Multiscale Modeling via Particle Methods

Steve Plimpton
Sandia National Labs

Sid Fuchs Mechanical Engineering Seminar Series
LSU - Nov 2011

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

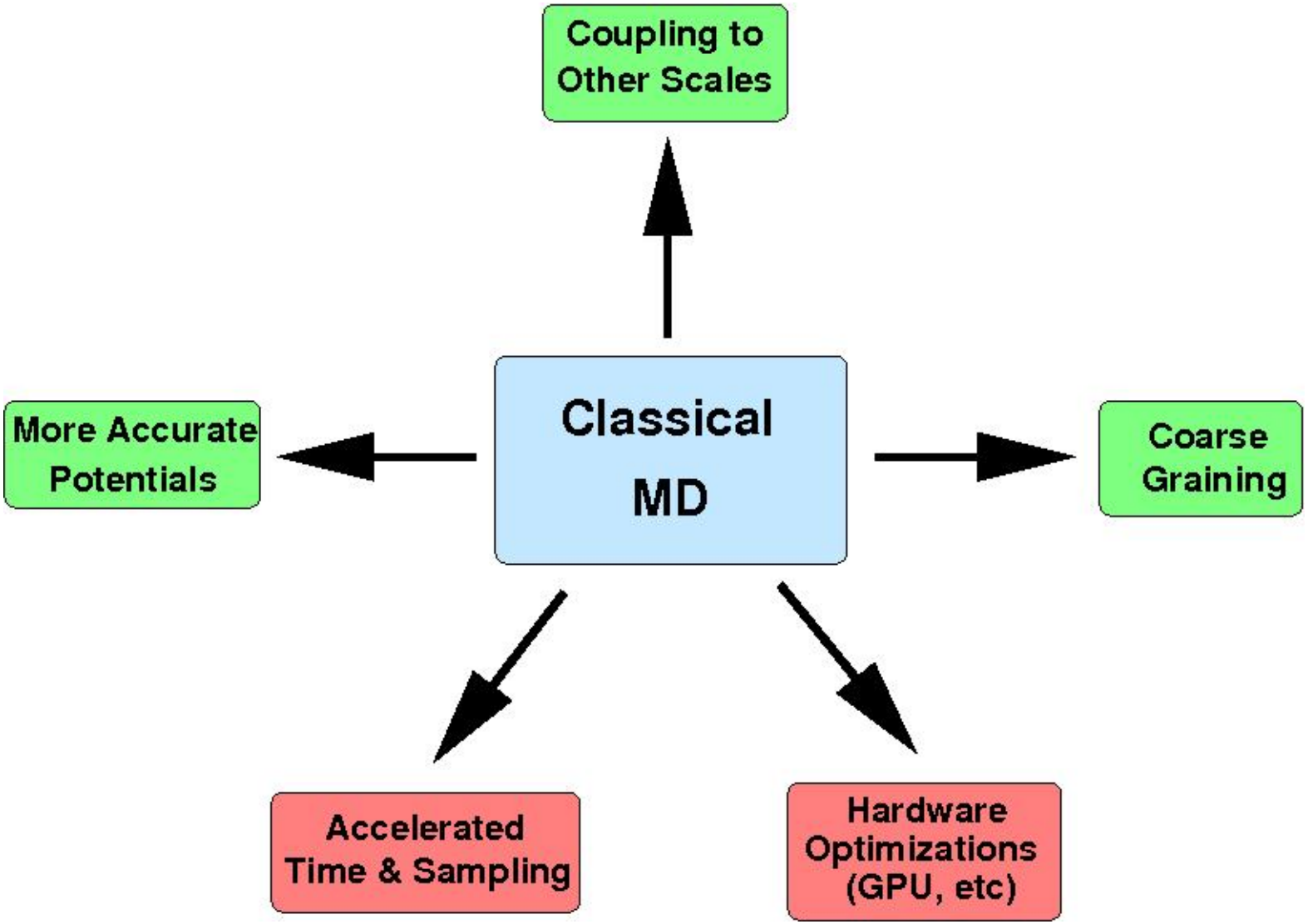
Multiscale Modeling via Particle Methods

Steve Plimpton
Sandia National Labs

Sid Fuchs Mechanical Engineering Seminar Series
LSU - Nov 2011

Go

Research directions in classical MD



Multiscale is hard

- Parameter passing between scales (hard)
- Loose coupling of two or more models (harder)
- Tight coupling of two or more models (hardest)

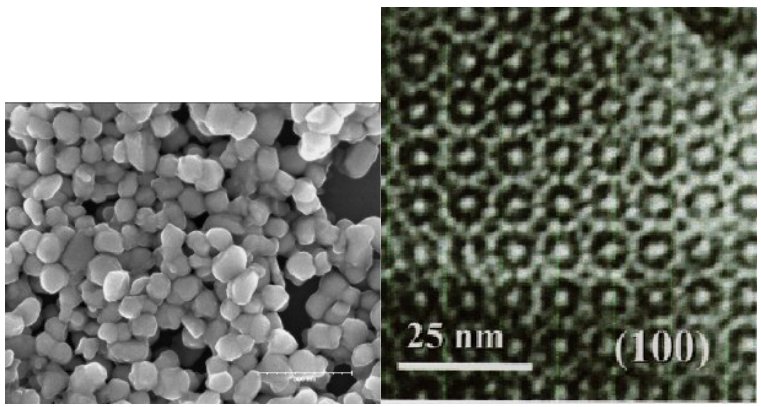
Particle suspensions

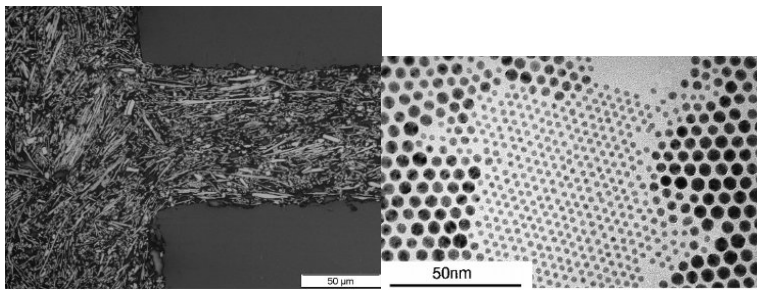
- Colloids = large particles, sub-micron to few microns in diameter, squishy or hard, bare or coated, spherical or irregular in shape
- Nanoparticles = small colloids, 2-100 nm in diameter
- Suspension = background fluid

Particle suspensions

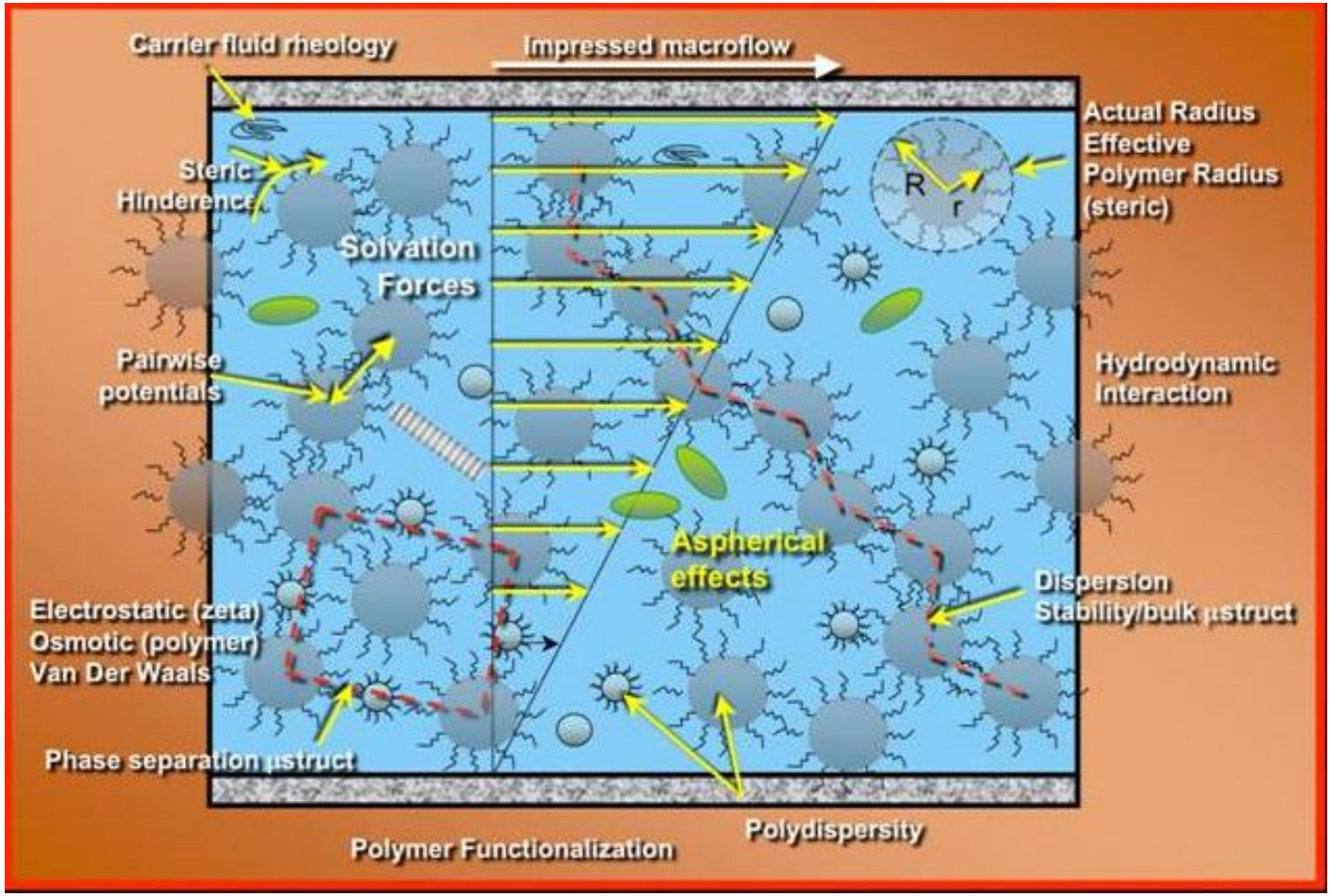
- Colloids = large particles, sub-micron to few microns in diameter, squishy or hard, bare or coated, spherical or irregular in shape
- Nanoparticles = small colloids, 2-100 nm in diameter
- Suspension = background fluid

- Applications:
  - bulk: paints, gels, pastes
  - films: self-assembly of nano-structured materials
- Processing steps:
  - extrusion, flow, drying, self-assembly
- Measure/predict:
  - diffusion, rheology, aggregation/dispersion



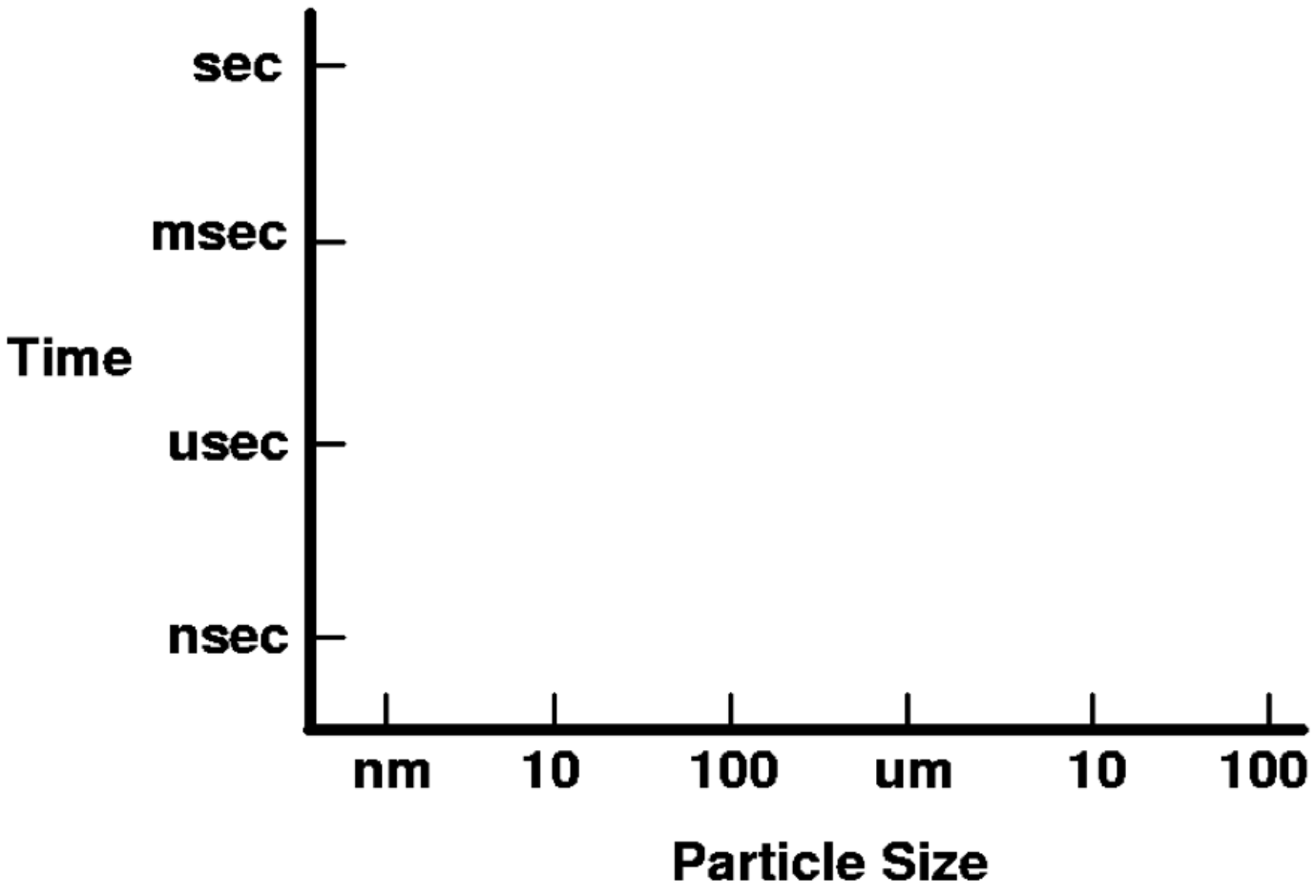


What we want to model

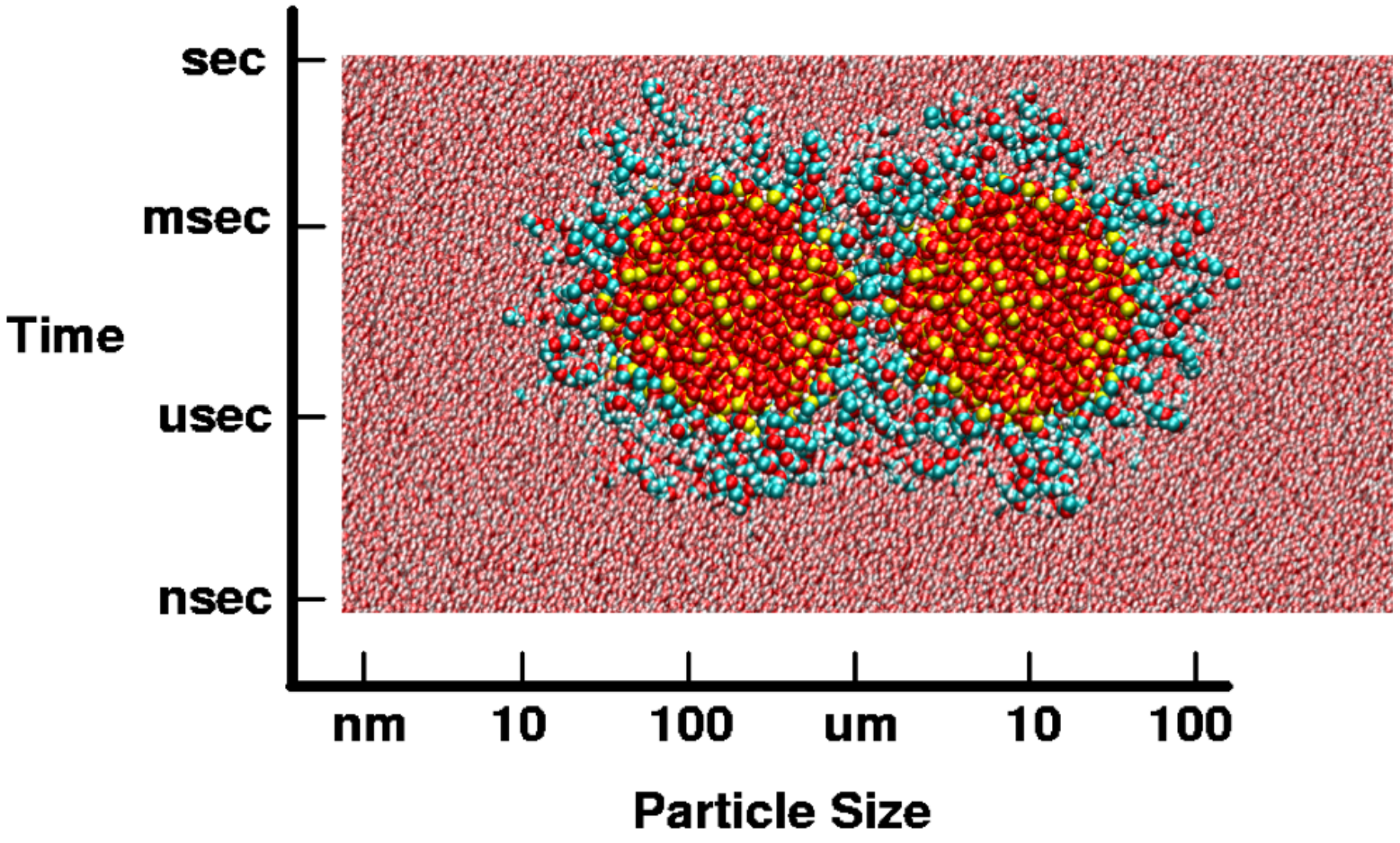


Spherical vs aspherical, bare vs coated, polydisperse, agglomeration, response to shear, ...

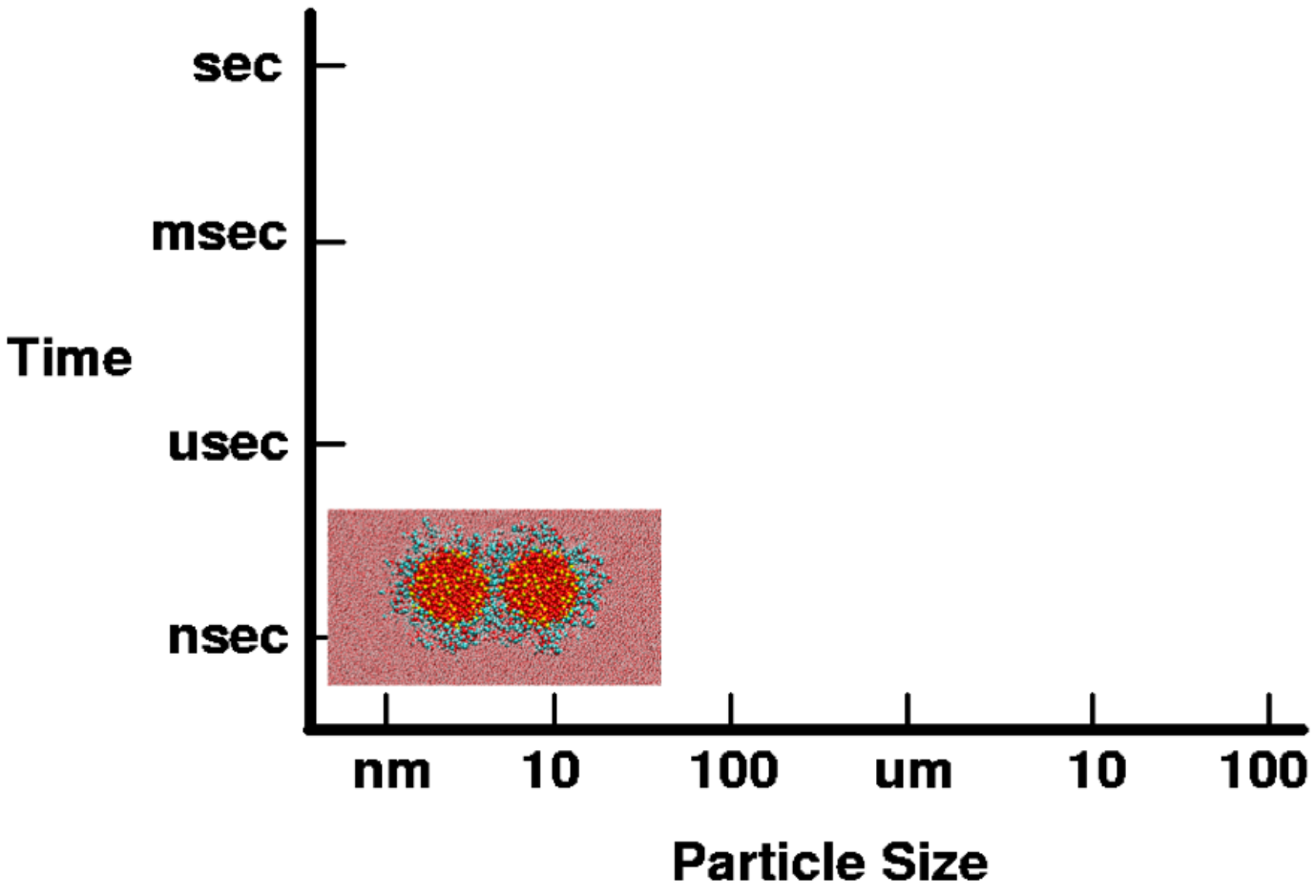
Length and time scales



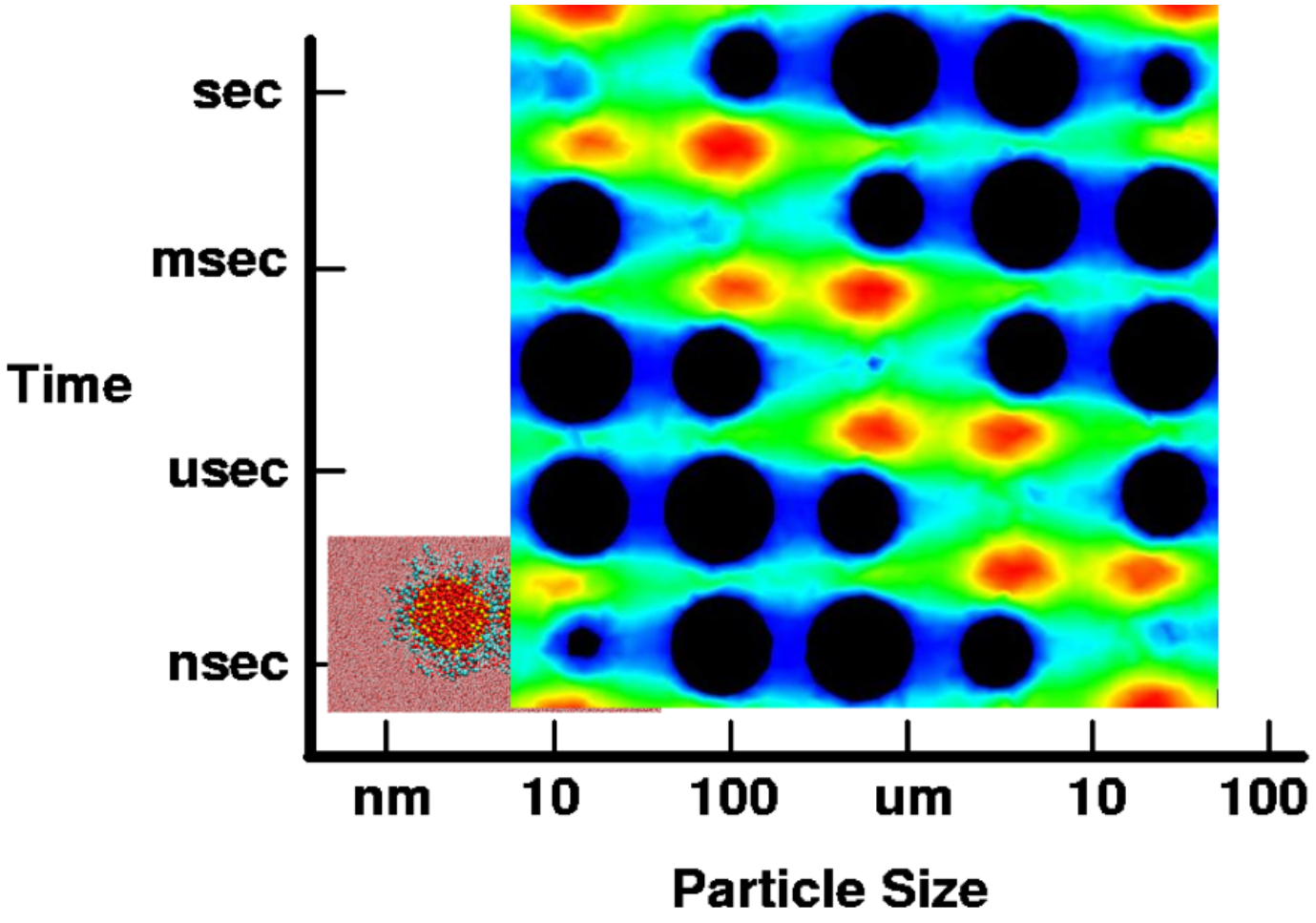
Length and time scales



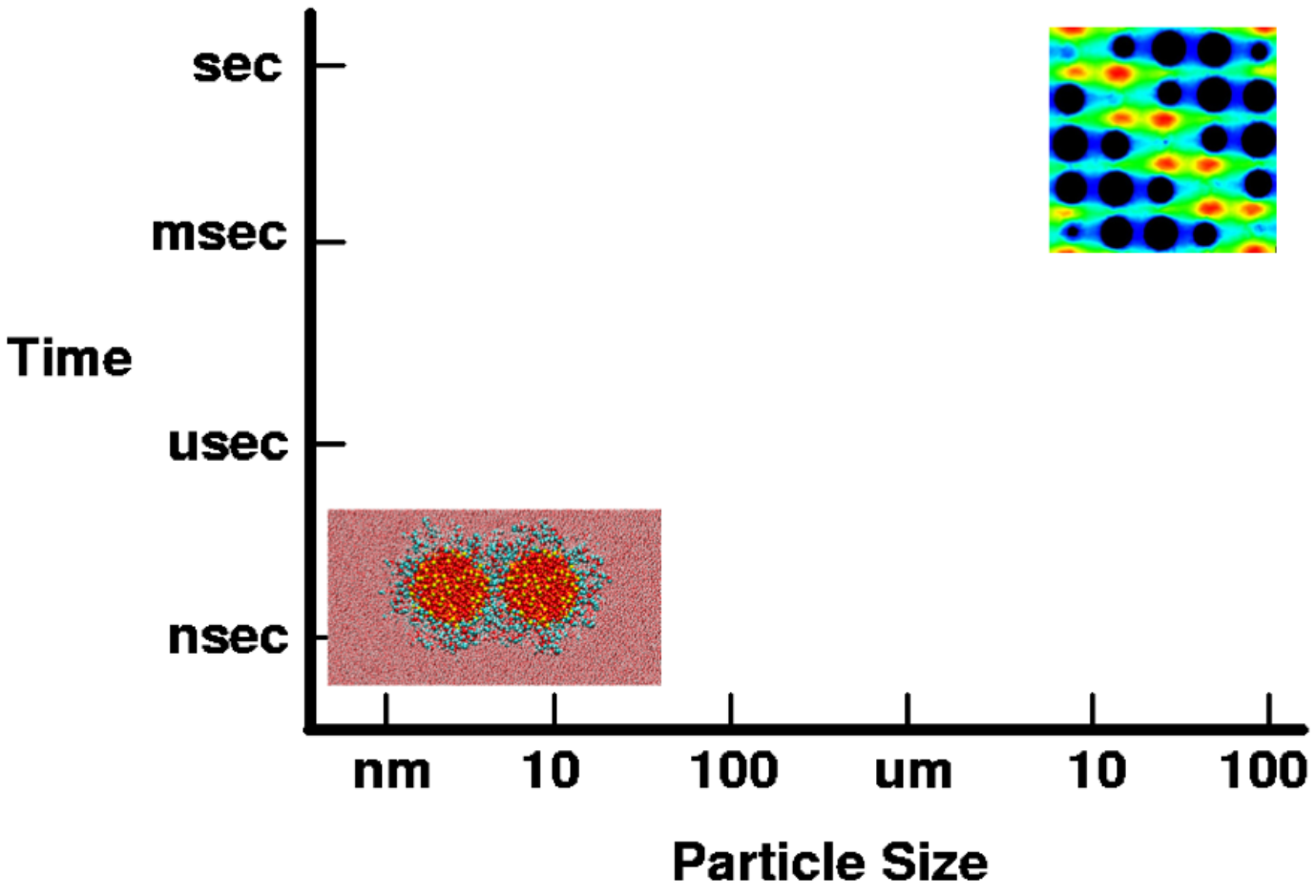
Length and time scales



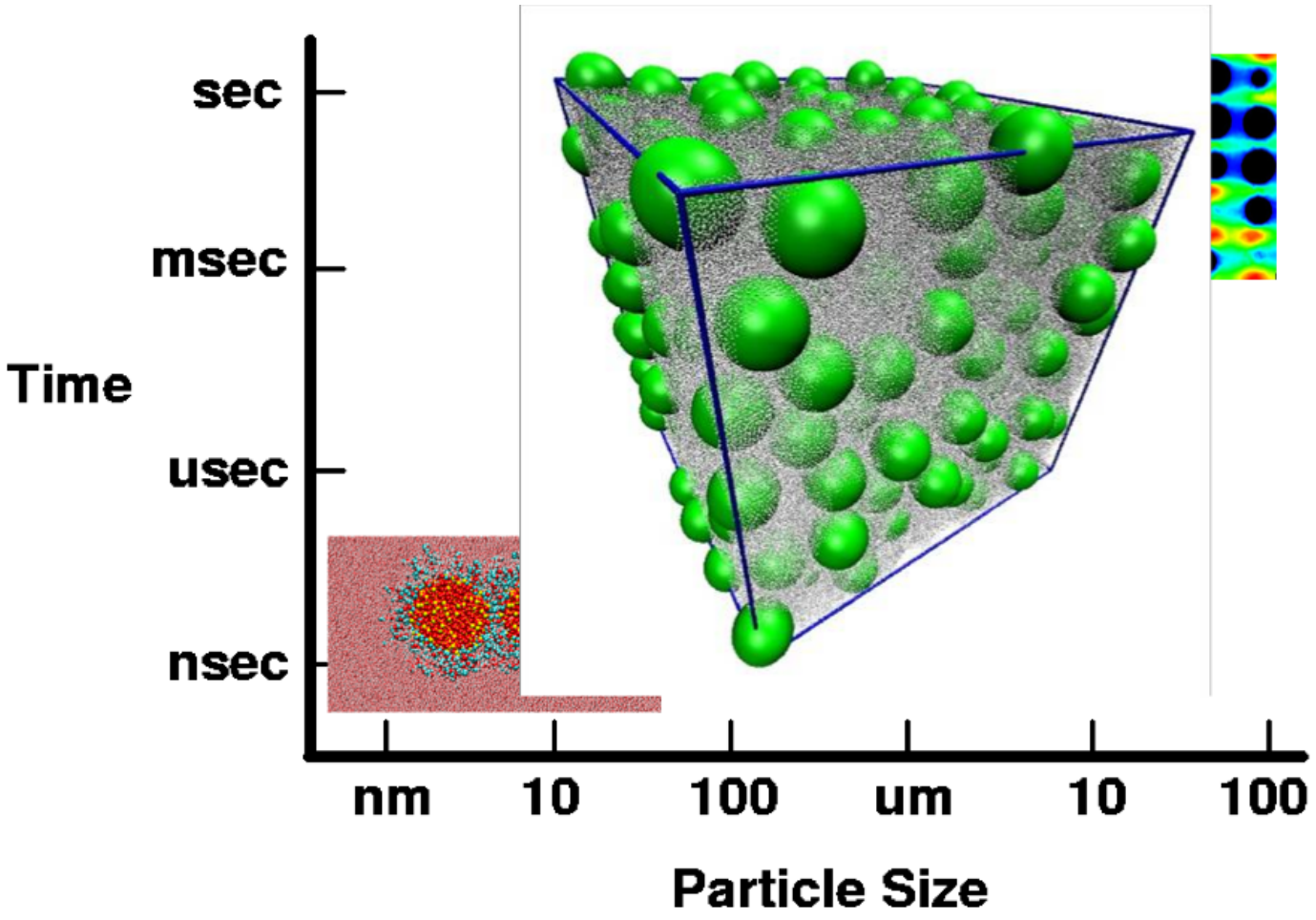
Length and time scales



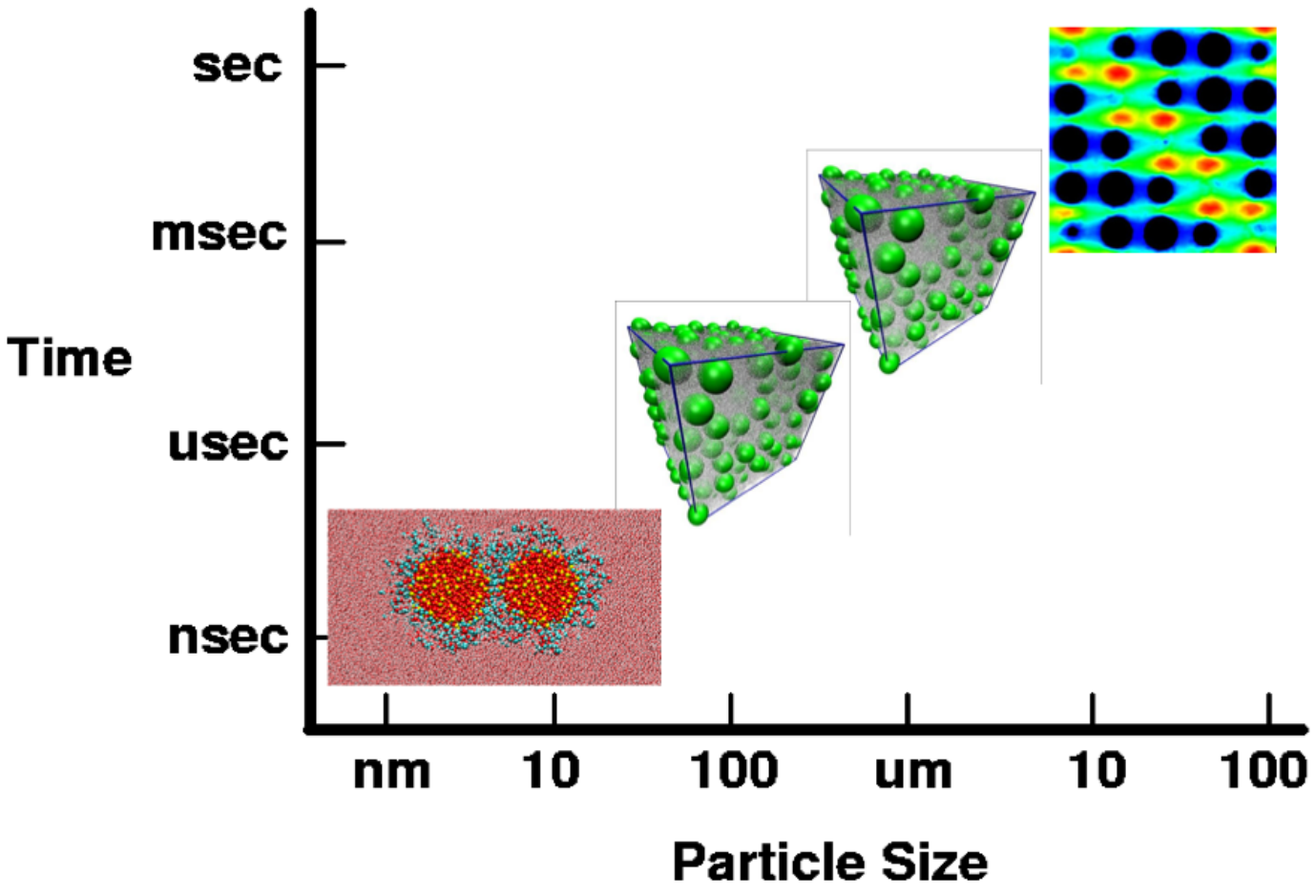
Length and time scales



Length and time scales

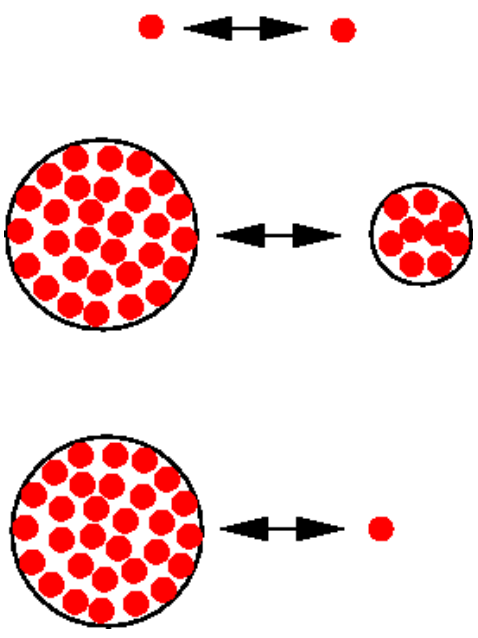


Length and time scales



Coarse-grained nanoparticle interactions

- Integrated LJ potential over volume of nanoparticle
  Everaers (PRE 2003)



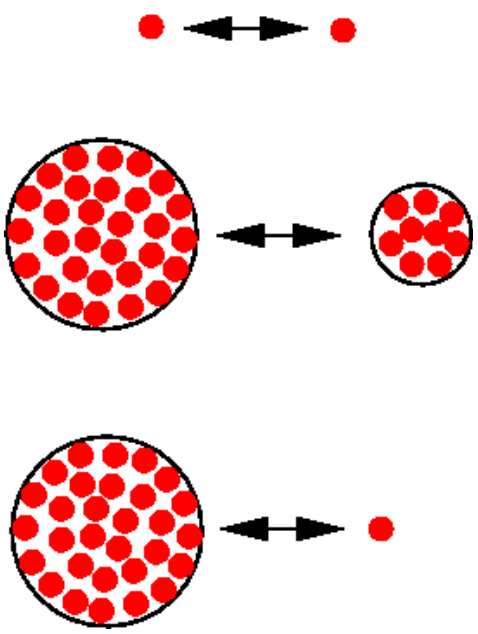
$$U_A = -\frac{A_{cc}}{6}\left[\frac{2a_1a_2}{r^2-(a_1+a_2)^2}+\frac{2a_1a_2}{r^2-(a_1-a_2)^2}+\ln\left(\frac{r^2-(a_1+a_2)^2}{r^2-(a_1-a_2)^2}\right)\right]$$

$$\begin{aligned} U_R = \frac{A_{cc}}{37800}\frac{\sigma^6}{r}\Bigg[& \frac{r^2-7r\,(a_1+a_2)+6\,(a_1^2+7a_1a_2+a_2^2)}{(r-a_1-a_2)^7} \\ & +\frac{r^2+7r\,(a_1+a_2)+6\,(a_1^2+7a_1a_2+a_2^2)}{(r+a_1+a_2)^7} \\ & -\frac{r^2+7r\,(a_1-a_2)+6\,(a_1^2-7a_1a_2+a_2^2)}{(r+a_1-a_2)^7} \\ & -\frac{r^2-7r\,(a_1-a_2)+6\,(a_1^2-7a_1a_2+a_2^2)}{(r-a_1+a_2)^7}\Bigg] \end{aligned}$$

$$U = U_A + U_R, \qquad r < r_c$$

Coarse-grained nanoparticle interactions

- Integrated LJ potential over volume of nanoparticle
  Everaers (PRE 2003)



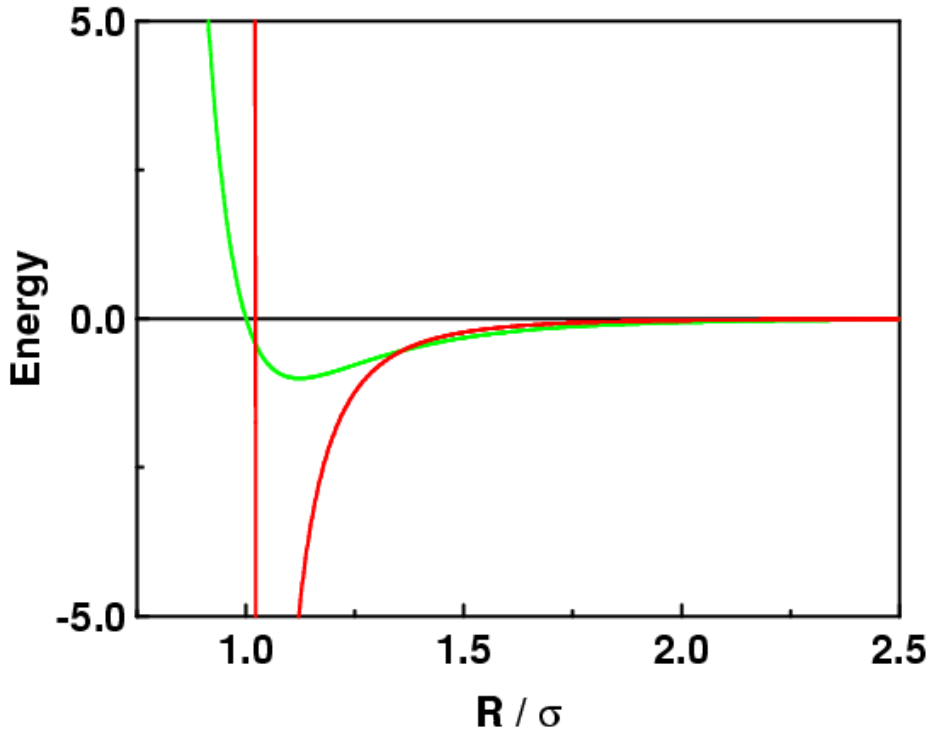
$$U_A = -\frac{A_{cc}}{6}\left[\frac{2a_1a_2}{r^2-(a_1+a_2)^2}+\frac{2a_1a_2}{r^2-(a_1-a_2)^2}+\ln\left(\frac{r^2-(a_1+a_2)^2}{r^2-(a_1-a_2)^2}\right)\right]$$

$$\begin{aligned} U_R = \frac{A_{cc}}{37800}\frac{\sigma^6}{r}\Bigg[& \frac{r^2-7r\,(a_1+a_2)+6\,(a_1^2+7a_1a_2+a_2^2)}{(r-a_1-a_2)^7} \\ & +\frac{r^2+7r\,(a_1+a_2)+6\,(a_1^2+7a_1a_2+a_2^2)}{(r+a_1+a_2)^7} \\ & -\frac{r^2+7r\,(a_1-a_2)+6\,(a_1^2-7a_1a_2+a_2^2)}{(r+a_1-a_2)^7} \\ & -\frac{r^2-7r\,(a_1-a_2)+6\,(a_1^2-7a_1a_2+a_2^2)}{(r-a_1+a_2)^7}\Bigg] \end{aligned}$$

$$U = U_A + U_R, \qquad r < r_c$$

- Pairwise and analytic (albeit expensive), Hamaker constant, similar formulation for ellipsoids

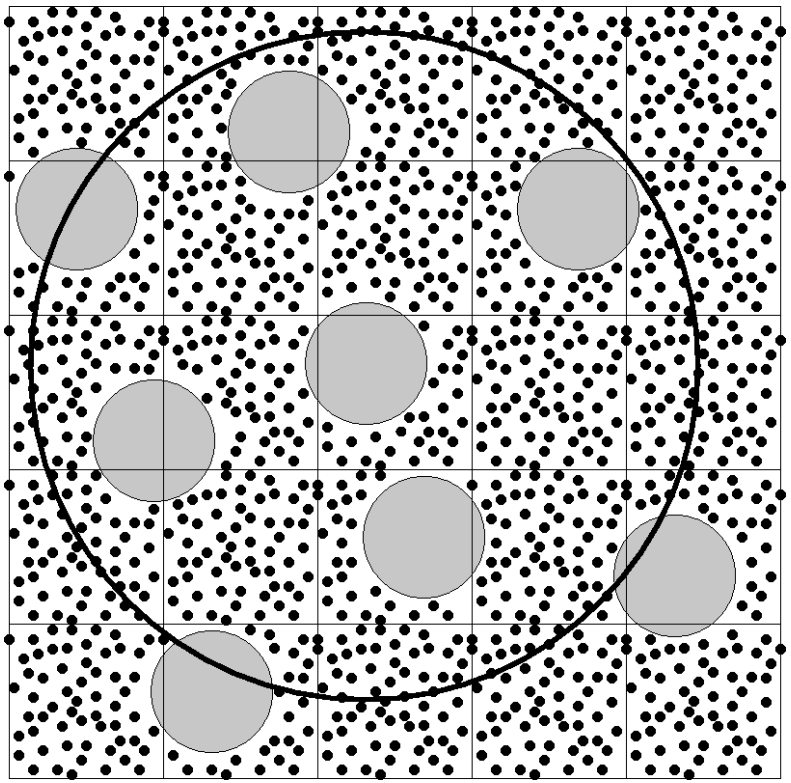
Colloid/colloid forces are now long-range



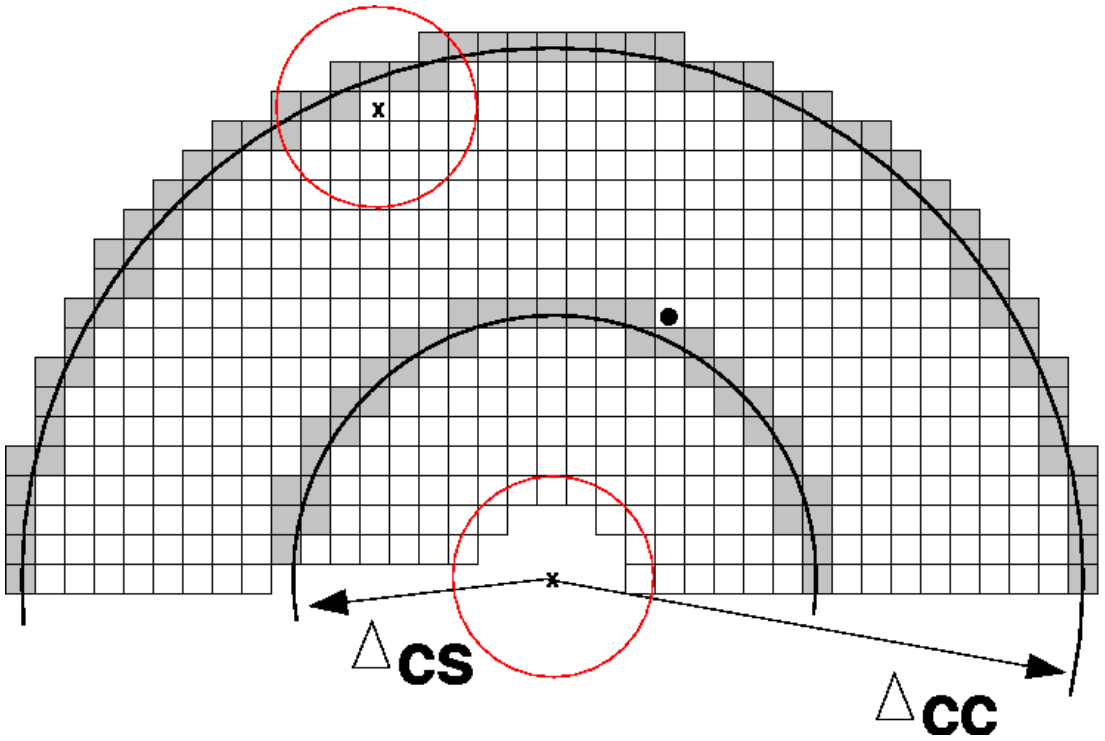
- Distance is plotted in particle diameters
- For colloid/solvent size ratio of 20:1, LJ cutoff of 2.5 sigma translates to: colloid/colloid cutoff = 50 sigma, colloid/solvent cutoff = 25 sigma

Finding neighbors in mixtures

- Goal: efficient Verlet lists
  - SS cutoff at 2.5
  - CS cutoff at 12.5
  - CC cutoff at 25
- Bin size = 1/2 of max cutoff
- Problem: compute R_{ij} for too many pairs
- Performance:
  0.5M particles, 100 S/C
  - 4.7 secs (pair)
  - 242 secs (neighbor)
  - 36 secs (communication)
- Exacerbated as size ratio grows



Faster neighbor finding



- Bin based on smallest cutoff
- Store 2 values with each stencil bin (closest/furthest corners)
- Only need compute R_{ij} in shaded ring/shell of bins
- Improved performance:

  4.7 secs (pair), 2.4 secs (neigh), 2.1 secs (comm)

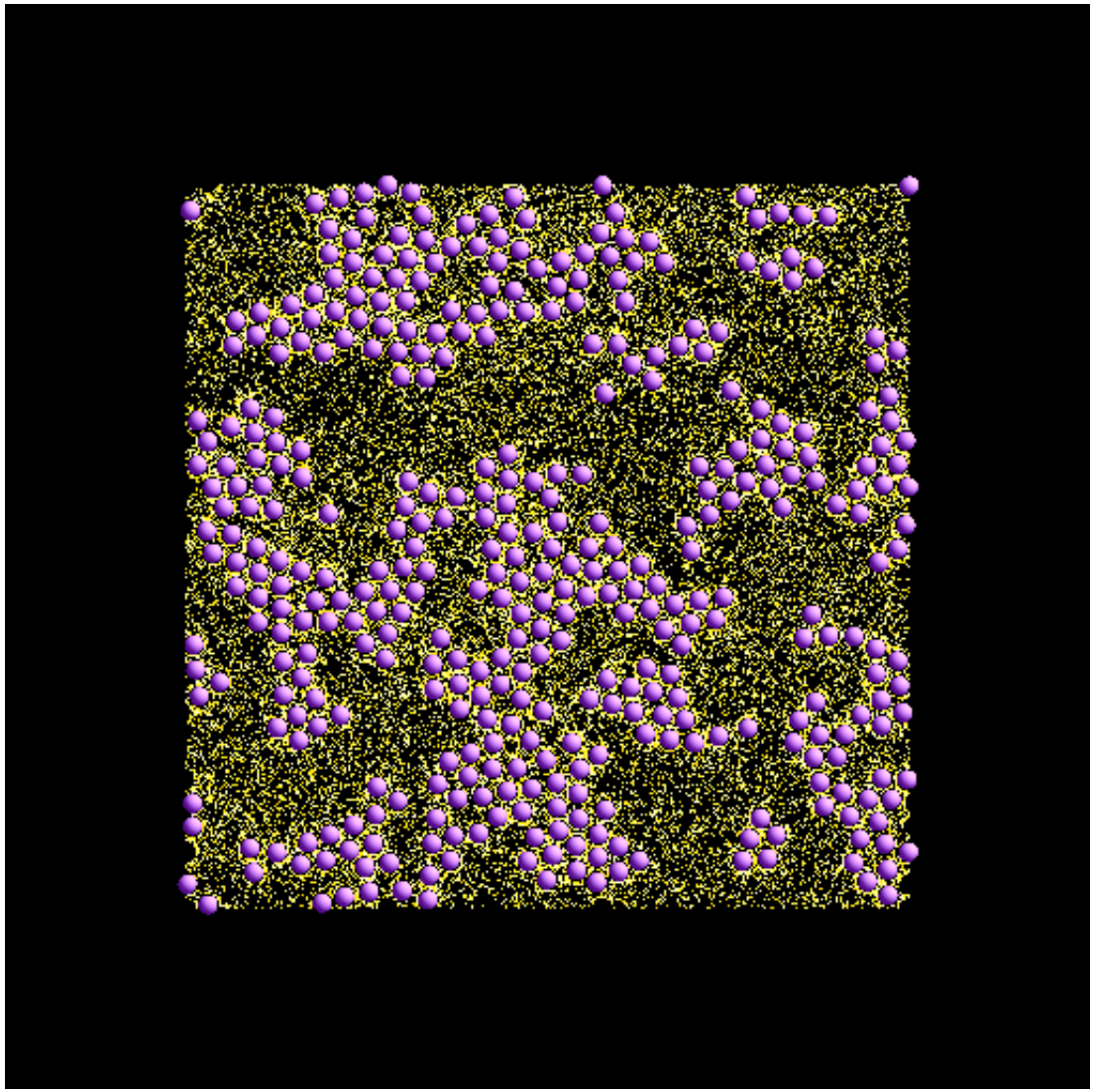
Performance improvement

3 size ratios, 3 volume fractions, CPU time for 100 steps

Ratio	P	N	old/old	new/old	new/new
5:1	27	200K	17.8	6.8	5.4
		143K	7.6	4.0	3.1
		87K	3.0	2.0	1.6
10:1	64	672K	471	19.2	11.2
		558K	284	15.9	8.2
		445K	165	11.3	5.6
20:1	125	2.3M	5630	88.6	38.6
		2.0M	4390	73.7	31.2
		1.7M	2750	56.9	22.0

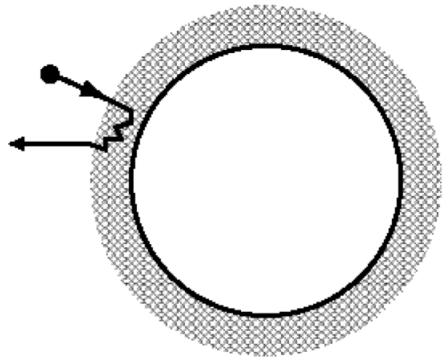
Bottom line: new algorithms as much as 100x faster

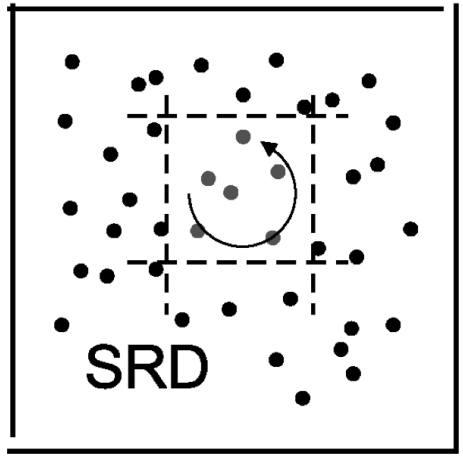
Shear of polymer chains



Further coarse graining via SRD particles

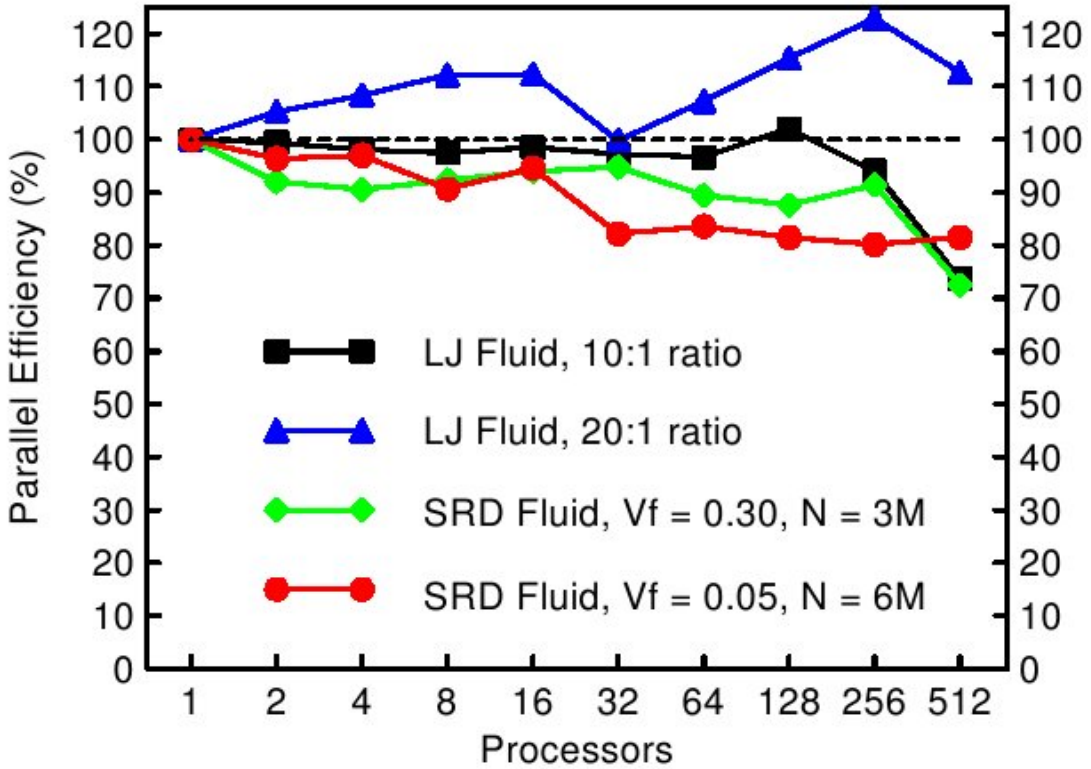
- SRD = stochastic rotation dynamics
  - *Malevanets (J Chem Phys 99), Padding (PRL 04), Hecht (PRE 05)*
  - intermediate Peclet numbers ~ 1
    Pe = ratio of advection to diffusion
- Basic idea:
  - SRDs are background solvent for colloids
  - two timescales: $t_{colloid}$ and t_{SRD}
  - small $t_{colloid}$:
    - colloids move, C/C interactions
    - SRDs advect (no self-interactions)
    - detect colloid-SRD collisions
  - large t_{SRD}:
    - bin SRDs, v is randomly rotated





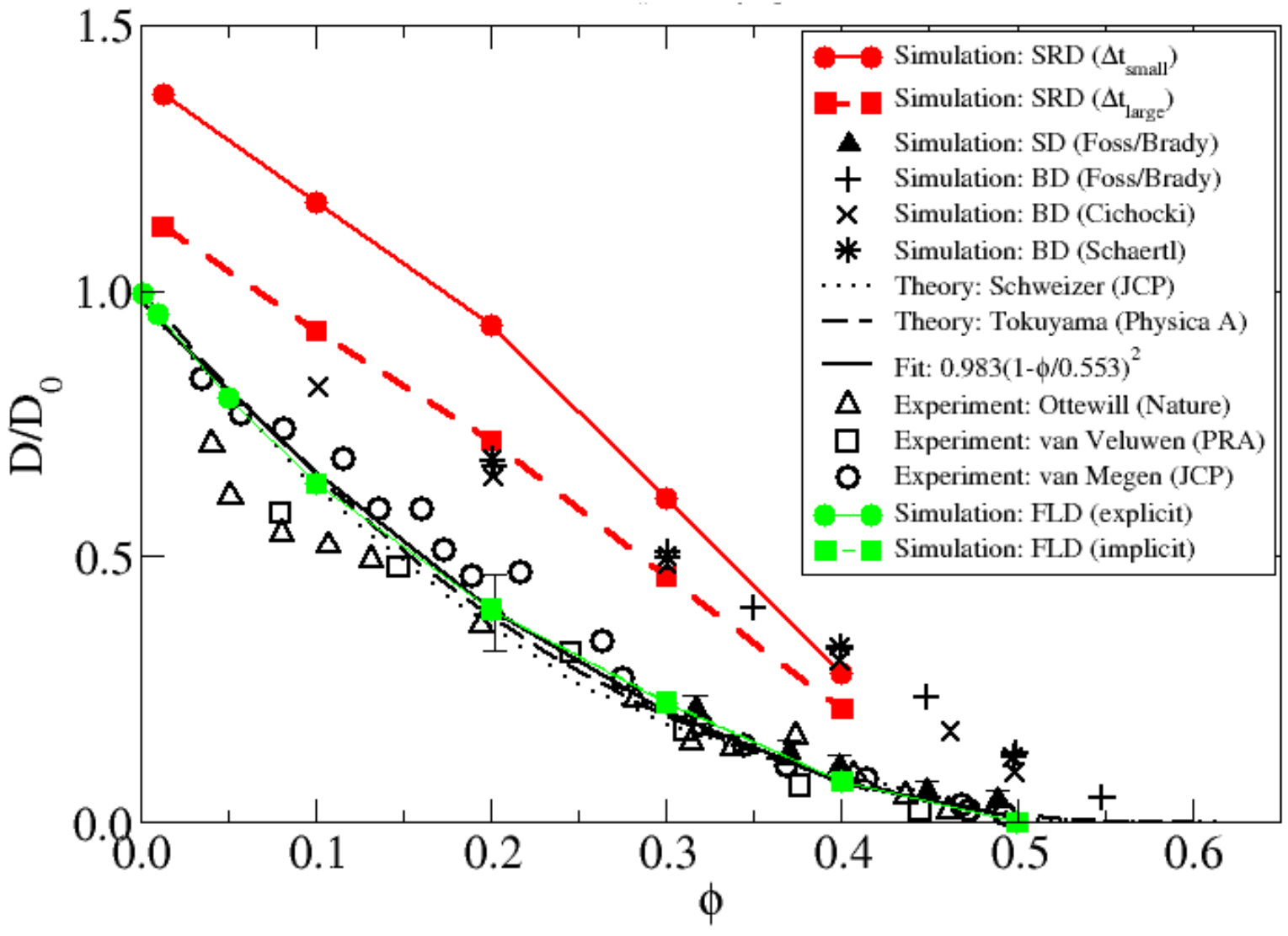
Parallel performance

- Key point: SRDs are cheap due to no S/S interactions
- Challenge: Keep them cheap when 1000s per colloid

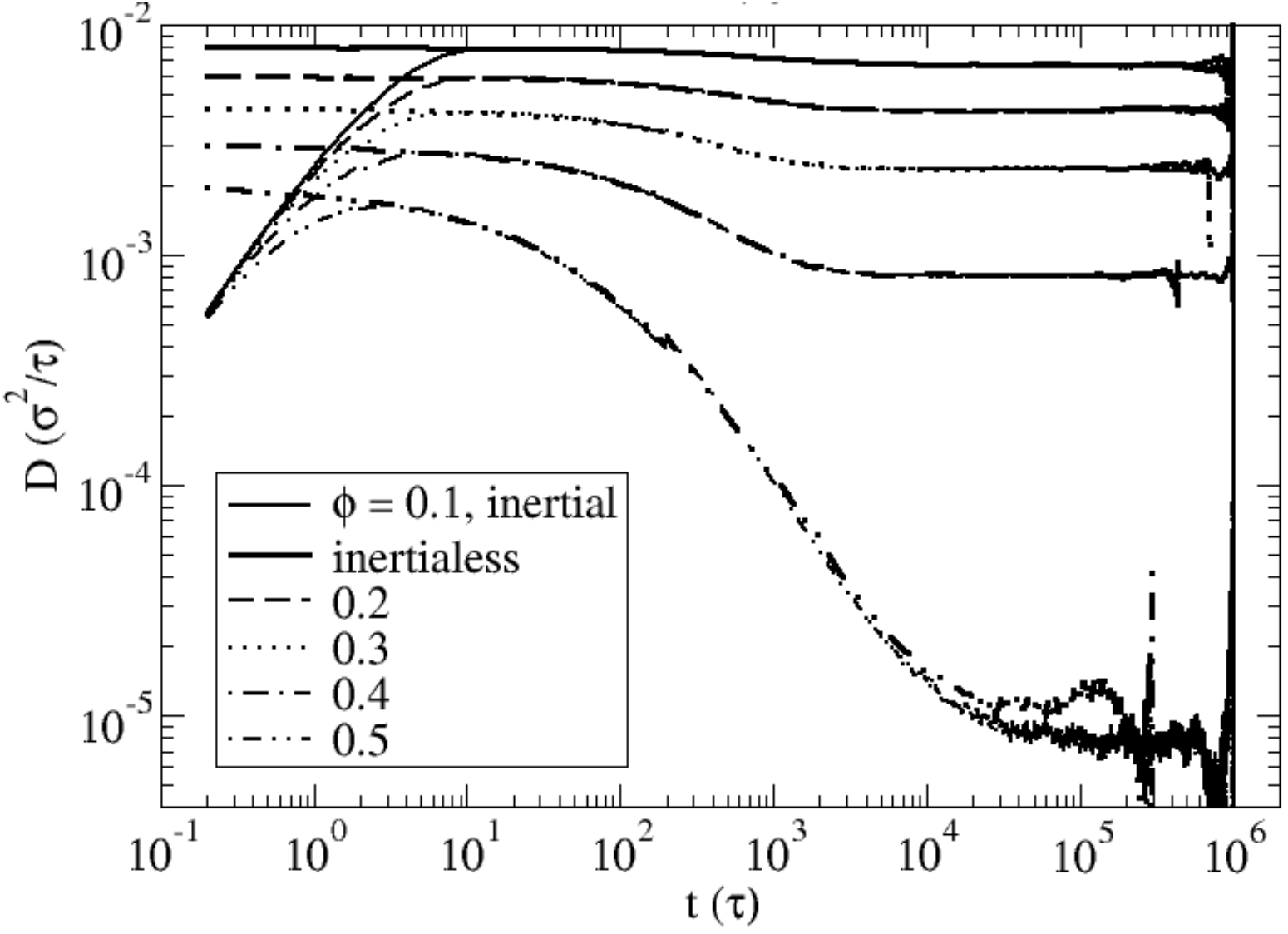


Savings vs explicit LJ solvent:
30x in speed (per particle), 20x in timestep

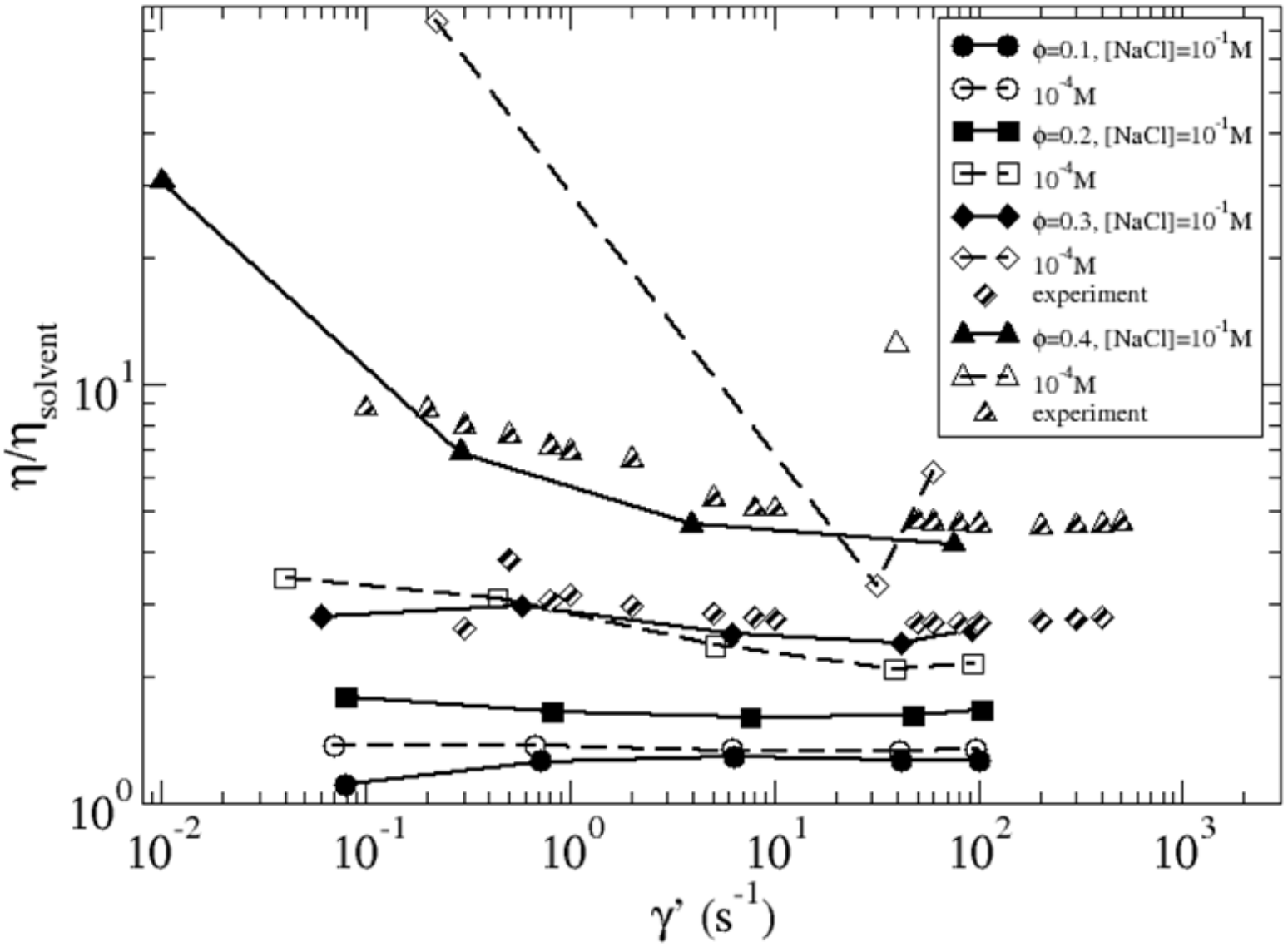
Diffusion coefficient versus volume fraction



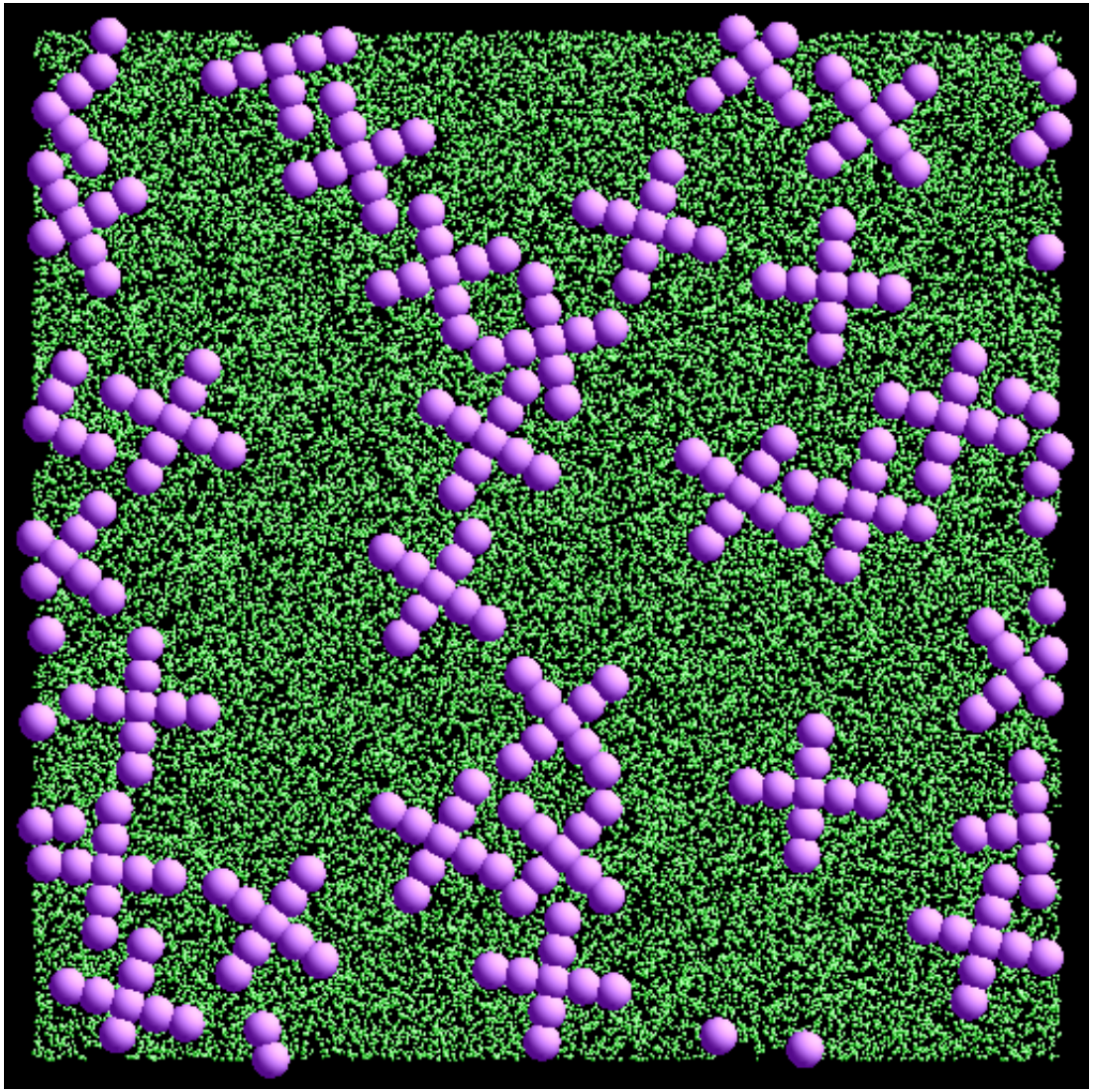
Diffusion via FLD across time scales

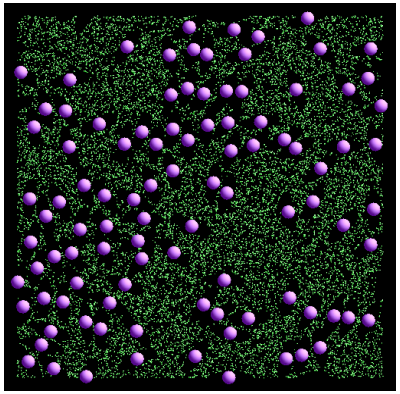


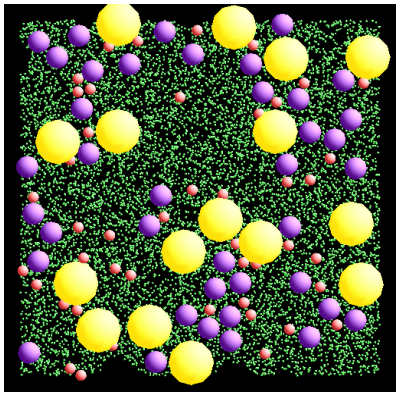
Shear viscosity for varying shear rate and volume fraction

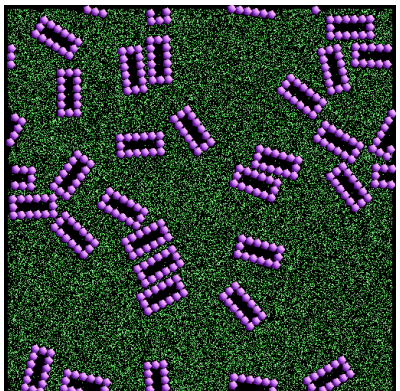


Composite aspherical particles

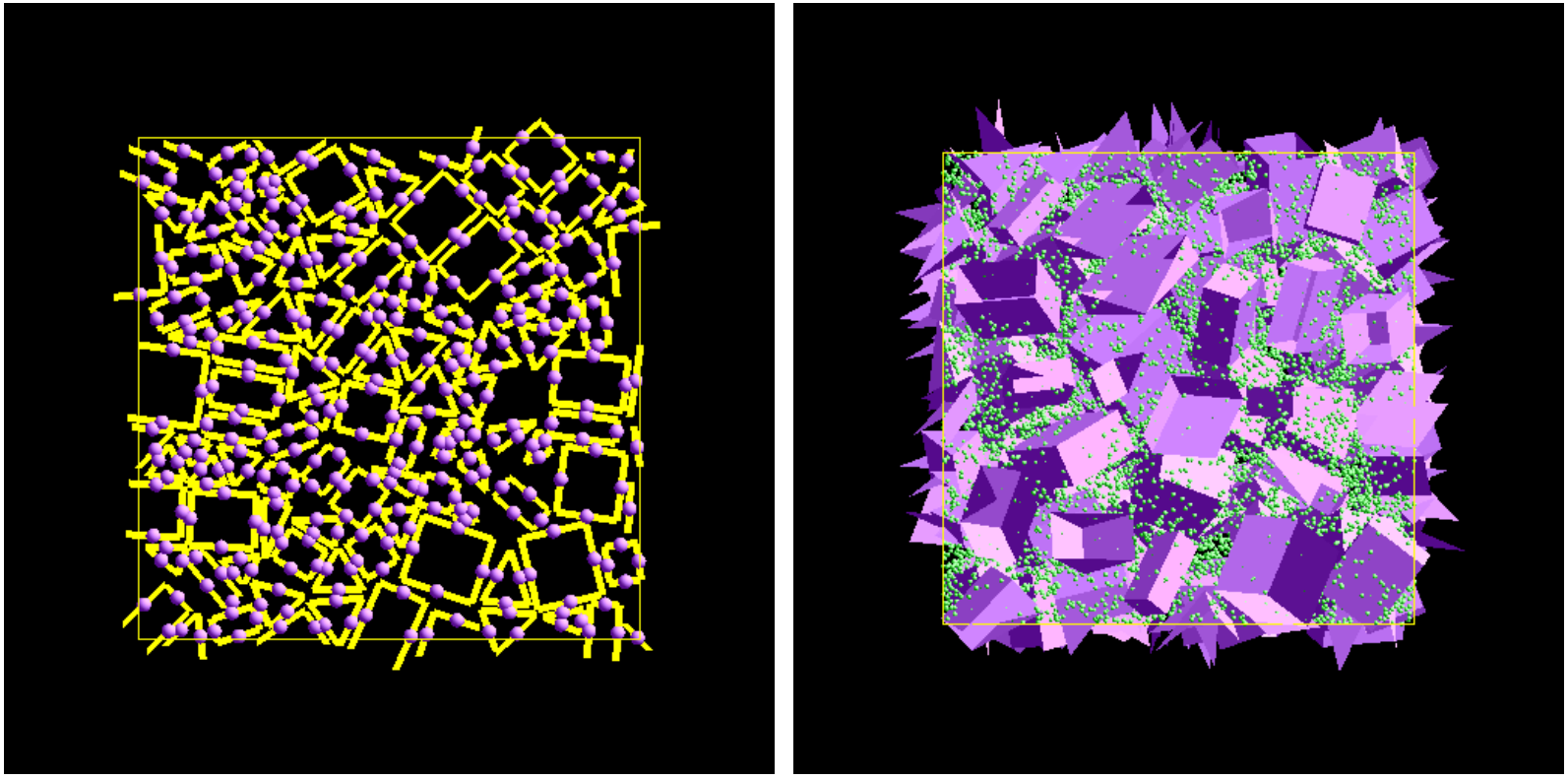




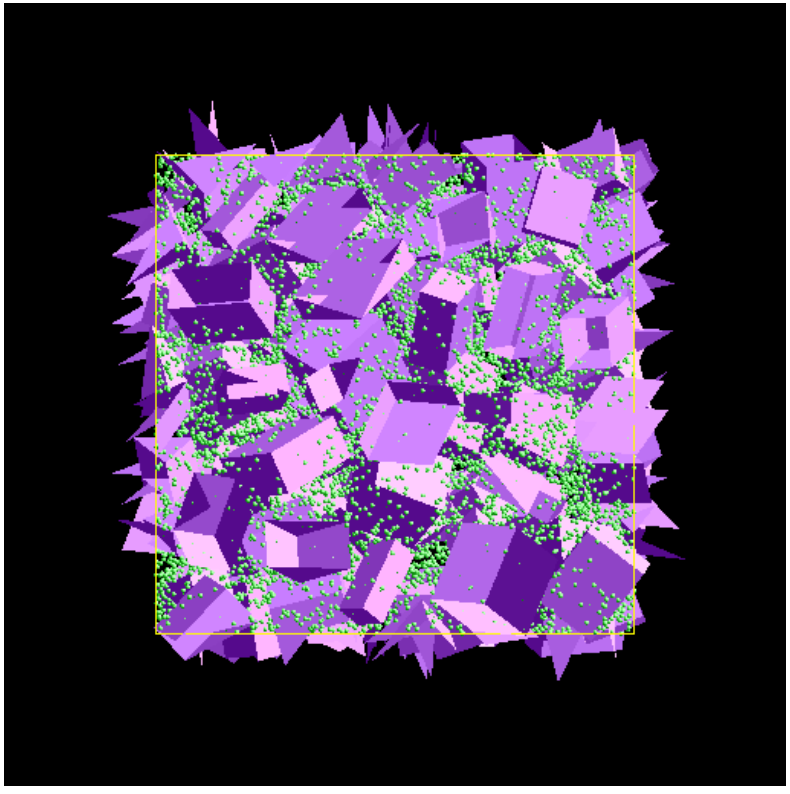


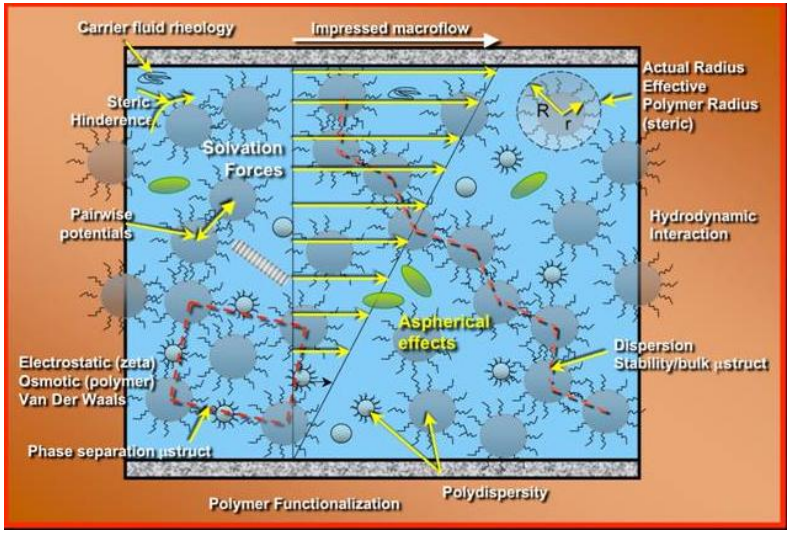


Generalized aspherical particles (2d and 3d)



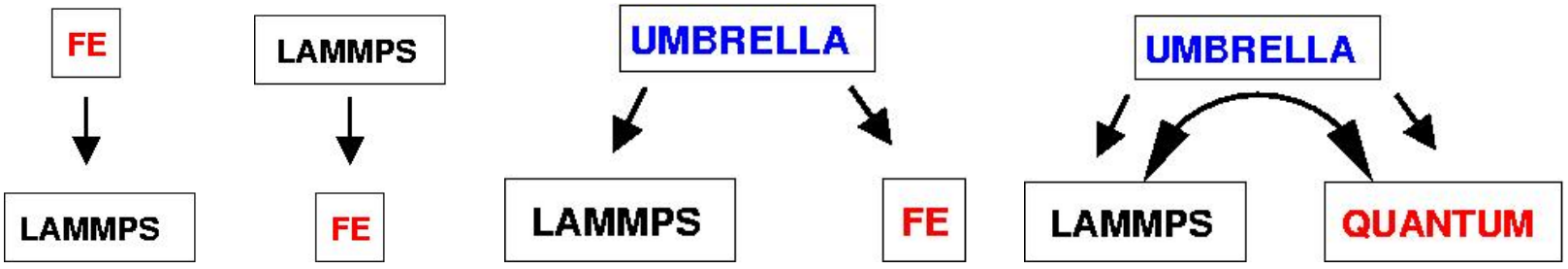
Generalized aspherical particles





Other mesoscale/continuum methods in LAMMPS:
FLD, DPD, SPH, Peridynamics, DEM (granular)

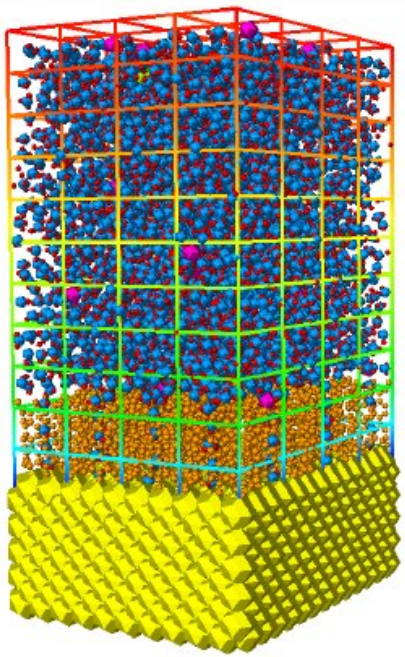
Examples of MD in multi-scale context



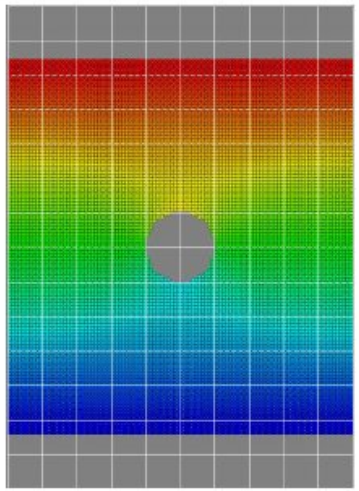
- MD + DFT: dynamics with quantum forces
- MD + FE: thermal/mechanical coupling to continuum
- MD + Navier-Stokes: fluidized granular bed
- MD + Navier-Stokes: flowing biomolecules
- MD + off-lattice kinetic MC: defect dynamics in solids
- MD + on-lattice kinetic MC: stress-driven grain growth

AtC: Atomistic to Continuum coupling

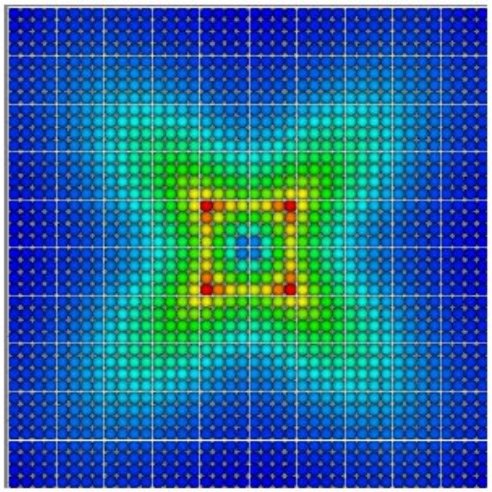
Reese Jones, Jon Zimmerman, Jeremy Templeton, Greg Wagner (Sandia)



Saltwater-electrode-CNT system: mesh overlaps exactly with water-CNT atom region



Circular hole in plate: mesh overlaps exactly with box, but atom region is subset

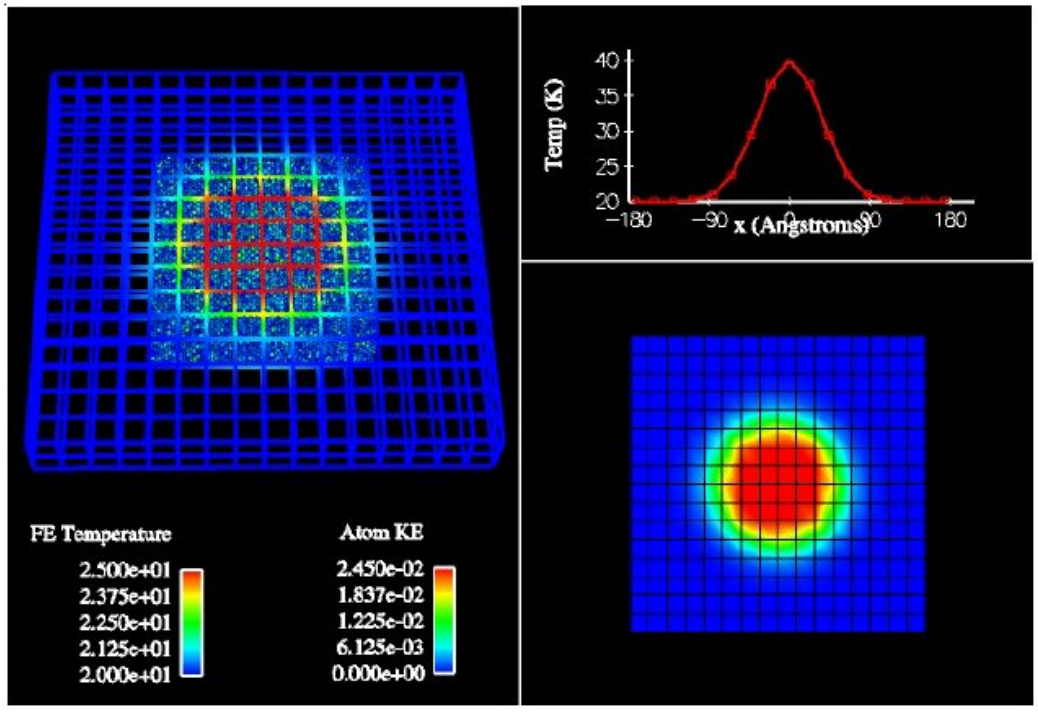


Elastic inclusion problem: mesh overlaps exactly with box and atoms

Particles in parallel, FE solution in serial

Thermal coupling with AtC package

2D diffusion problem

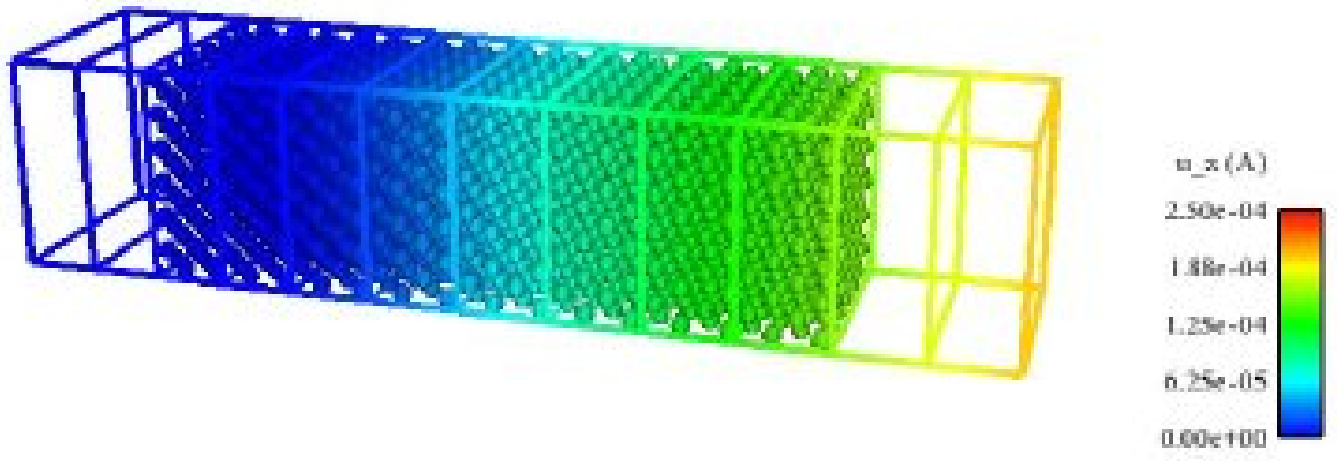


- Plate with embedded MD region (~33,000 atoms)
- Initialized to temperature field with gaussian profile
- Adiabatic boundary conditions at edges

Sandia National Laboratories

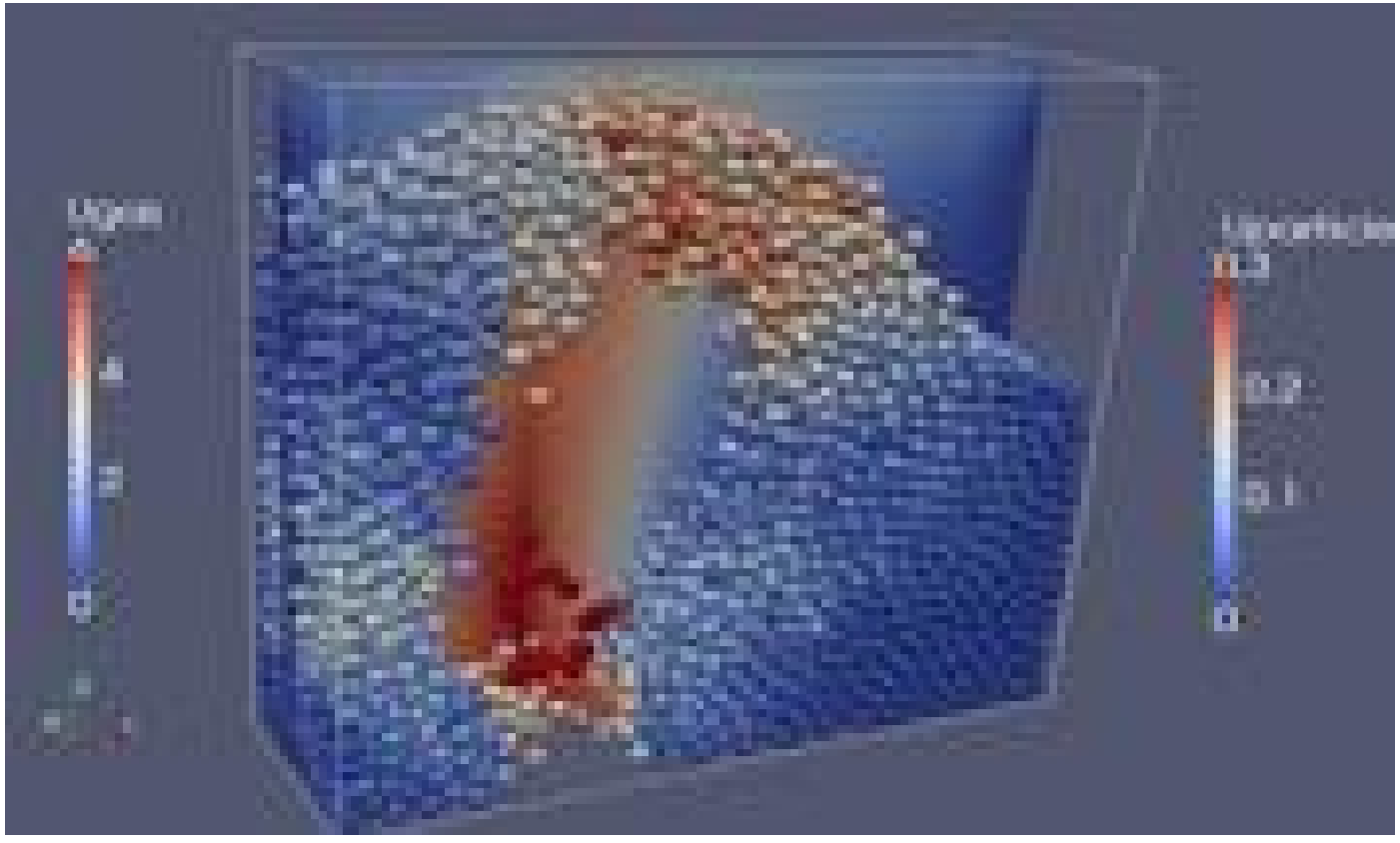
Mechanical coupling with AtC package

Elasto-dynamic response:



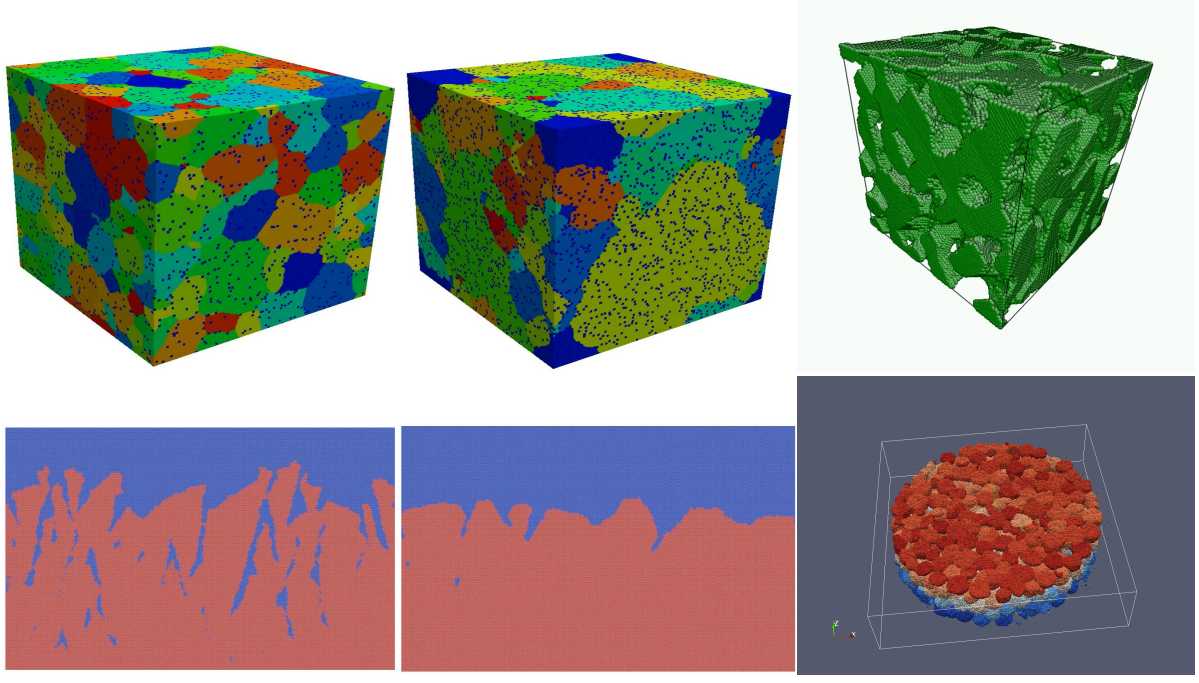
Granular materials + fluids via OpenFoam

Christoph Kloss (JKU) and LIGGGHTS package
www.liggghts.com/www.cfdem.com



Materials modeling via on-lattice KMC

- Variety of models for time evolution of processed materials
- Length scale = atomic to mesoscale (fcc or cubic lattices)
- Time scale = microseconds to days
- Hamiltonian encodes physics of interest via local interactions

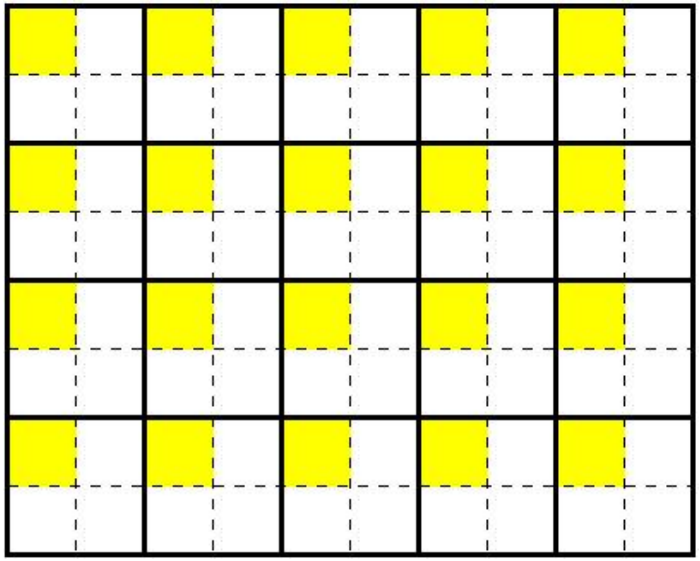


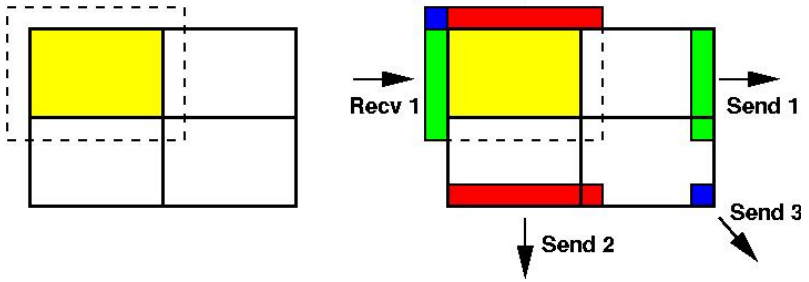
Parallel approximate KMC algorithm

- Adapted from semi-rigorous synchronous sub-lattice idea
  Shim & Amar, Phys Rev B 71, 125432 (2005)

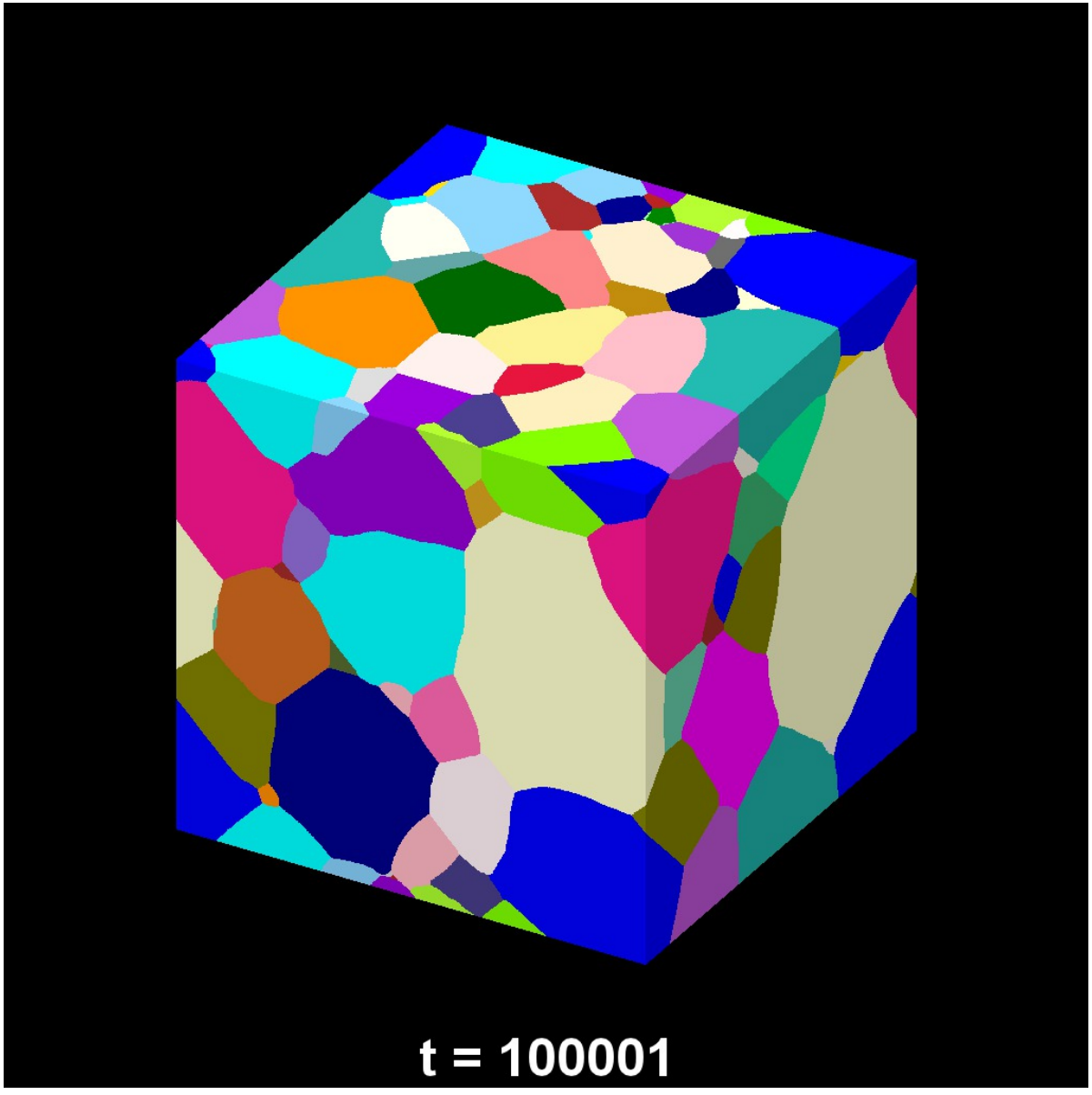
Parallel approximate KMC algorithm

- Adapted from semi-rigorous synchronous sub-lattice idea
  Shim & Amar, Phys Rev B 71, 125432 (2005)
- Split domain into sub-domains and sectors: 4 in 2d, 8 in 3d
- Each processor works on same sector at same time
- KMC chooses site, sites can have multiple events
- Alternate KMC within sector, comm of boundary sites



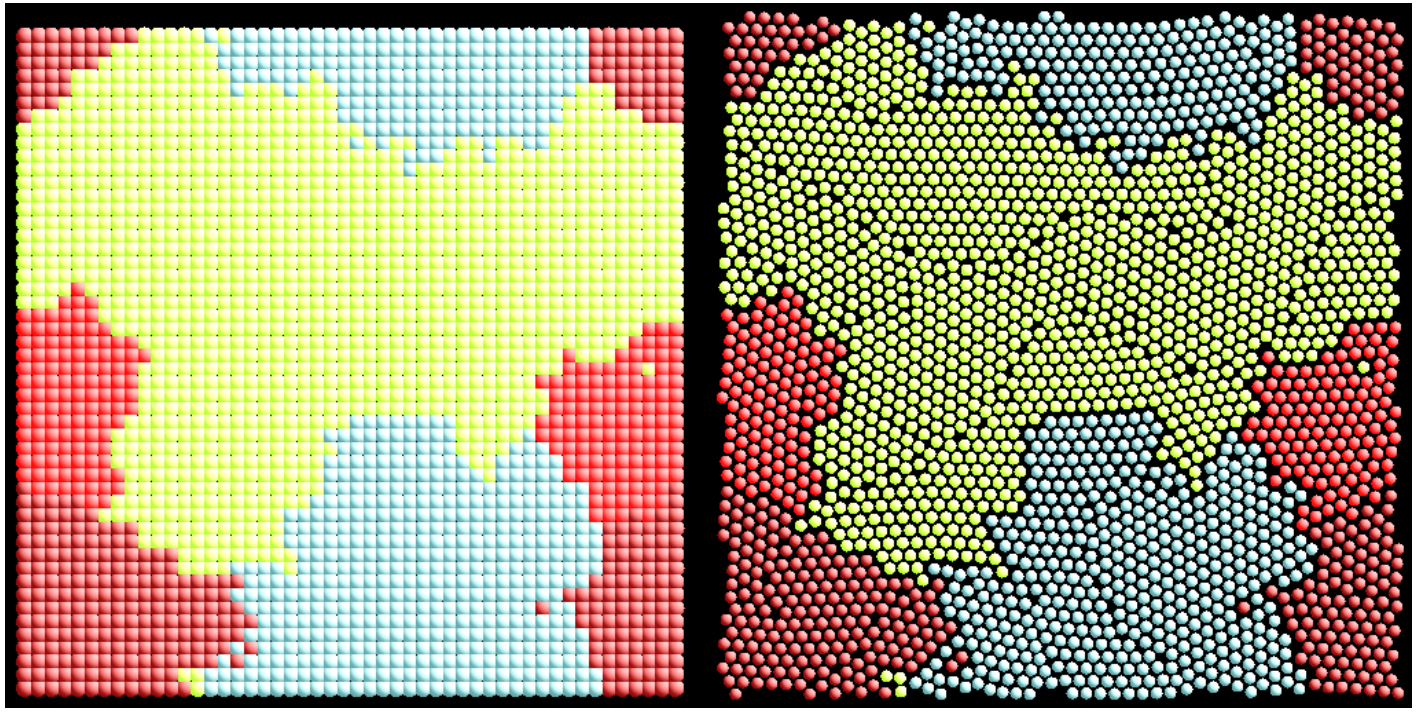


Microstructural evolution: normal grain growth



MD + kMC for stress-driven grain growth

- SPPARKS (kMC) runs Potts model for grain growth
  - Hamiltonian includes stress term
  - send grain structure to LAMMPS
- LAMMPS (MD) treats particles at grain boundary as larger
  - relaxes system
  - send per-particle stress to SPPARKS

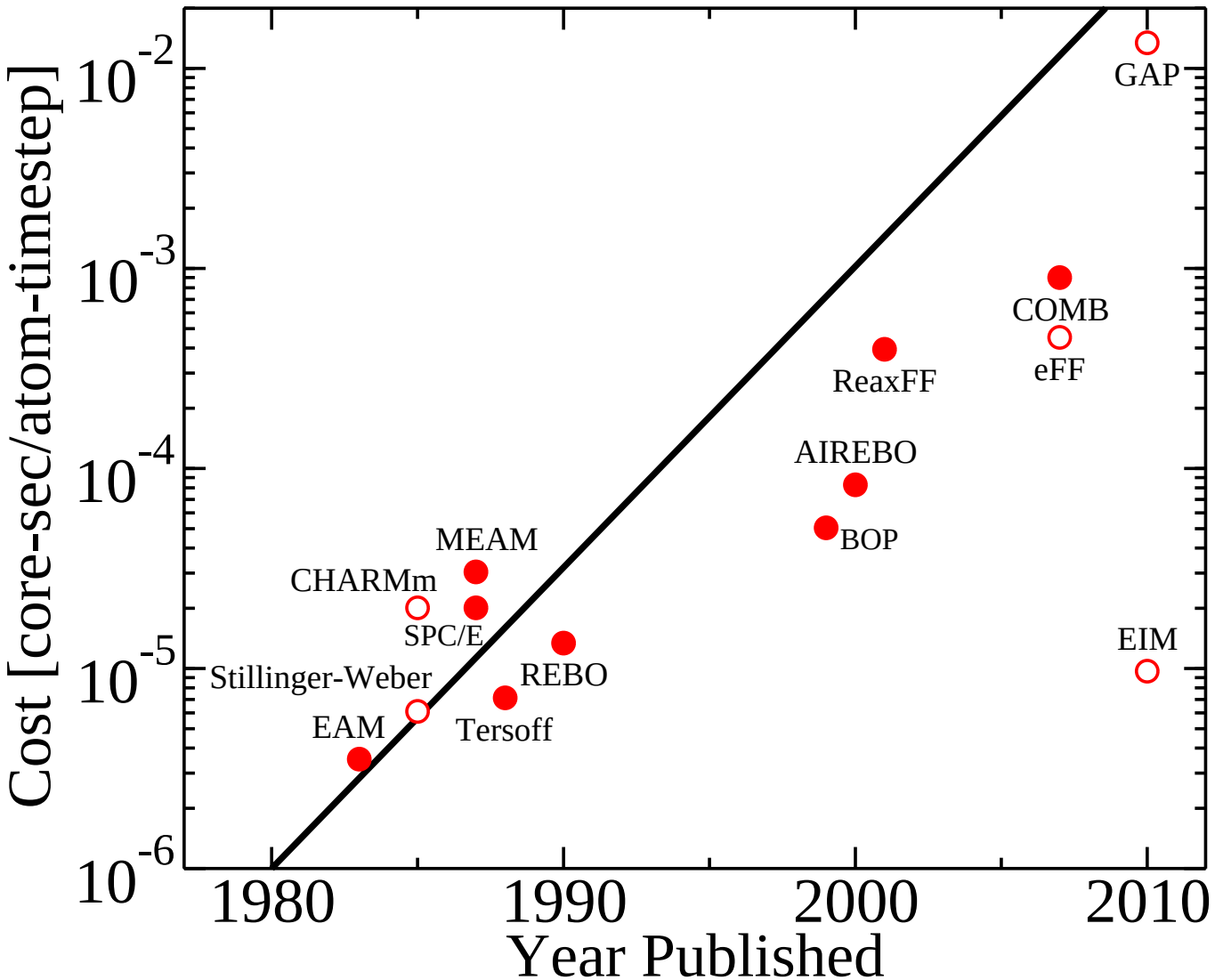


Empirical potentials are getting more expensive!

See lammps.sandia.gov/bench.html#potentials

Potential	System	Atoms	Timestep	CPU	LJ Ratio
Granular	chute flow	32000	0.0001 tau	5.08e-7	0.34x
FENE bead/spring	polymer melt	32000	0.012 tau	5.32e-7	0.36x
Lennard-Jones	LJ liquid	32000	0.005 tau	1.48e-6	1.0x
DPD	pure solvent	32000	0.04 tau	2.16e-6	1.46x
EAM	bulk Cu	32000	5 fmsec	3.59e-6	2.4x
Tersoff	bulk Si	32000	1 fmsec	6.01e-6	4.1x
Stillinger-Weber	bulk Si	32000	1 fmsec	6.10e-6	4.1x
EIM	crystalline NaCl	32000	0.5 fmsec	9.69e-6	6.5x
SPC/E	liquid water	36000	2 fmsec	1.43e-5	9.7x
CHARMM + PPPM	solvated protein	32000	2 fmsec	2.01e-5	13.6x
MEAM	bulk Ni	32000	5 fmsec	2.31e-5	15.6x
Peridynamics	glass fracture	32000	22.2 nsec	2.42e-5	16.4x
Gay-Berne	ellipsoid mixture	32768	0.002 tau	4.09e-5	28.3x
AIREBO	polyethylene	32640	0.5 fmsec	8.09e-5	54.7x
COMB	crystalline SiO2	32400	0.2 fmsec	4.19e-4	284x
eFF	H plasma	32000	0.001 fmsec	4.52e-4	306x
ReaxFF	PETN crystal	16240	0.1 fmsec	4.99e-4	337x
ReaxFF/C	PETN crystal	32480	0.1 fmsec	2.73e-4	185x
VASP/small	water	192/512	0.3 fmsec	26.2	17.7e6
VASP/medium	CO2	192/1024	0.8 fmsec	252	170e6
VASP/large	Xe	432/3456	2.0 fmsec	1344	908e6

Moore's Law for potentials



Summary of challenges

- Challenges for multiscale via parameter passing:
  - overlapping 2 methods in length/time scales
  - consistent answers from 2 methods for real materials
- Challenges for multiscale via loose coupling:
  - physics of coupling
  - not having model limited by shortest timescale

Summary of challenges

- Challenges for multiscale via parameter passing:
  - overlapping 2 methods in length/time scales
  - consistent answers from 2 methods for real materials
- Challenges for multiscale via loose coupling:
  - physics of coupling
  - not having model limited by shortest timescale

- General challenge:
  - Reaching experimental length/time scales

Thanks

- DOE and NINE funding
- CRADA with Corning, 3M, BASF
- Joint work with:
  Aidan Thompson, Flint Pierce, Jeremy Lechman, Gary Grest,
  Randy Schunk (Sandia), Pieter in't Veld (BASF)

- LAMMPS (MD): lammps.sandia.gov
- SPPARKS (kMC): www.sandia.gov/~sjplimp/spparks.html
- WWW sites have paper citations