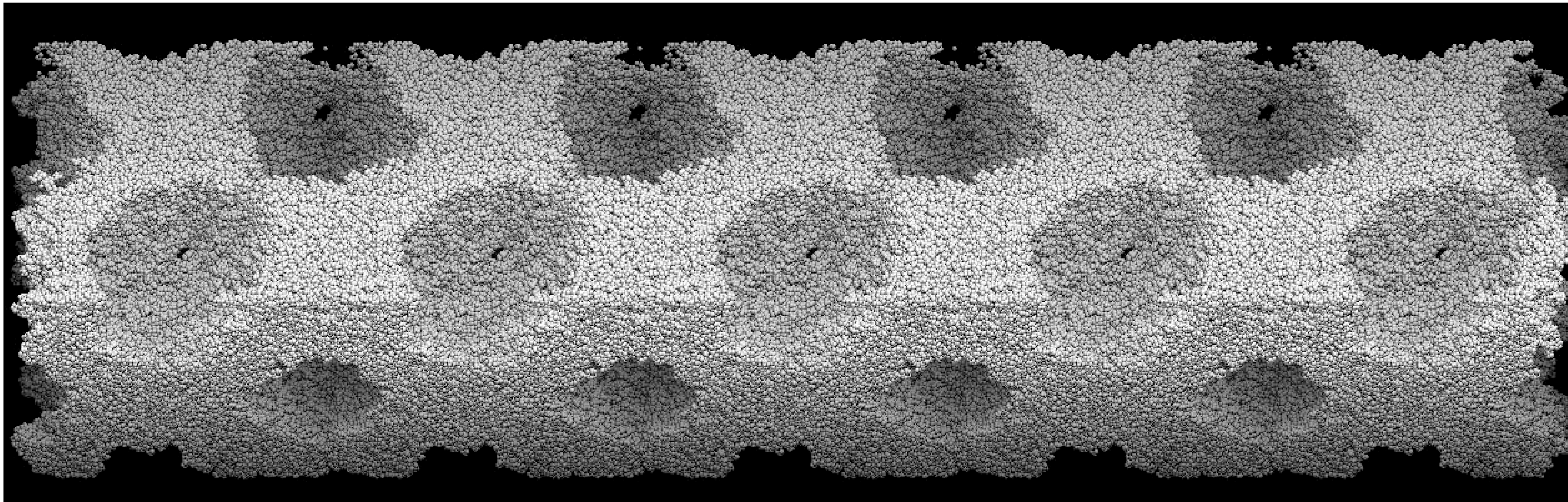
See accompanying files
nanoparticle.data
nanoparticle.in

Sample Research: Shock studies in hydrocarbon foam

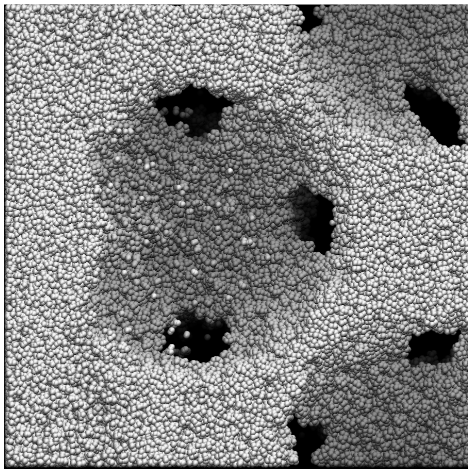
Objective: Measure shock response of polymer foam

Procedure: Apply shock driver method and measure pressure, density, temperature and hot spot formation behind the shock front





Sample Research: Shock studies in hydrocarbon foam



See accompanying files
shock.data
shock.in