SAND2011-1435C

Grand canonical Monte Carlo simulations of gas uptake in microporous materials using LAMMPS

Paul S. Crozier

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King's College Seminar

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A brief introduction to MD

- MD: molecular dynamics
- F = ma
- Classical dynamics
- Rapidly grown in popularity and use in research
- Computationally intensive, especially computation of nonbonded interactions
- Uses force fields: mathematical models of interatomic interactions

MD uses empirical force fields

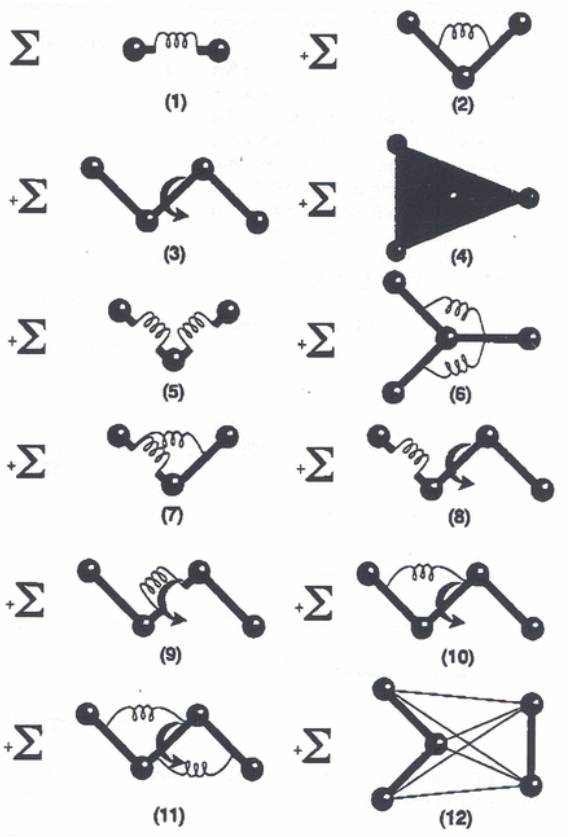
- Particles interact via empirical potentials
  - analytic equations, fast to compute
  - coefficients fit to expt or quantum calcs

$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad r < r_c$$

$$E = K(r - r_0)^2$$

- Potential energy = Φ = f(x)
- Force = -Grad Φ

- Pair-wise forces
  - Van der Waals (dipole-dipole)
  - Coulombic (charge-charge)
- Many-body forces
  - EAM, Tersoff, bond-order, ReaxFF
- Molecular forces
  - springs, torsions, dihedrals, ...
- Long-range Coulombic forces
  - Ewald, particle-mesh methods, FFTs



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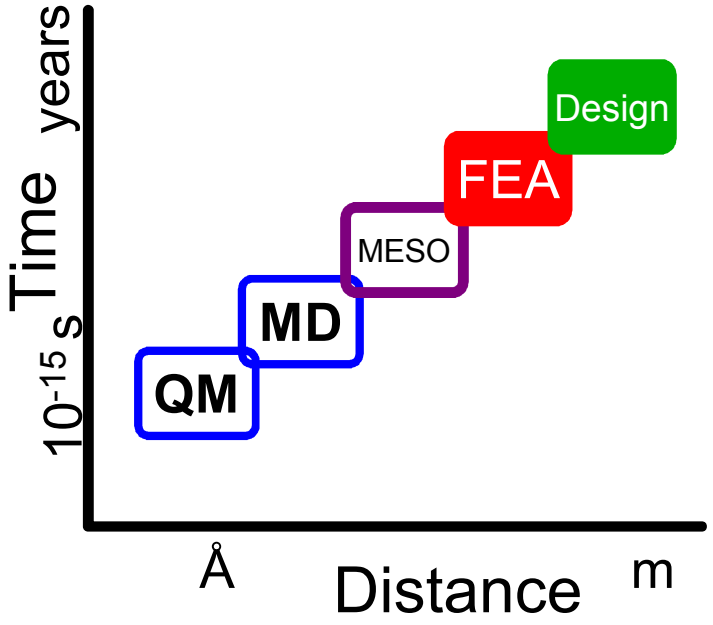
MD in the Middle

- **Quantum mechanics**
  - **electronic degrees of freedom, chemical reactions**
  - **Schrodinger equation, wave functions**
  - **sub-femtosecond timestep, 1000s of atoms, O(N^3)**
- **Atomistic models**
  - **molecular dynamics (MD), Monte Carlo (MC)**
  - **point particles, empirical forces, Newton's equations**
  - **femtosecond timestep, millions of atoms, O(N)**
- **Mesoscale to Continuum**
  - **finite elements or finite difference on grids**
  - **coarse-grain particles: DPD, PeriDynamics, ...**
  - **PDEs, Navier-Stokes, stress-strain**
  - **microseconds → seconds, microns → meters, O($N^{3/2}$)**



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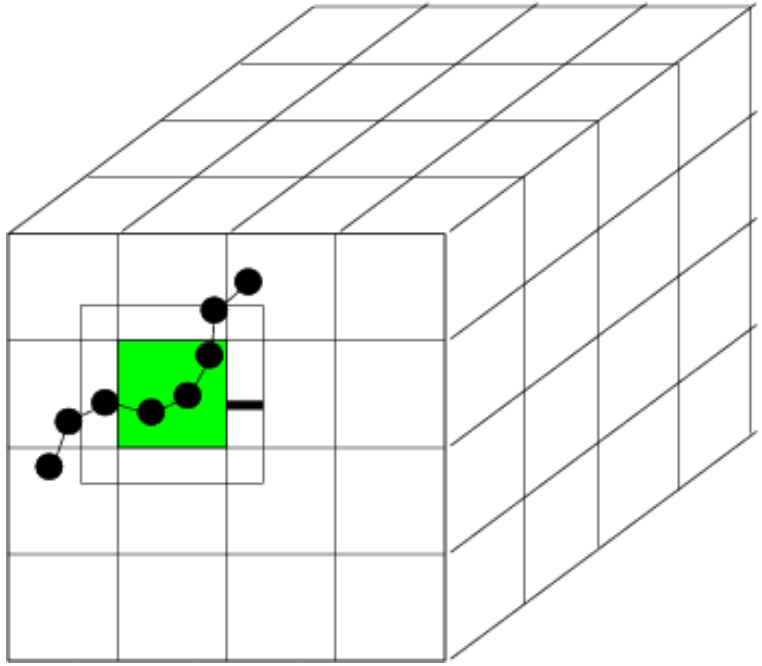
Parallelism via Spatial-Decomposition

- Physical domain divided into 3d boxes, one per processor
- Each proc computes forces on atoms in its box
  using info from nearby procs
- Atoms "carry along" molecular topology
  as they migrate to new procs
- Communication via
  nearest-neighbor 6-way stencil



- Optimal scaling for MD: N/P
  so long as load-balanced

- Computation scales as N/P
- Communication scales
  sub-linear as $(N/P)^{2/3}$
  (for large problems)
- Memory scales as N/P

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A brief introduction to LAMMPS

LAMMPS: Large-scale Atomic/Molecular Massively Parallel Simulator

- Massively parallel, general purpose MD code.
- Developed at Sandia National Laboratories, with contributions from many labs throughout the world.
- Roughly 140,000 lines of code.
- 14 major releases since September 2004
- Continual (many times per week) releases of patches (bug fixes and patches)
- Freely available for download under GPL

  lammps.sandia.gov

  Tens of thousands of downloads since September 2004

  Open source, easy to understand C++ code

  Easily extensible

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How to download, install, and use LAMMPS

- **Download page:**
  lammps.sandia.gov/download.html

- **Installation instructions:**
  lammps.sandia.gov/doc/Section_start.html
  go to lammps/src
  type "make *your_system_type*"

- **To perform a simulation:**
  lmp < *my_script.in*

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How to get help with LAMMPS

1. **Excellent User's Manual:**
   lammps.sandia.gov/doc/Manual.html

2. **User's e-mail list:**
   lammps.sandia.gov/mail.html

3. **Contact the developers:**
   Steve Plimpton, sjplimp@sandia.gov
   Aidan Thompson, athomps@sandia.gov
   Paul Crozier, pscrozi@sandia.gov
   Mike Brown, wmbrown@sandia.gov

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Force fields available in LAMMPS

- **Biomolecules:** CHARMM, AMBER, OPLS, COMPASS (class 2), long-range Coulombics via PPPM, point dipoles, ...
- **Polymers:** all-atom, united-atom, coarse-grain (bead-spring FENE), bond-breaking, …
- **Materials:** EAM and MEAM for metals, Buckingham, Morse, Yukawa, Stillinger-Weber, Tersoff, Al-REBO, Reaxx FF, ...
- **Mesoscale:** granular, DPD, Gay-Berne, colloidal, peri-dynamics, ...
- **Hybrid:** can use combinations of potentials for hybrid systems: water on metal, polymers/semiconductor interface, colloids in solution, …

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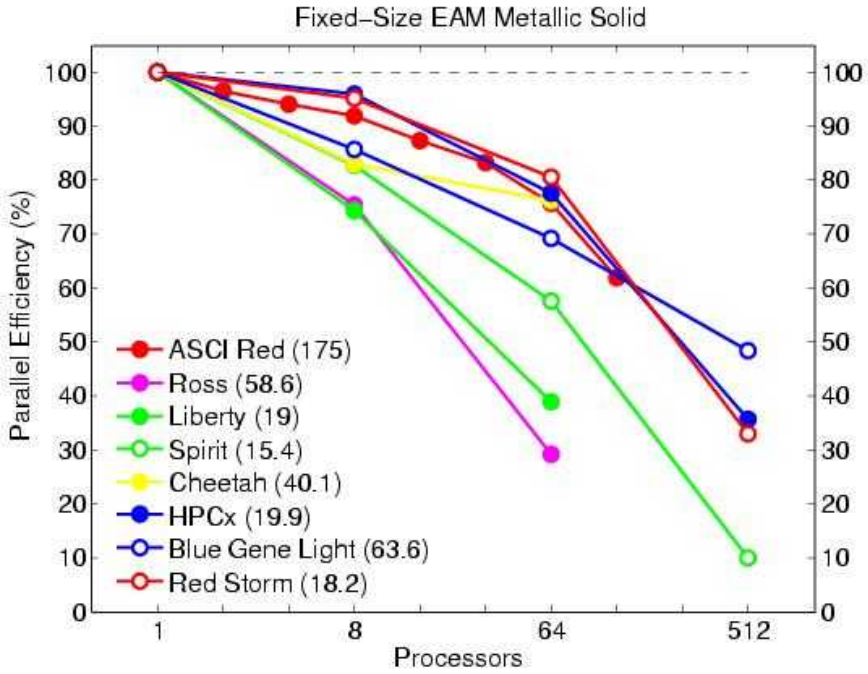
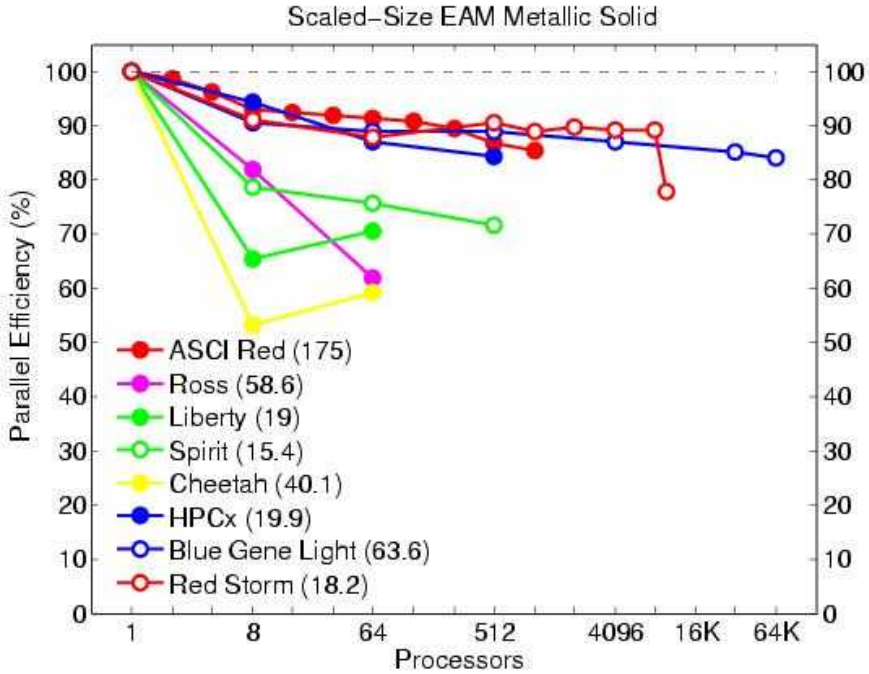
LAMMPS's parallel performance

- Fixed-size (32K atoms) and scaled-size (32K atoms/proc) parallel efficiencies
- Metallic solid with EAM potential





- Billions of atoms on 64K procs of Blue Gene or Red Storm
- Opteron processor speed: 5.7E-6 sec/atom/step (0.5x for LJ, 12x for protein)

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Easily add your own LAMMPS feature

- New user or new simulation → always want new feature not in code
- Goal: make it as easy as possible for us and others to add new features
  - called “styles” in LAMMPS:
  - particle type, pair or bond potential, scalar or per-atom computation
  - "fix": BC, force constraint, time integration, diagnostic, ...
  - input command: create_atoms, set, run, temper, ...
  - 75% of current 100K+ lines of LAMMPS is add-on styles
- Enabled by C++
  - "virtual" parent class for all pair potentials
  - defines interface: compute(), coeff(), restart(), ...
  - add feature: add 2 lines to header file, add files to src dir, re-compile
  - feature won't exist if not used, won't conflict with rest of code
- Of course, someone has to write the code for the feature!

What are microporous materials and what are their uses?

"**A microporous material is a material containing pores with diameters less than 2 nm.** Porous materials are classified into several kinds by their size."

"Microporous materials have pore diameters of less than 2 nm, mesoporous materials have pore diameters between 2 nm and 50 nm and macroporous materials have pore diameters of greater than 50 nm."

- **Facilitate contaminant-free exchange of gases.** Mold spores, bacteria, and other airborne contaminants will become trapped, while allowing gases to pass through the material.
- **Microporous materials are also used in first aid.**

http://en.wikipedia.org/wiki/Microporous_material

- **Radioactive materials separation or storage.**

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What are ZIFs?

ZIF = zeolitic imidazolate framework

"ZIFs are one kind of metal-organic frameworks' subsidiaries which could be used to keep industrial emissions of carbon dioxide out of the atmosphere. One litre of the crystals could store about 83 litres of CO2. **The crystals are non-toxic and require little energy to create**, making them an attractive possibility for carbon capture and storage. **The porous structures can be heated to high temperatures without decomposing** and can be boiled in water or solvents for a week and remain stable, making them suitable for use in hot, energy-producing environments like power plants."

"Like zeolites and other porous materials, zeolitic imidazolate framework membranes can be used for the **separation of gases** because of its highly porous structure, large accessible pore volume with fully exposed edges and faces of the organic links, pore apertures in the range of the kinetic diameter of several gas molecules, and high CO_2 adsorption capacity."

http://en.wikipedia.org/wiki/Zeolitic_imidazolate_frameworks

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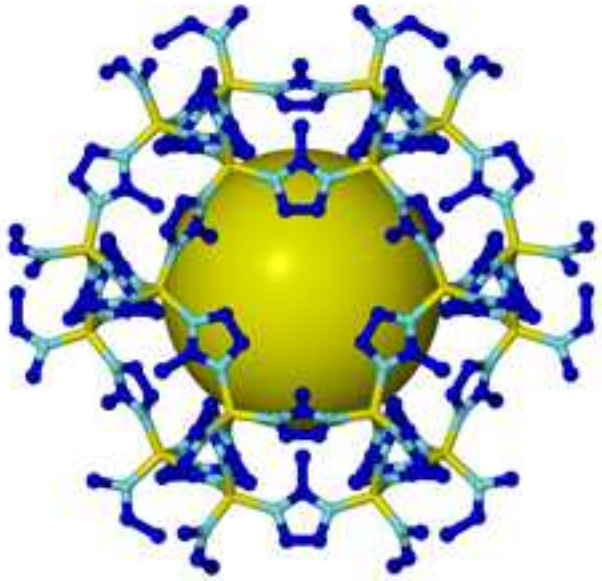
ZIF-8

Synonym:	2-Methylimidazole zinc salt, ZIF 8
CAS Number:	59061-53-9
Empirical Formula (Hill Notation):	$C_8H_{12}N_4Zn$
Molecular Weight:	229.60



Crystal structure of ZIF-8 with void space shown in yellow.

Figure credit: Praveen K. Thallapally

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What questions about iodine uptake in ZIF-8 might we hope to address with molecular simulation?

1. How much I_2 can ZIF-8 hold? (What is the loading vs pressure relationship? Can we compute a loading iostherm?)

2. How mobile is I_2 once it is adsorbed within the ZIF-8 framework?

3. What is the structure of I_2-loaded ZIF-8 and where are the main binding locations?

4. How well do simulation results compare with available experimental measurements?

What simulation tools might we use to address our questions?

Molecular dynamics (MD): is computer simulation of physical movements by atoms and molecules. http://en.wikipedia.org/wiki/Molecular_dynamics

Monte Carlo (MC): This approach relies on statistical mechanics rather than molecular dynamics. Instead of trying to reproduce the dynamics of a system, it generates states according to appropriate Boltzmann probabilities. (http://en.wikipedia.org/wiki/Monte_Carlo_molecular_modeling)

Grand canonical Monte Carlo (GCMC): a very versatile and powerful Monte Carlo technique that explicitly accounts for **density fluctuations at fixed volume and temperature**. This is achieved by means of **trial insertion and deletion of molecules**. Although this feature has made it the preferred choice for the study of interfacial phenomena, in the last decade grand-canonical ensemble simulations have also found widespread applications in the study of bulk properties. Such applications had been hitherto limited by the very low particle insertion and deletion probabilities, but the development of the configurational bias grand canonical technique has very much improved the situation. (http://www.sklogwiki.org)

Gibbs ensemble Monte Carlo (GEMC): The Gibbs ensemble Monte Carlo method has been specifically designed to **characterize phase transitions**. It was mainly developed by Panagiotopoulos (Refs. 1 and 2) to avoid the problem of finite size interfacial effects. **In this method, an NVT (or NpT) ensemble containing two (or more) species is divided into two (or more) boxes.** In addition to the usual particle moves in each one of the boxes, the algorithm includes moves steps to change the volume and composition of the boxes at mechanical and chemical equilibrium. Transferring a chain molecule from a box to the other requires the use of an efficient method to insert chains. The configurational bias method is specially recommended for this purpose. (http://www.sklogwiki.org)

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Which molecular simulation tool is best suited for each task?

How much I_2 can ZIF-8 hold?	Molecular dynamics (MD)
How mobile is I_2 once it is adsorbed within the ZIF-8 framework?	Monte Carlo (micro-canonical) (MC)
What is the structure of I_2-loaded ZIF-8 and where are the main binding locations?	Grand canonical Monte Carlo (GCMC)
	Gibbs ensemble Monte Carlo (GEMC)

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Which molecular simulation tool is best suited for each task?

How much I_2 can ZIF-8 hold?

How mobile is I_2 once it is adsorbed within the ZIF-8 framework?

What is the structure of I_2-loaded ZIF-8 and where are the main binding locations?

Molecular dynamics (MD)

Monte Carlo (micro-canonical) (MC)

Grand canonical Monte Carlo (GCMC)

Gibbs ensemble Monte Carlo (GEMC)

Why would we want to use LAMMPS to perform molecular simulation of gas uptake into a ZIF?

Can already do the following for free:

- Molecular dynamics
- Model ZIF-8 force fields we'd like to use
- I/O: we already know how to work with LAMMPS input, output, versatile scripting options, etc.
- Many useful computes, fixes, available.
- Combine features in new useful combinations.
- Runs efficiently on available HPC resources.
- Great user support.
- New features can be donated to the community.

Can't do (yet): GCMC

What would we have to add to LAMMPS to be able to do GCMC simulations?

- A new “fix” (i.e. BC, constraint, mid-step instruction).
- Let’s call it “fix GCMC.”
- Need to find a textbook GCMC algorithm to implement.
- Should include the following features:
  - Support particle creation/destruction.
  - Compute pre- and post-creation/deletion potential energies.
  - Work efficiently, and in parallel on multiple processors.
  - Written in LAMMPS coding style and include documentation so that it can be shared.
  - Be compatible with other LAMMPS features (MD, ensembles, force fields, computes, etc.)
  - Allow creation/deletion of molecules.
  - Report relevant statistics to users.

GCMC algorithm by Frenkel and Smit *

```
 SUBROUTINE mcexc                    attempt to exchange a particle
                                     with a reservoir
 if (ranf().lt.0.5) then             decide to remove or add a particle
   if (npart.eq.0) return            test whether there is a particle
   o=int(npart*ranf())+1             select a particle to be removed
   call ener(x(o),eno)               energy particle o
   arg=npart*exp(beta*eno)           acceptance rule (5.6.9)
+       /(zz*vol)
   if (ranf().lt.arg) then
     x(o)=x(npart)                   accepted: remove particle o
     npart=npart-1
   endif
 else
   xn=ranf()*box                     new particle at a random position
   call ener(xn,enn)                 energy new particle
   arg=zz*vol*exp(-beta*enn)         acceptance rule (5.6.8)
+       /(npart+1)
   if (ranf().lt.arg) then
     x(npart+1)=xn                   accepted: add new particle
     npart=npart+1
   endif
 endif
 return
 end
```

* Frenkel and Smit, "*Understanding Molecular Simulation*," Academic Press, London, 2002.

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Excerpts from LAMMPS's new fix GCMC

(GCMC algorithm: select move, deletion, or insertion)

```
// perform ncycles MC cycles

for (int i = 0; i < ncycles; i++) {
  int random_int_fraction = static_cast<int>(random->uniform()*ncycles) + 1;
  if (random_int_fraction <= nmcmoves) {
    attempt_move();
  } else {
    if (random->uniform() < 0.5) {
      attempt_deletion();
    } else {
      attempt_insertion();
    }
  }
}
```

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Excerpts from LAMMPS's new fix GCMC

(move algorithm)

```
int success = 0;
iwhichglobal = static_cast<int> (ngas*random->uniform());
if ((iwhichglobal >= ngas_before) && (iwhichglobal < ngas_before + ngas_local)) {
  iwhichlocal = iwhichglobal - ngas_before;
  i = local_gas_list[iwhichlocal];
  double energy_before = energy(i,x[i]);
  coord[0] = x[i][0] + displace*(random->uniform() - 0.5);
  coord[1] = x[i][1] + displace*(random->uniform() - 0.5);
  coord[2] = x[i][2] + displace*(random->uniform() - 0.5);
  double energy_after = energy(i,coord);
  if (random->uniform() < exp(-beta*(energy_after - energy_before))) {
    x[i][0] = coord[0];
    x[i][1] = coord[1];
    x[i][2] = coord[2];
    success = 1;
  }
}
```

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Excerpts from LAMMPS's new fix GCMC

(deletion algorithm)

```
// choose particle randomly across all procs and delete it
// keep ngas, ngas_local, ngas_before, and local_gas_list current after each deletion

int success = 0;
iwhichglobal = static_cast<int> (ngas*random->uniform());
if ((iwhichglobal >= ngas_before) && (iwhichglobal < ngas_before + ngas_local)) {
  iwhichlocal = iwhichglobal - ngas_before;
  i = local_gas_list[iwhichlocal];
  double deletion_energy = energy(i,atom->x[i]);
  if (random->uniform() < ngas*exp(beta*deletion_energy)/(zz*volume)) {
    avec->copy(atom->nlocal-1,i);
    atom->nlocal--;
    local_gas_list[iwhichlocal] = local_gas_list[ngas_local-1];
    ngas_local--;
    success = 1;
  }
}
```

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Excerpts from LAMMPS's new fix GCMC

(insertion algorithm)

```
success = 0;
if (flag) {
  int nall = atom->nlocal + atom->nghost;
  double insertion_energy = energy(nall,coord);
  if (random->uniform() < zz*volume*exp(-beta*insertion_energy)/(ngas+1)) {
    atom->avec->create_atom(ntype,coord);
    int m = atom->nlocal - 1;
    atom->type[m] = ntype;
    atom->mask[m] = 1 | groupbit;
    atom->v[m][0] = random->gaussian()*sigma;
    atom->v[m][1] = random->gaussian()*sigma;
    atom->v[m][2] = random->gaussian()*sigma;

    int nfix = modify->nfix;
    Fix **fix = modify->fix;
    for (int j = 0; j < nfix; j++)
      if (fix[j]->create_attribute) fix[j]->set_arrays(m);

    if (atom->nlocal > nmax) {
      nmax = atom->nmax;
      local_gas_list = (int *) memory->srealloc(local_gas_list,nmax*sizeof(int),"GCMC:local_gas_list");
    }

    local_gas_list[ngas_local] = atom->nlocal;
    ngas_local++;
    success = 1;
  }
}
```

How do we know that we've implemented the algorithm correctly?

Verification exercise: code-to-code comparison versus an established Monte Carlo code (Towhee).

Gas = Kr **(with LJ parameters from Pellenq and Levitz)**

T = 300 K

μ = -10.284 kcal/mol

P = ?

If ideal gas: $$\mu = -k_B T \ln \left[\left(\frac{2\pi m k_B T}{h_0^2} \right)^{3/2} \frac{V}{N} \right]$$

✓**$P_{(ideal\ gas)}$ = 1 bar**

✓**Also, from Towhee calculation: $P_{(Towhee)}$ = 1 bar**

✓**Corrected a sign error in the new code that caused a slight discrepancy**

✓**Now, with our new fix GCMC for LAMMPS, we have: $P_{(LAMMPS)}$ = 1 bar**

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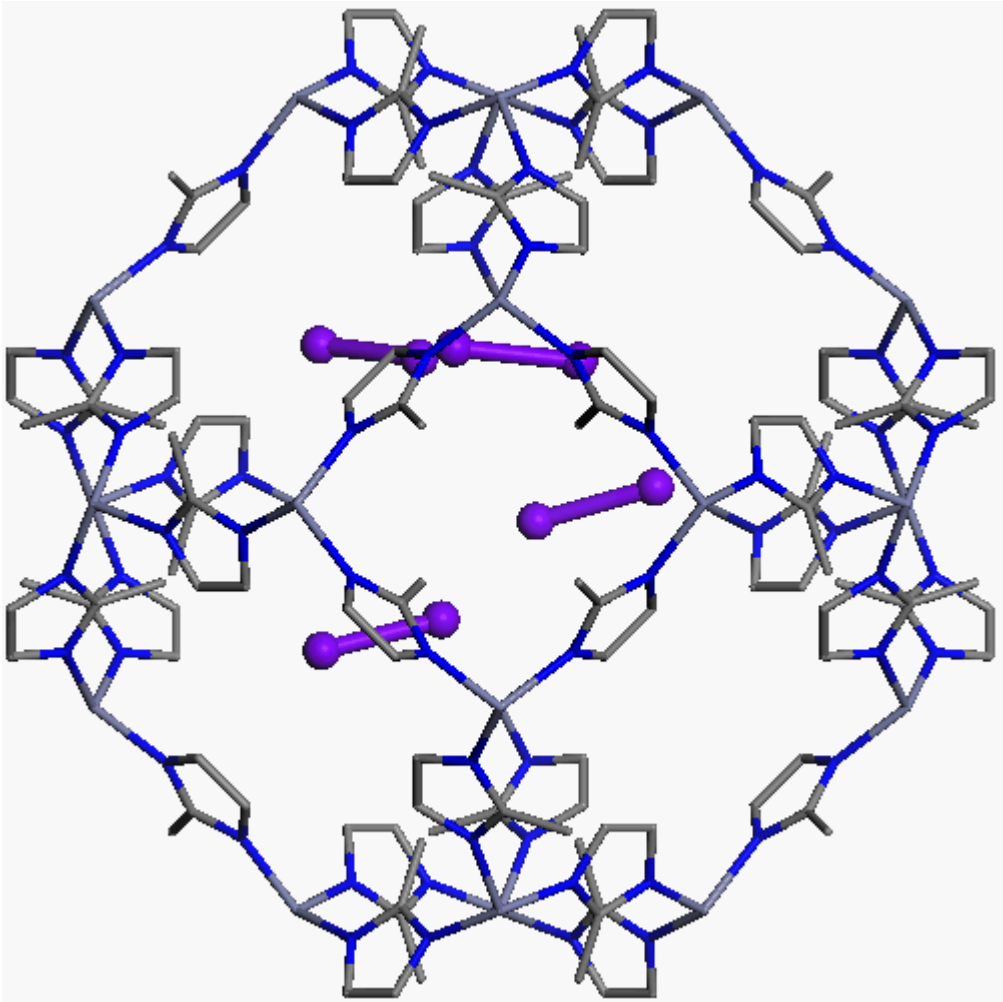
MD movie: 4 I_2 molecules in one ZIF-8 cage



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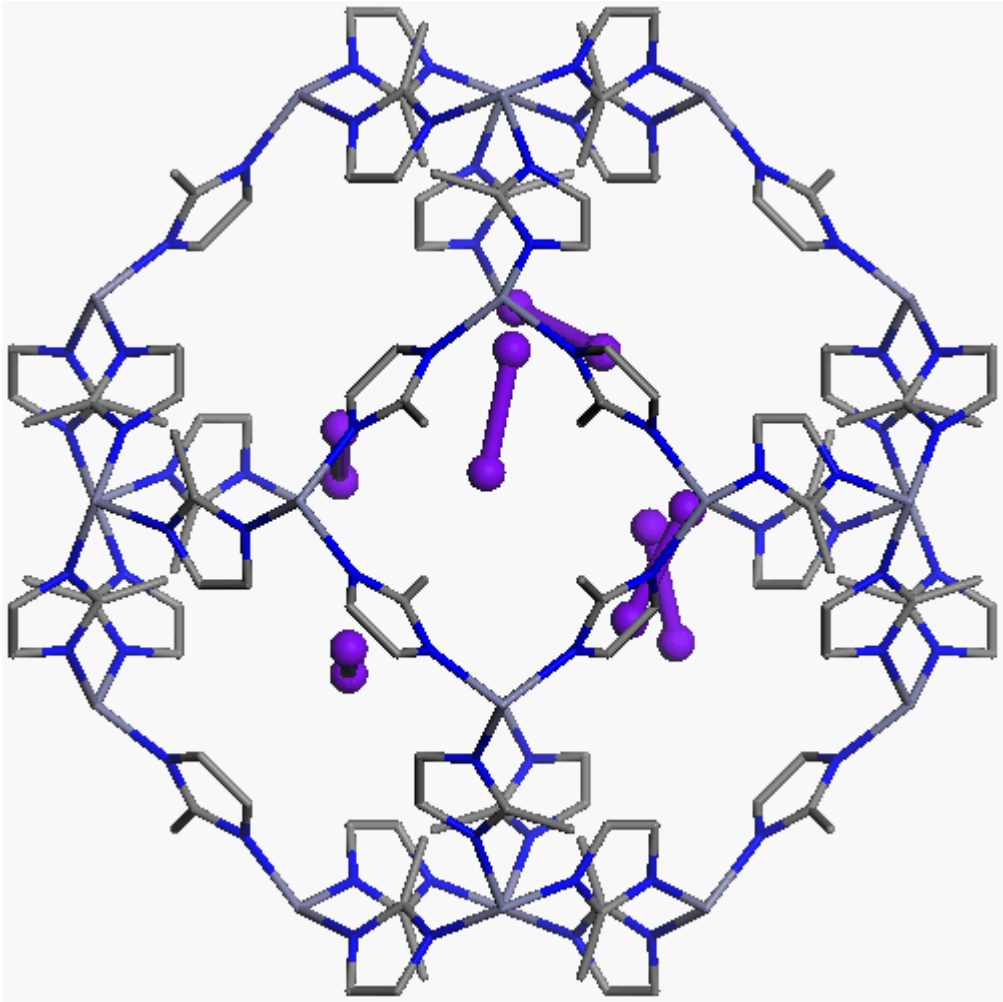
MD movie: 6 I_2 molecules in one ZIF-8 cage



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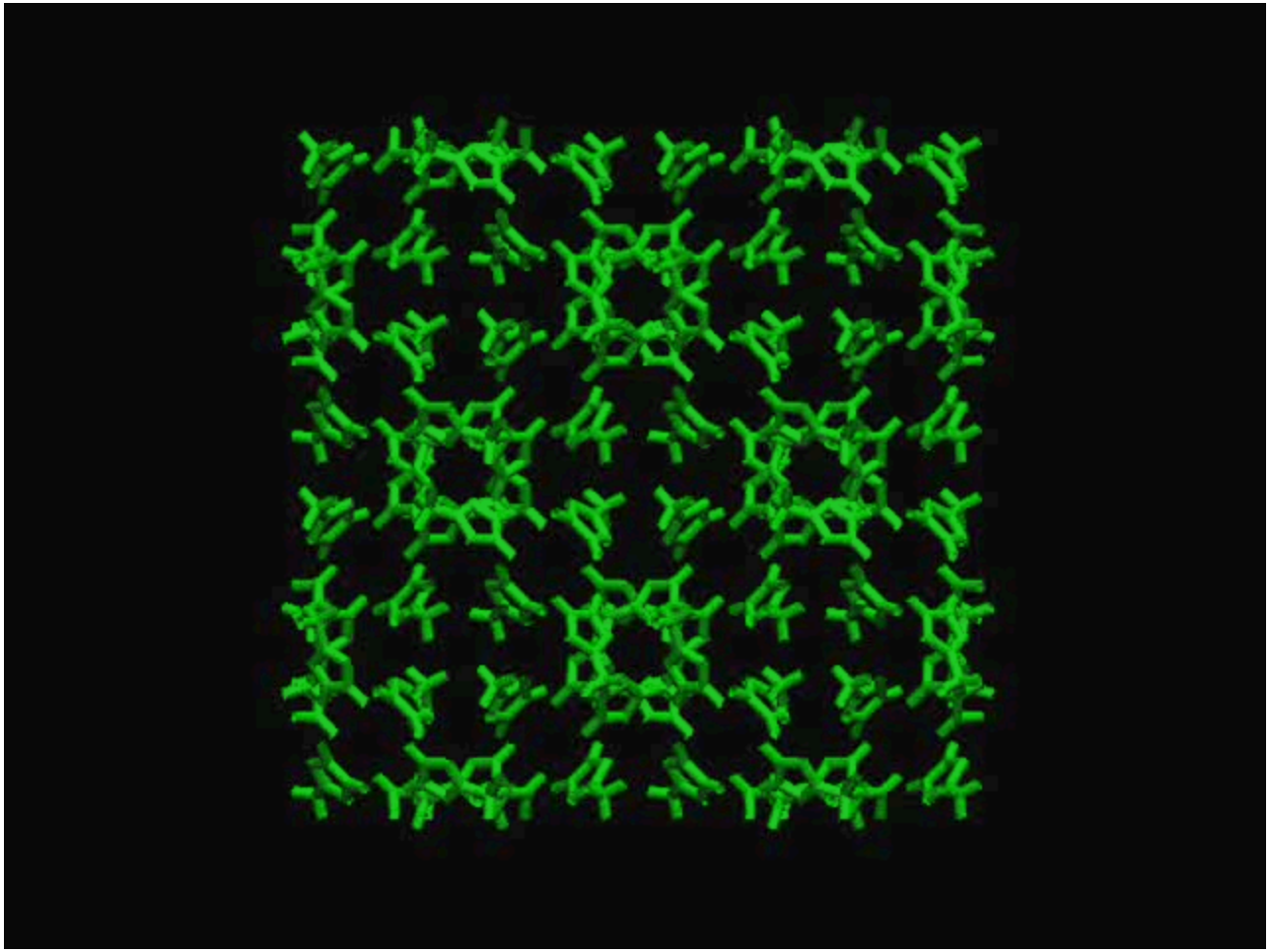
GCMC loading movie



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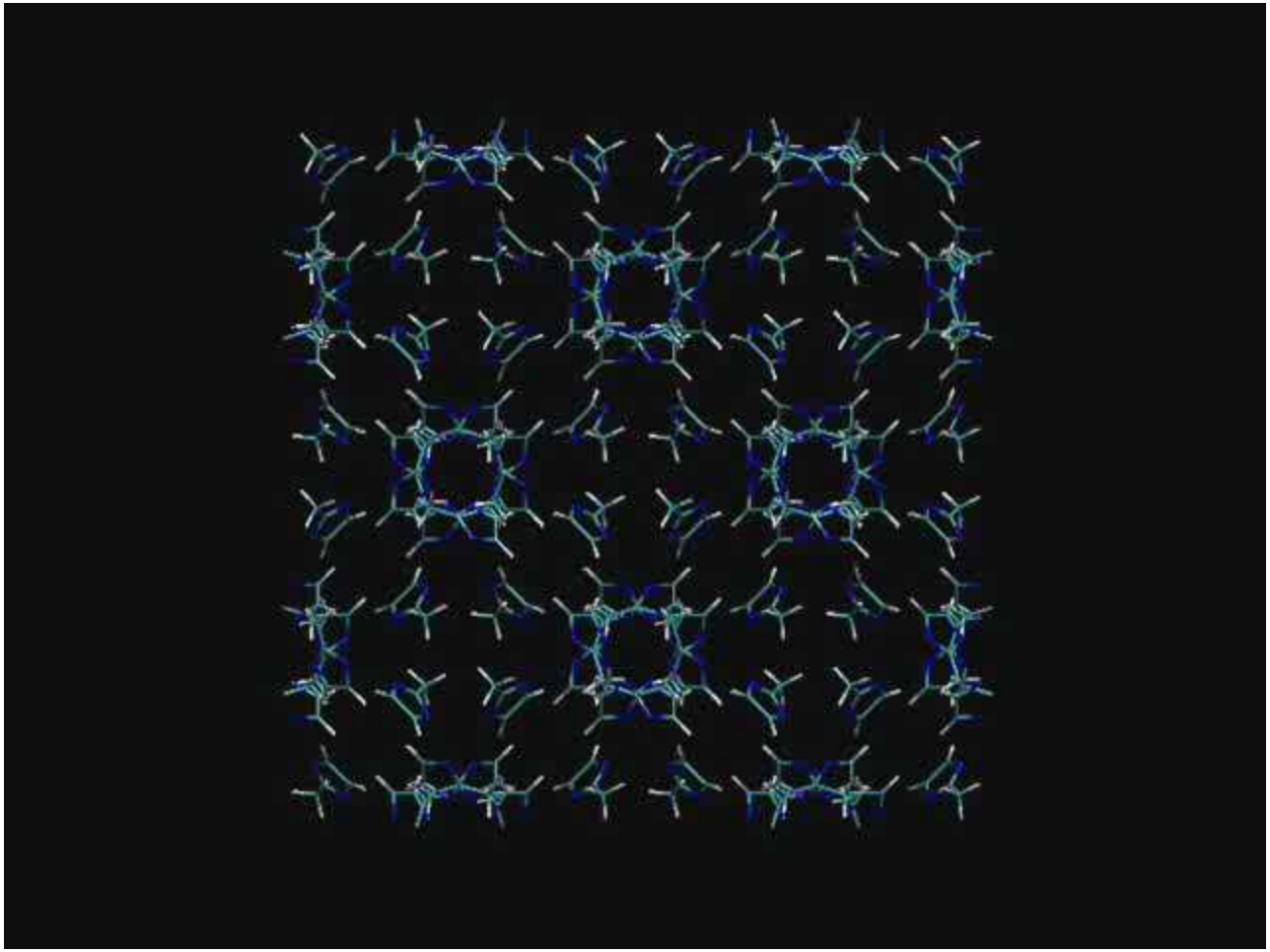
GCMC saturation movie



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Additional work on “fix GCMC”

Likely to be done soon:

1. Ensure compatibility with all LAMMPS atom styles.
2. Add molecule capability, including MC exchanges, moves, and rotations of molecules.
3. Send code & docs out to more beta testers for feedback.
4. Add ability to measure and report chemical potential.
5. Improve the documentation in preparation for release.
6. Send updated code & docs out to beta testers and Steve.
7. Release code & docs on main LAMMPS website.

Maybe later if there’s time:

8. Make it work with long-range electrostatics.
9. Make it scale: better parallel simulation.
10. Add fancier MC moves (configurational bias, etc.).

Additional Material

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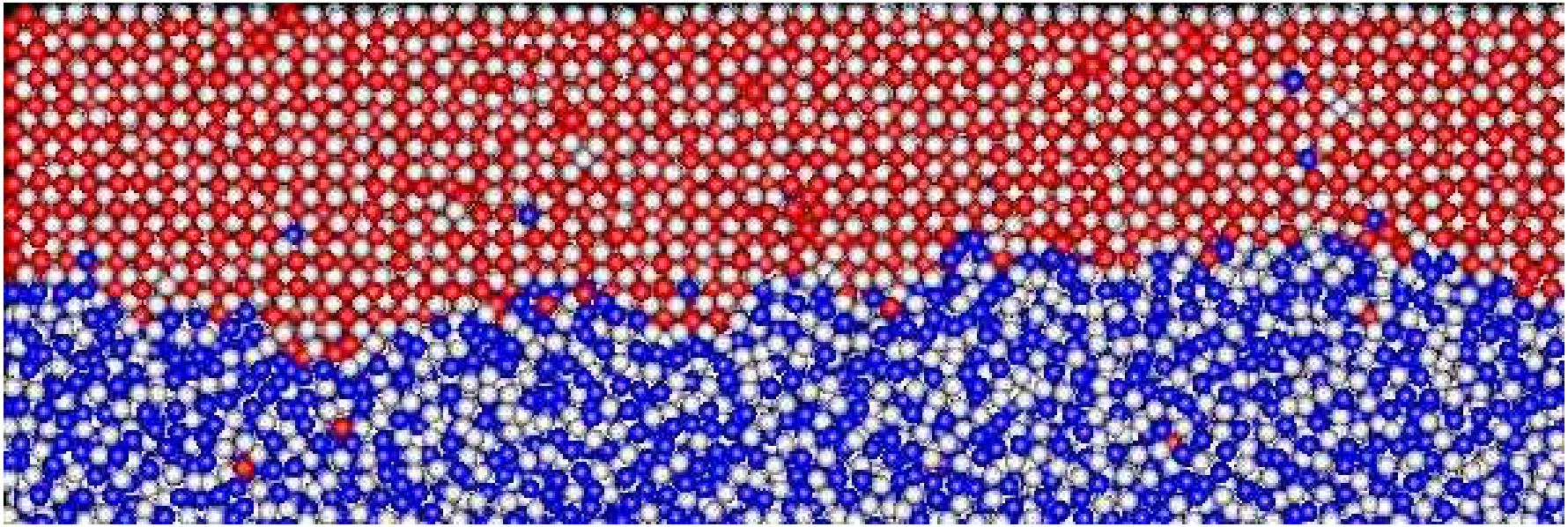
Melt Interface in NiAl

- Mark Asta (UC Davis) and Jeff Hoyt (Sandia)
- Careful thermostatting and equilibration of alloy system
- Track motion and structure of melt interface



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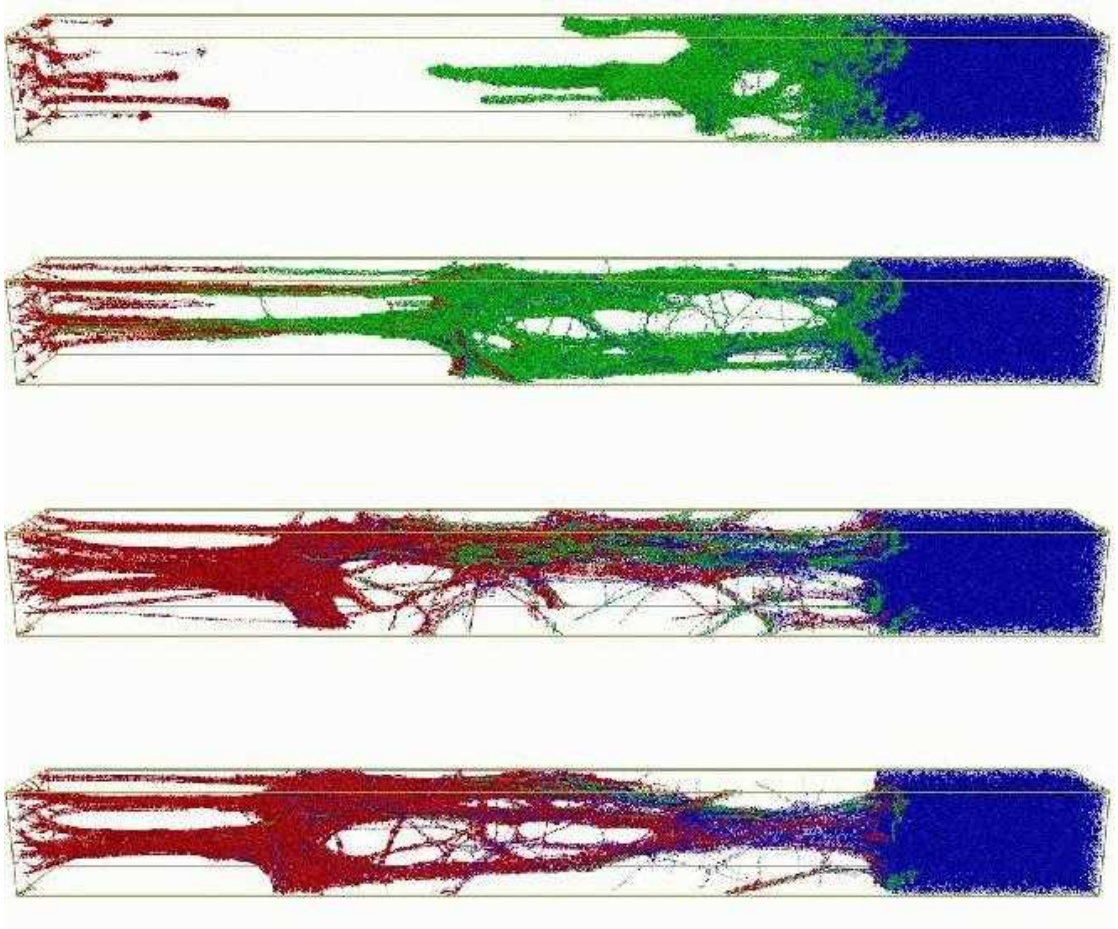
Polymer Adhesive Properties

- Mark Stevens and Gary Grest (Sandia)
- Bead/spring polymer model, allow for bond breaking



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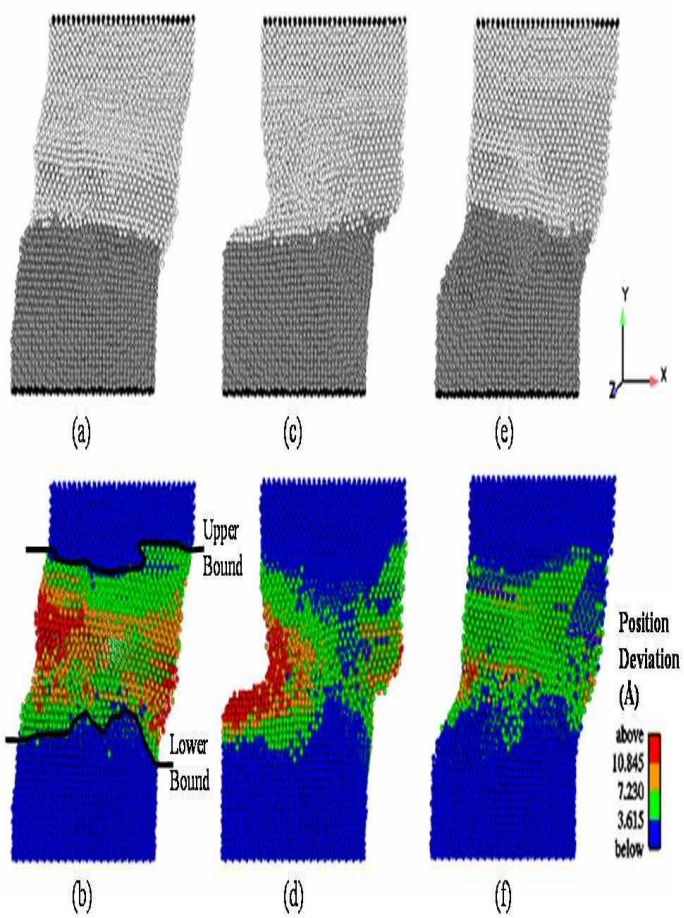
Shear Response of Cu Bicrystal

- David McDowell group (GA Tech)
- Defect formation, stress relaxation, energetics of boundary region



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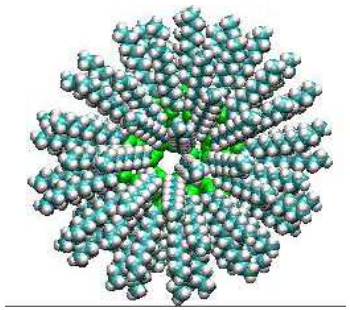
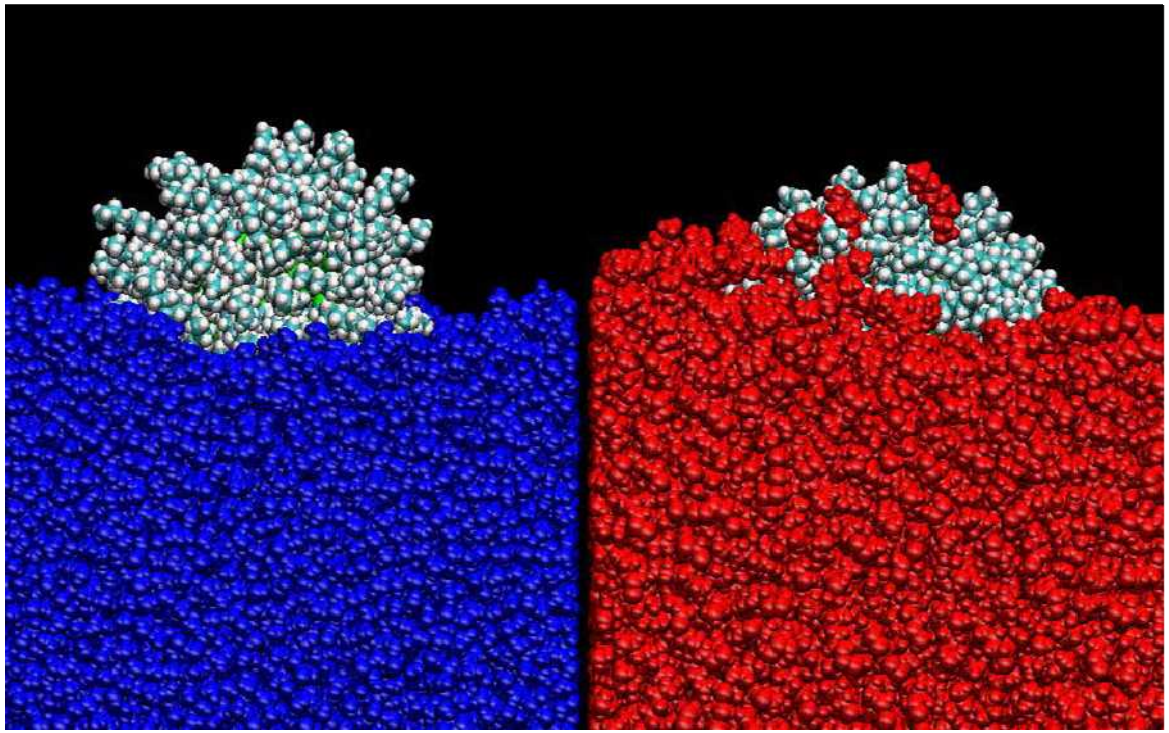
Coated Nanoparticles at Interfaces

- Matt Lane, Gary Grest (Sandia)
- S sites on Au nanoparticle, alkane-thiol chains, methyl-terminated, 3 ns sim





water

decane

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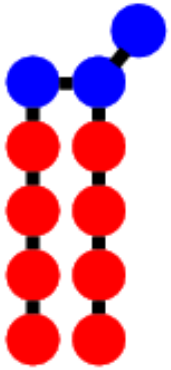
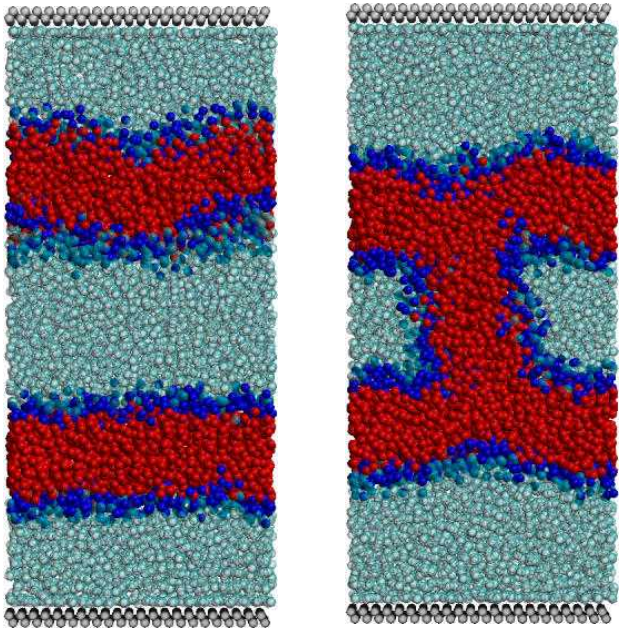
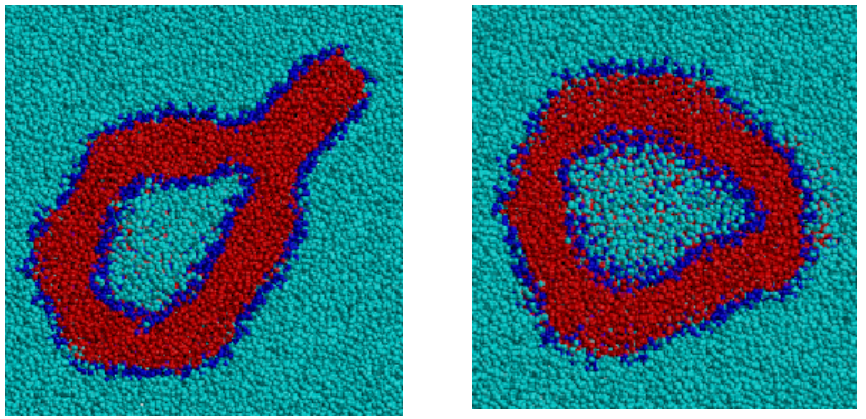
3d Membrane Self-Assembly

- Mark Stevens (Sandia)
- Coarse-grain lipid model in monomeric solvent
- Angle terms for rigidity
- Hydrophilic head-group & solvent, hydrophobic tail
- 100Ks of particles for millions of timesteps
- Bilayer & vesicle formation







15K monomers for 1M steps

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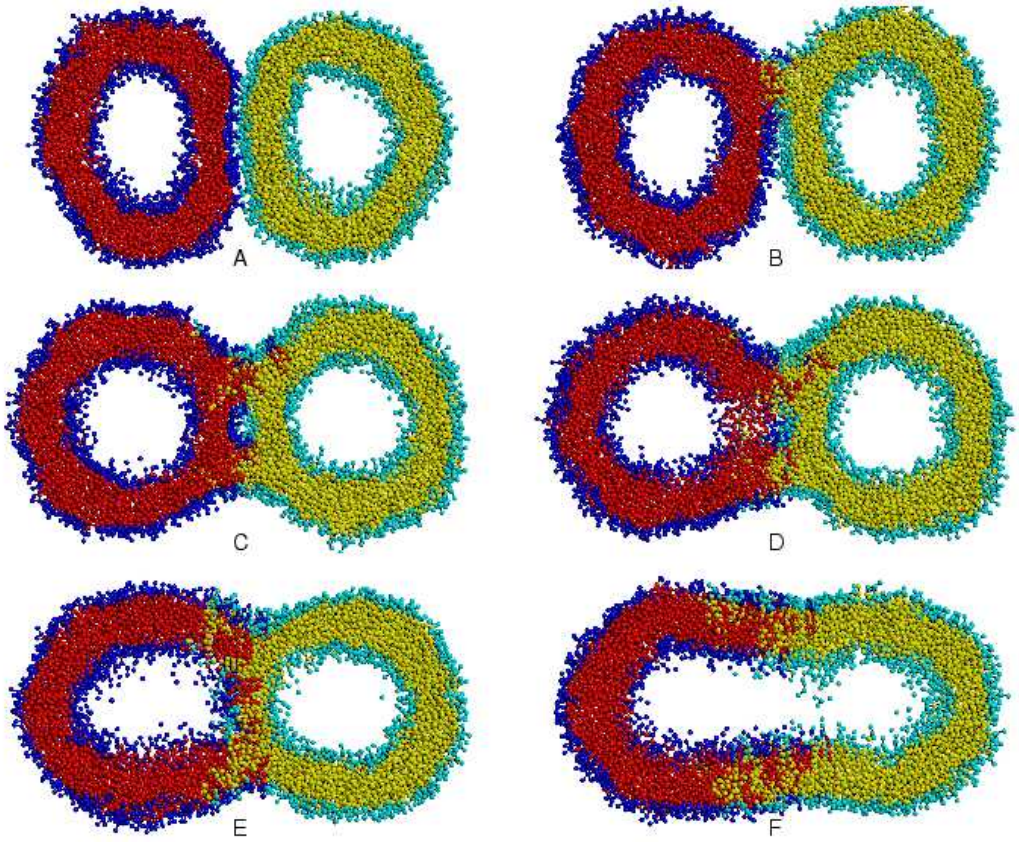
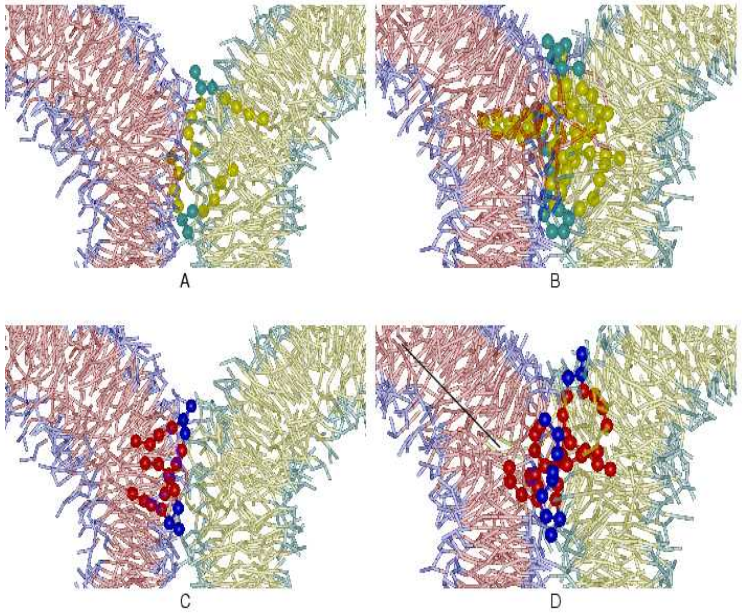
Membrane Fusion





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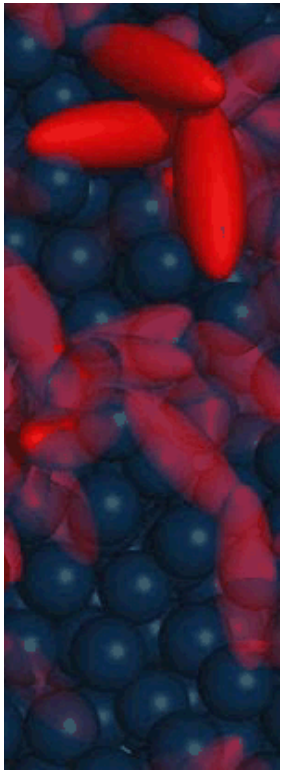
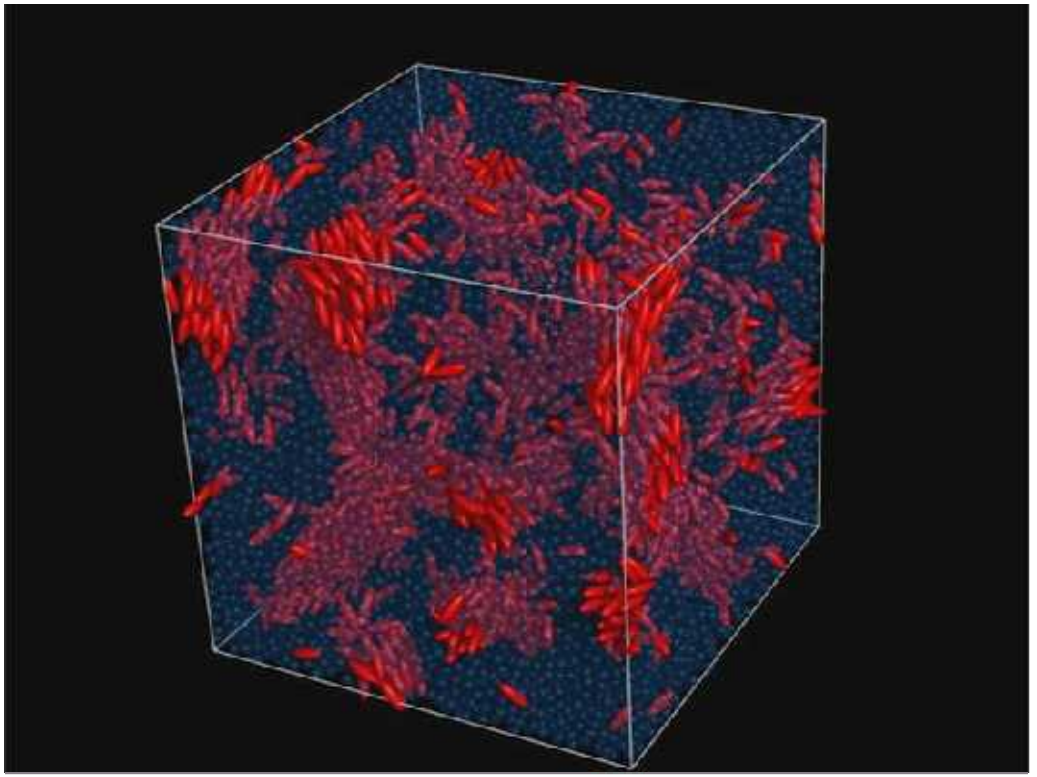
Aspherical Nanoparticles

- Mike Brown (Sandia)
- Ellipsoidal particles interacting via Gay-Berne potentials (LC), LJ solvent
- Nanodroplet formation in certain regimes of phase space





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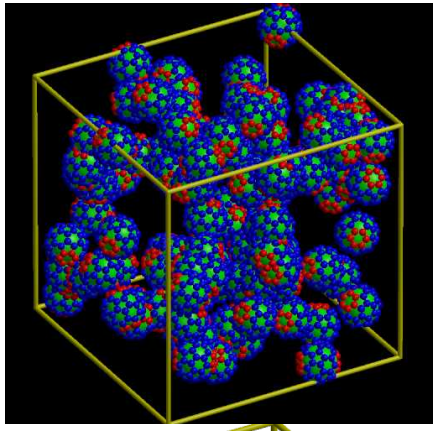
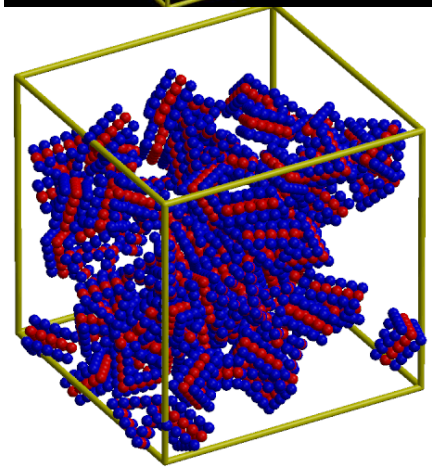
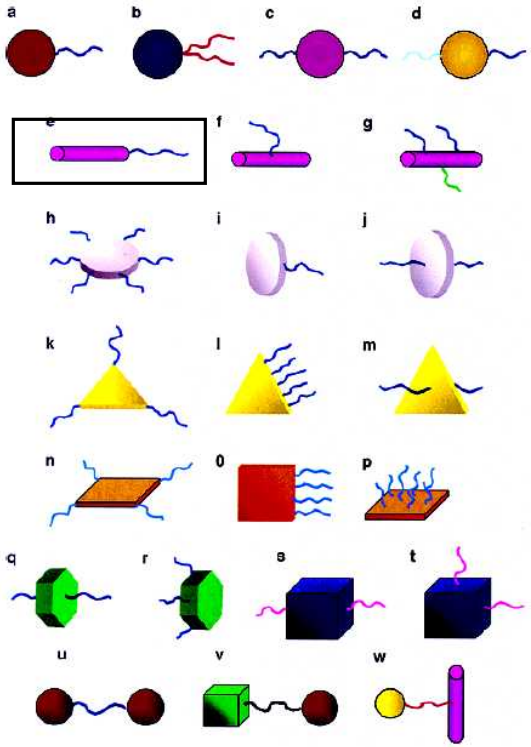
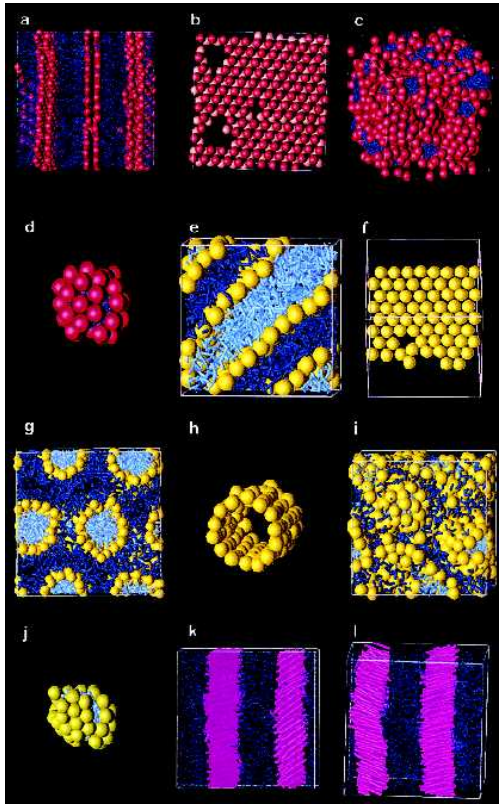
Rigid Nanoparticle Self-Assembly

- Multiple rigid bodies
- Quaternion integration
- Brownian dynamics
- Self-assembly → phases









(Sharon Glotzer *et al.*, *Nano Letters*, **3**, 1341 (2003).

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LAMMPS's Reactive Force Fields Capability

Why Reactive Force Fields?

- Material behavior often dominated by chemical processes
- HE, Complex Solids, Polymer Aging
- Quantum methods limited to hundreds of atoms
- Ordinary classical force fields limited accuracy
- We need to have the best of both worlds $\Rightarrow$Reactive force fields

Why build Reactive Force Fields into LAMMPS?

- Reactive force fields typically exist as custom serial MD codes
- LAMMPS is a general parallel MD code

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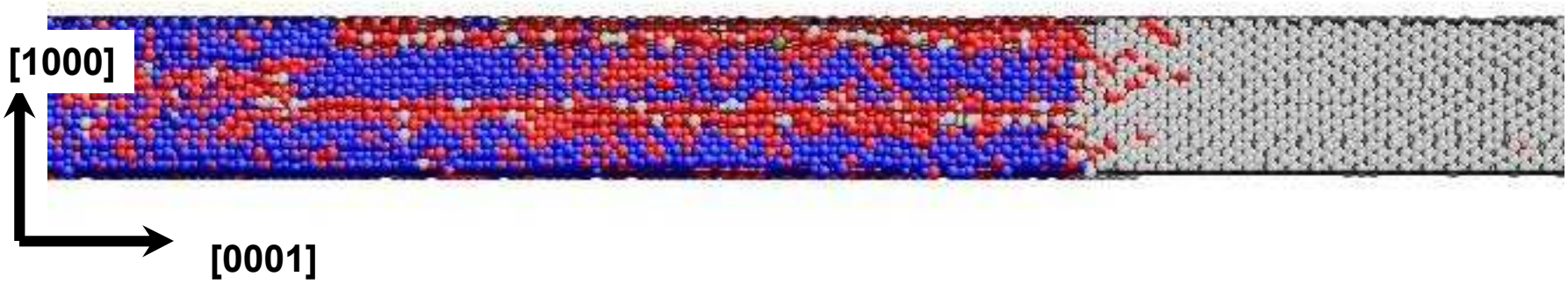
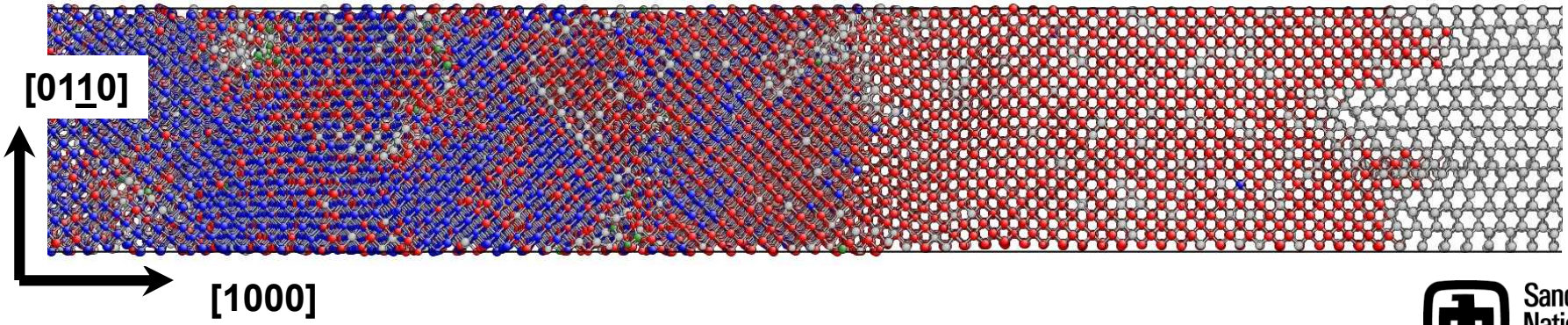
MD Simulation of Shock-induced Structural Phase Transformation in Cadmium Selenide

c-direction: 2-Wave Structure: rocksalt emerges directly from elastically compressed material



a-direction: 3-Wave Structure: tetragonal region forms between elastic wave and rocksalt phase



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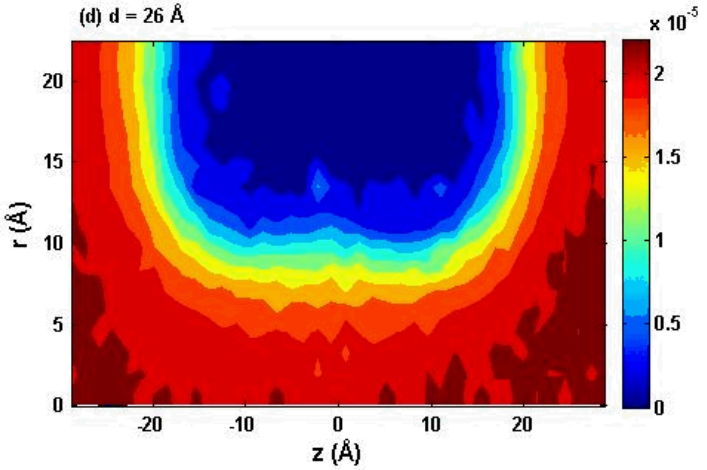
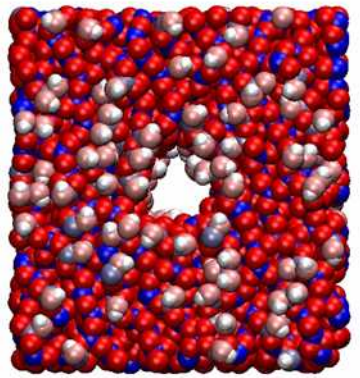
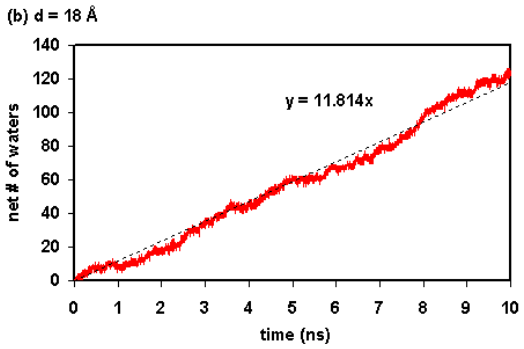
Non-equilibrium MD simulations of brackish water flow through silica and titania nanopores

- Small flow field successfully induces steady state solvent flow through amorphous SiO_2 and TiO_2 nanopores in NEMD simulations.
- Complex model systems built through a detailed processs involving melting, quenching, annealing, pore drilling, defect capping, and equilibration.
- 10-ns simulations carried out for a variety of pore diameters for for both SiO_2 and TiO_2 nanopores.
- Densities, diffusivities, and flows of the various species computed spatially, temporally, and as a function of pore diameter.

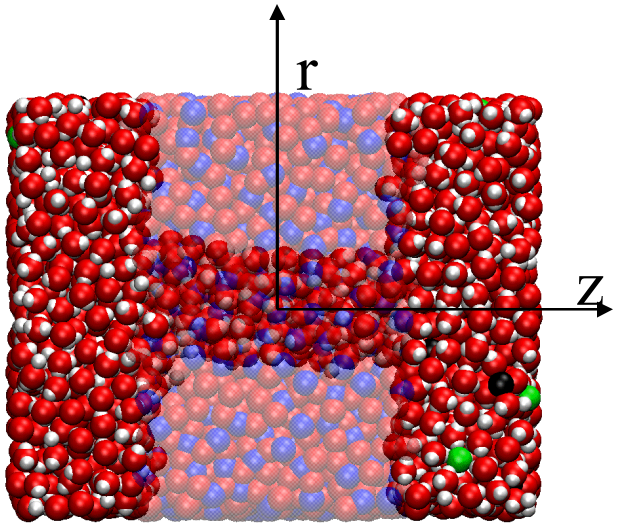


Spatial map of water diffusivities in a 26 Å TiO_2 nanopore.





Water flux through an 18 Å TiO_2 nanopore.



- Water is tightly bound to hydrophilic TiO_2 surface, greatly hampering mobility within 5 Å of the surface.
- Simulations show that amorphous nanopores of diameter at least 14 Å can conduct water as well as Na+ and Cl- ions.
- No evidence of selectivity that allows water passage and precludes ion passage --- functional groups on pore interior may be able to achieve this.

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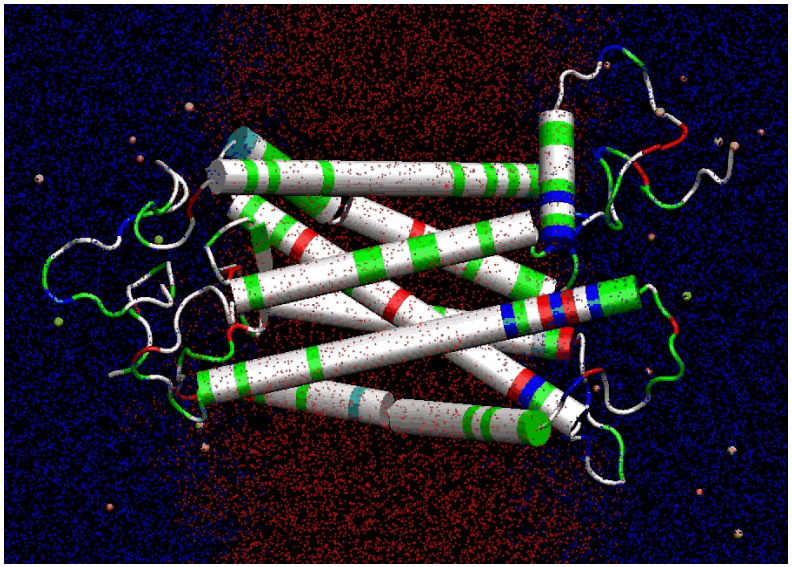
Rhodopsin photoisomerization simulation

- 190 ns simulation
  - 40 ns in dark-adapted state (*J. Mol. Biol.*, **333**, 493, (2003))
  - 150 ns after photoisomerization
- CHARMM force field
- P^3M full electrostatics
- Parallel on ~40 processors; more than 1 ns simulation / day of real time
- Shake, 2 fs time step, velocity Verlet integrator
- Constant membrane surface area
- System description
  - All atom representation
  - 99 DOPC lipids
  - 7441 TIP3P waters
  - 348 rhodopsin residues
  - 41,623 total atoms
  - L_x=55 Å, L_y=77 Å, L_z=94-98 Å



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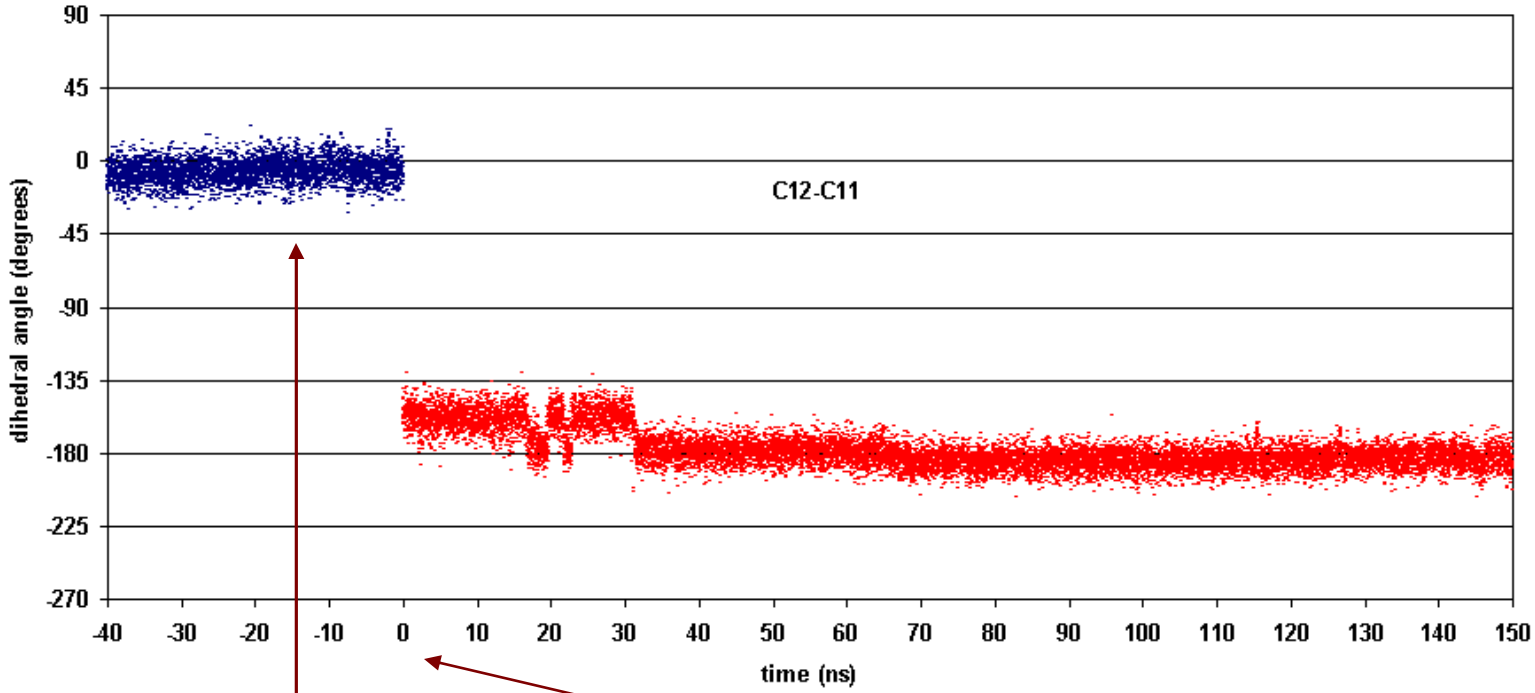
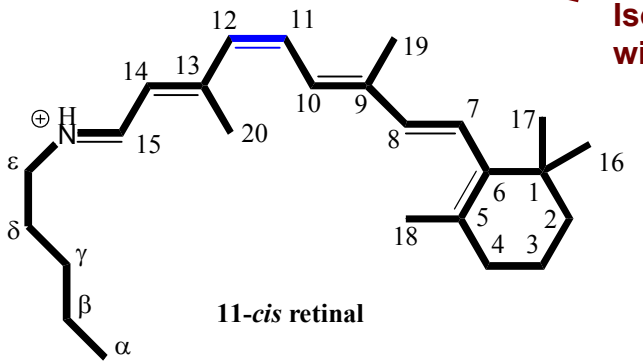
Photoisomerization of retinal

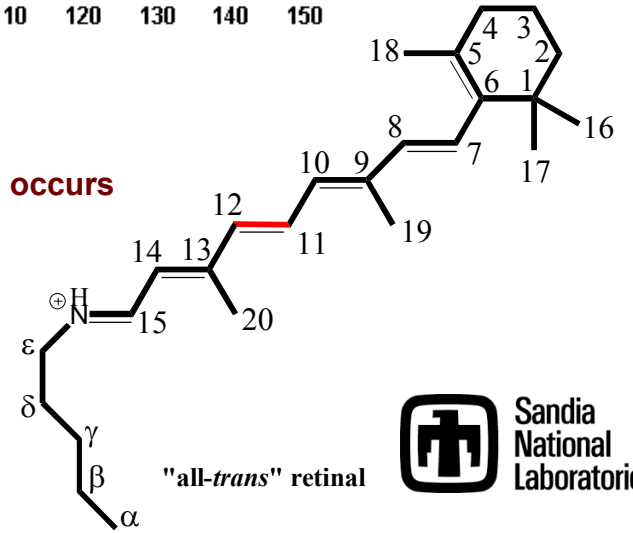


Dihedral remains in *trans* during subsequent 150 ns of relaxation

40-ns simulation in dark-adapted state

Isomerization occurs within 200 fs.





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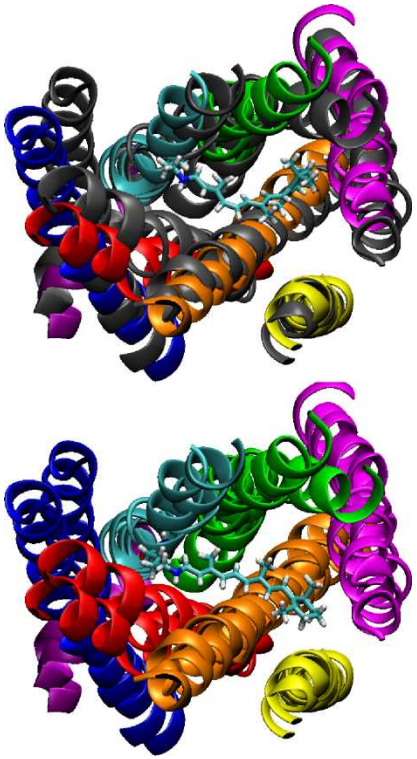
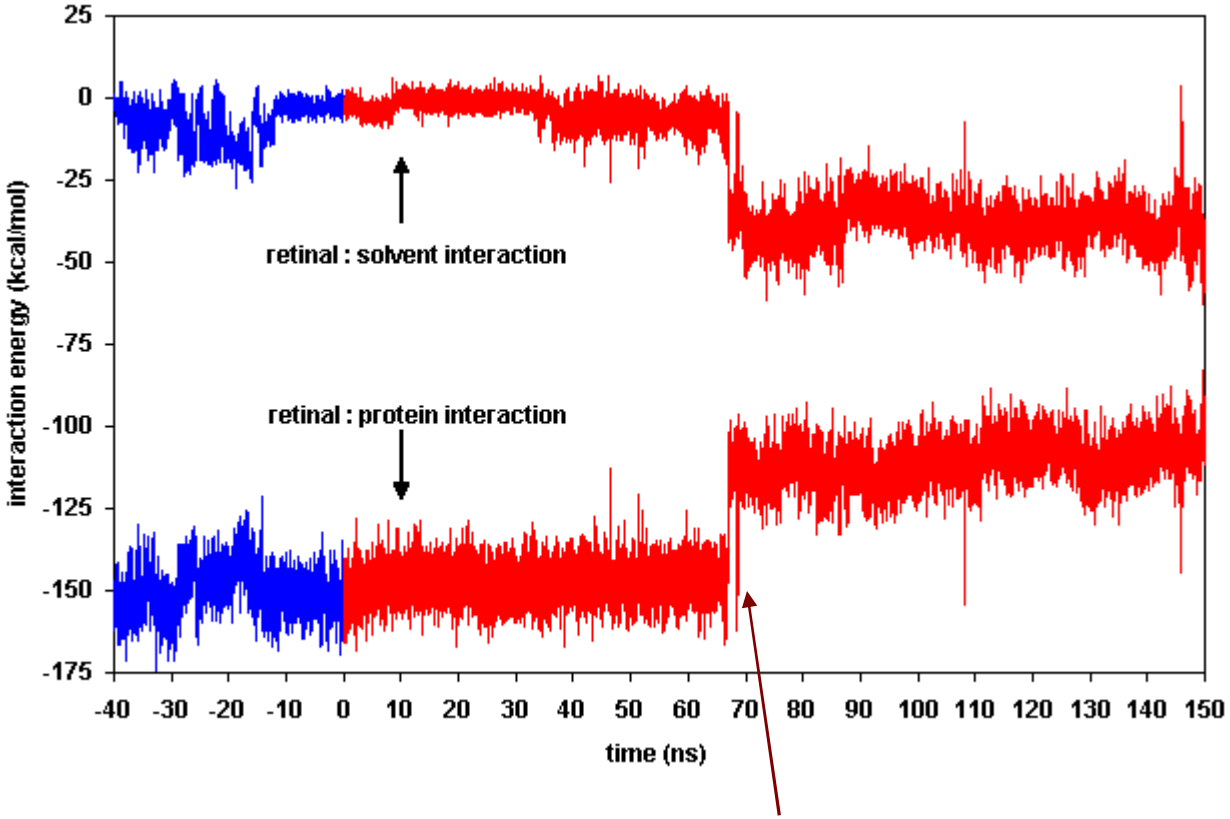
Transition in retinal's interaction environment

Retinal's interaction with the rest of the rhodopsin molecule weakens and is partially compensated by a stronger solvent interaction





Most of the shift is caused by breaking of the salt bridge between Glu 113 and the PSB

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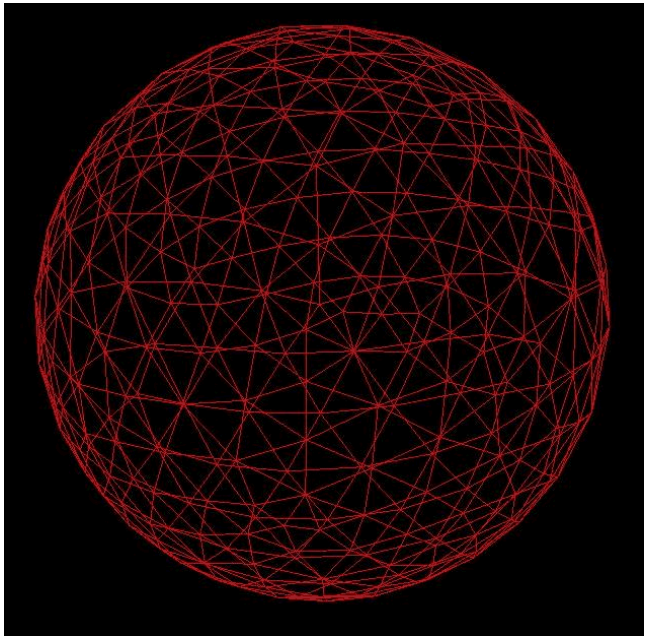
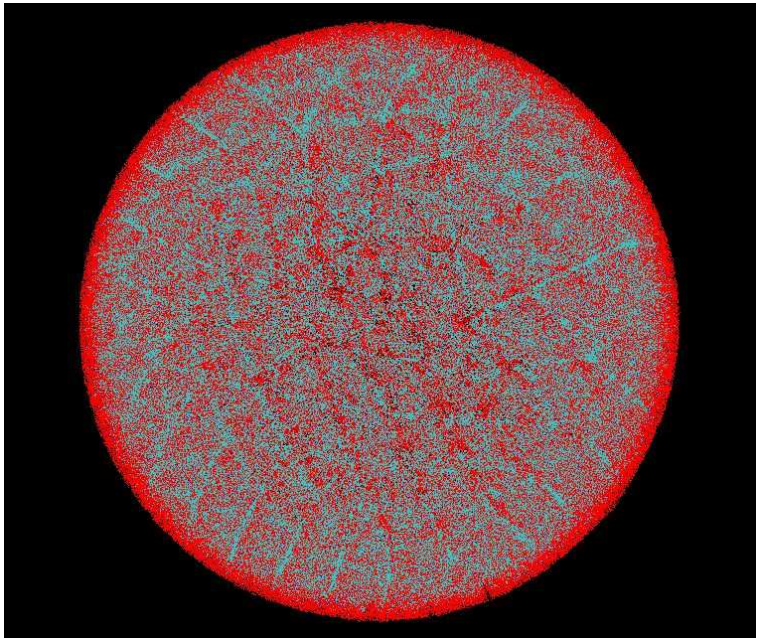
Whole vesicle simulation





- Enormous challenge due to sheer size of the system
  - 5 million atoms prior to filling box with water
  - Estimate > 100 million atoms total
- Sphere of tris built using Cubit software, then triangular patches of DOPC lipid bilayers were cut and placed on sphere surface.

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Radiation damage simulations

- Radiation damage is directly relevant to several nuclear energy applications
  - Reactor core materials
  - Fuels and cladding
  - Waste forms
- Experiments are not able to elucidate the mechanism involved in structural disorder following irradiation
- Classical simulations can help provide atomistic detail for relaxation processes involved
- Electronic effects have been successfully used in cascade simulations of metallic systems

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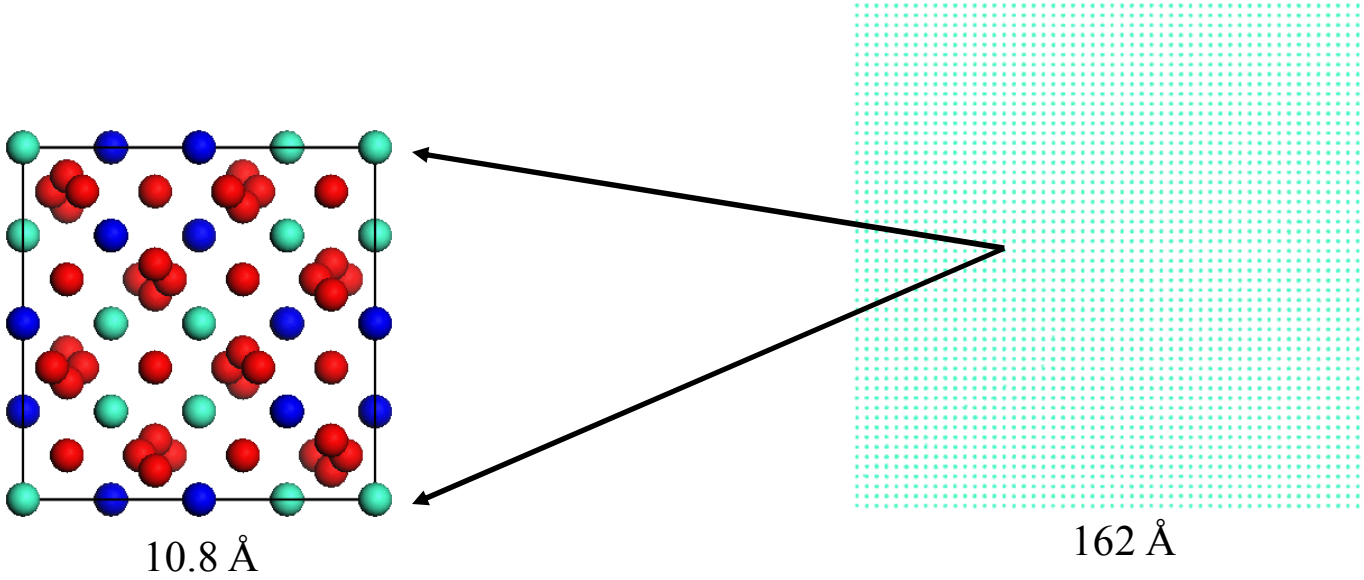
MD model for radiation damage simulations

- Gadolinium pyrochlore waste form ($Gd_2Zr_2O_7$)
- Natural pyrochlores are stable over geologic times and shown to be resistant to irradiation (Lumpkin, *Elements* **2006**).
- Recent simulations (without electronic effects) exist for comparison (Todorov et al, *J. Phys. Condens. Matter* **2006**).



1 unit cell, 88 atoms

15 x 15 x 15 supercell, 297k atoms
(only Gd atoms shown)

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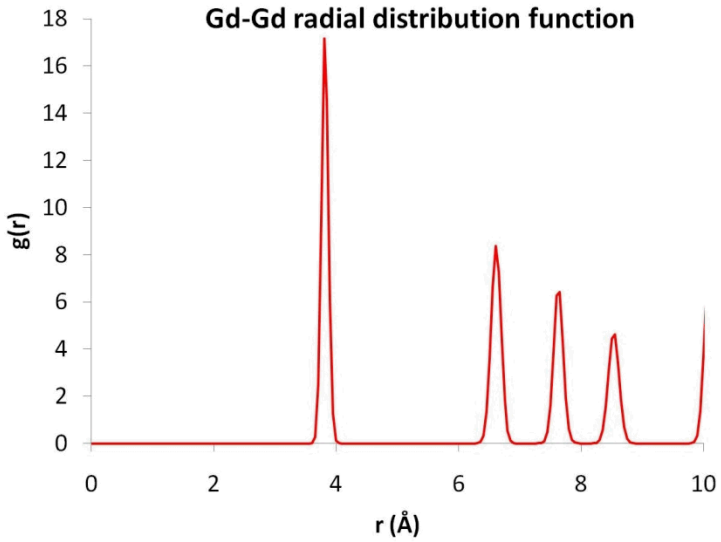
Defect analysis

- How the defect analysis works:
  1. Shape matching algorithm was used.*
  2. Nearest neighbors defined as those atoms in the first RDF peak.
  3. Clusters formed by each Gd atom and its nearest Gd neighbors are compared with clusters formed by those neighbors and their nearest Gd neighbors.
  4. If the cluster shapes match, the atom is considered “crystalline”; otherwise, it is considered “amorphous.”

- Why only Gd atoms were used:
  1. RDF analysis produces clear picture of crystal structure.
  2. Clearly shows the cascade damage.



* Auer and Frenkel, *J. Chem. Phys.* **2004**
Ten et al, *J. Chem. Phys.* **1996**

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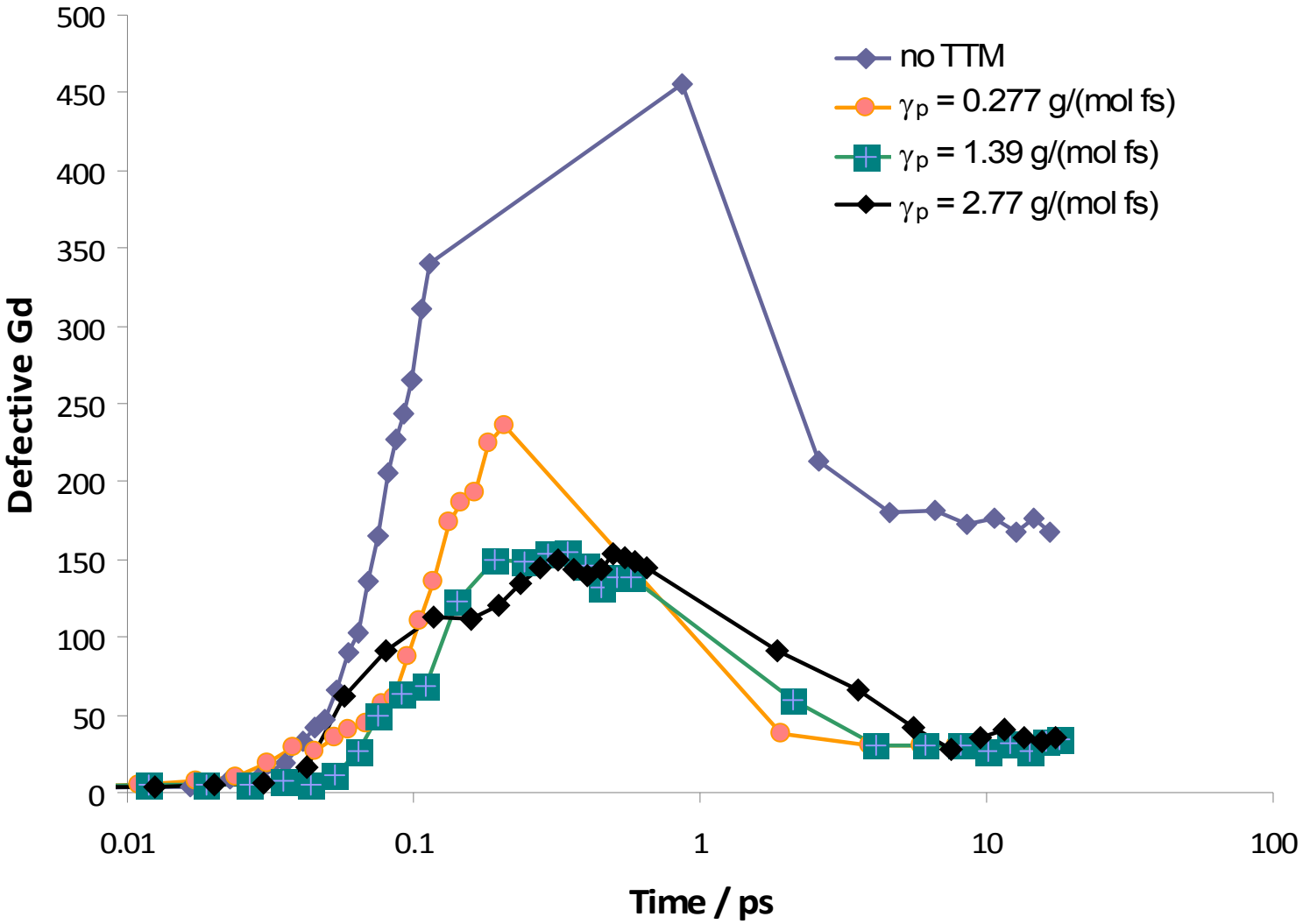
Results of defect analysis



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Future areas of LAMMPS development

- Alleviations of time-scale and spatial-scale limitations
- Improved force fields for better molecular physics
- New features for the convenience of users

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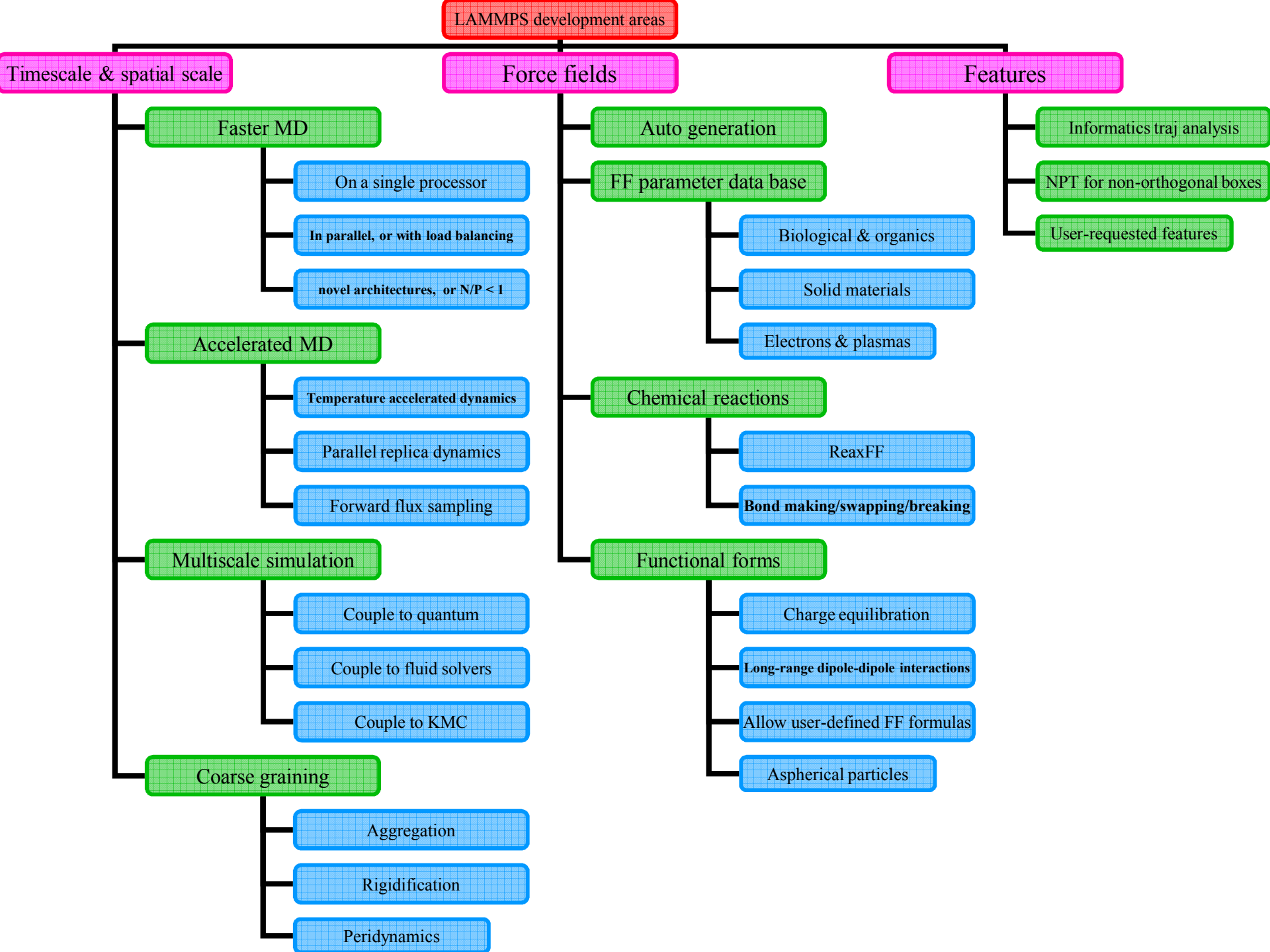
LAMMPS development areas
Timescale & spatial scale
Faster MD
On a single processor
In parallel, or with load balancing
novel architectures, or N/P < 1
Accelerated MD
Temperature accelerated dynamics
Parallel replica dynamics
Forward flux sampling
Multiscale simulation
Couple to quantum
Couple to fluid solvers
Couple to KMC
Coarse graining
Aggregation
Rigidification
Peridynamics
Force fields
Auto generation
FF parameter data base
Biological & organics
Solid materials
Electrons & plasmas
Chemical reactions
ReaxFF
Bond making/swapping/breaking
Functional forms
Charge equilibration
Long-range dipole-dipole interactions
Allow user-defined FF formulas
Aspherical particles
Features
Informatics traj analysis
NPT for non-orthogonal boxes
User-requested features