Coarse-graining breakout session

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Outline

Meso/macroscopic models in LAMMPS

- *Contributed talk: Svetoslav Nikolov*

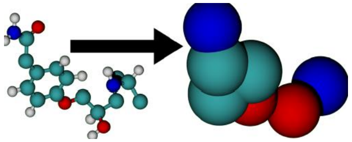
  "Modeling non-linear micromechanics
  of hydrogels using dissipative particle dynamics"
- DPD, SPH, SMD
- Hydrodynamics: SRD, Lattice Boltzmann, FLD, Mango-Selm, …
- Granular
- Peridynamics

Molecular <u>and</u> macroscopic:

- USER-ATC package

'Detailed' MD to coarse-grained MD

- Iterative Boltzmann, force matching, …
- Tools: VOTCA, fix mscg, PyCGTOOL, Auto_MARTINI
- CG force fields: MARTINI, USER-ELBA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1. Graham et al, J Chem Info Modeling 2017; 2.

Meso/macroscopic models in LAMMPS

"Top-down" : particles are simply a numerical device for solving governing physics

→ typically mass, momentum conservation, i.e. fluid dynamics (NS)

→ many other physics also possible

DPD:

See George Karniadakis talk! → **USER-MESO**

See Tim Mattox talk! → USER-DPD: NPT, NPH, equation of state → includes chemical reaction

pair_style dpd: 'plain vanilla' DPD

pair_style dpd/tstat: apply pairwise DPD thermostat to any pair-style

angular-momentum conserving variant?

SPH:

Definitely not 'physical' particles, just a Lagrangian solver of continuum equations!

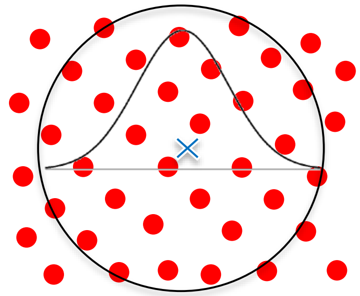
USER-SPH, USER-SMD (mitigates 'tensile instabilities')

iSPH – implicit time-stepping, coupled to Trilinos

Trask, Nathaniel, et al. *Comp Meth Appl Mech Eng* 2015

Related methods:

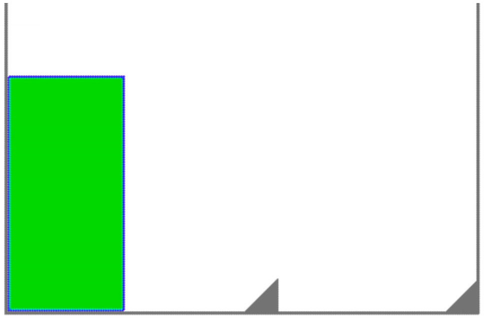
SDPD: 'thermostatted' SPH, i.e. solver for fluctuating hydrodynamics (Espanol and Revenga, PRE 2003)

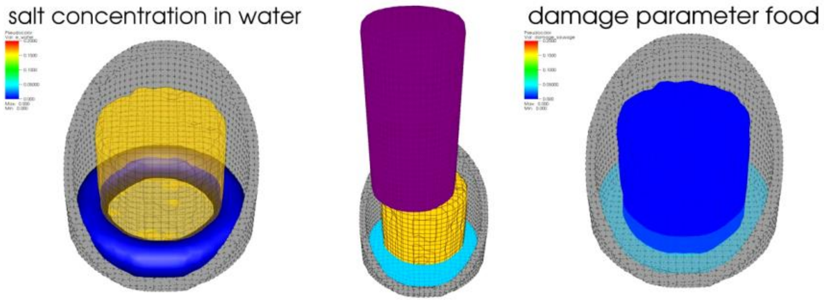


$$f(\mathbf{r}) \approx \sum \frac{m_j}{\rho_j} f(\mathbf{r}_j) W(|\mathbf{r} - \mathbf{r_j}|; h)$$

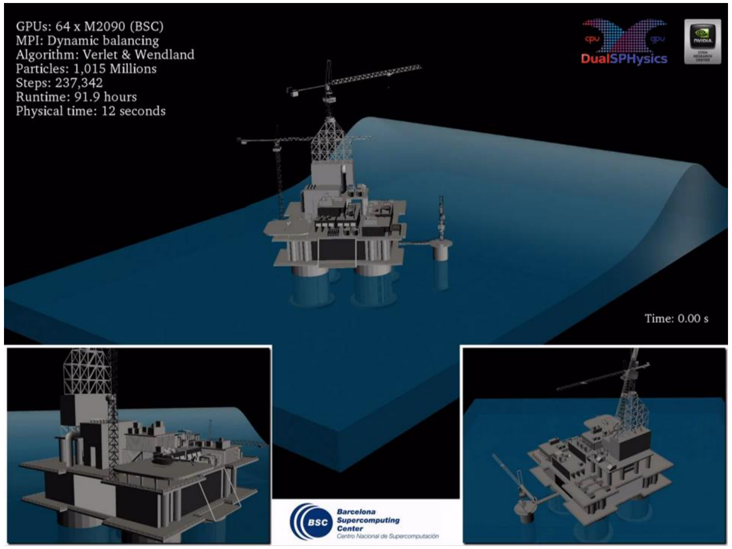
SPH gallery

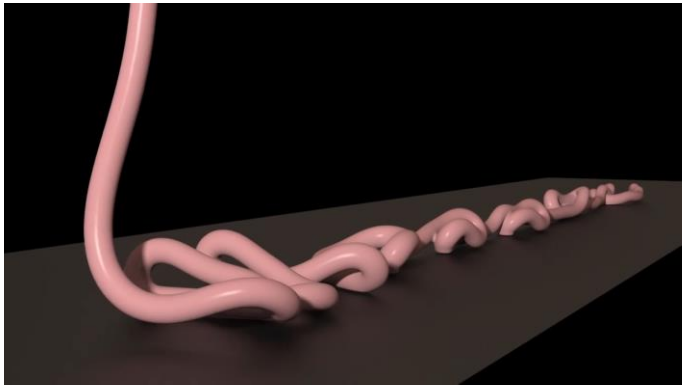
USER-SPH (Georg Ganzenmuller):



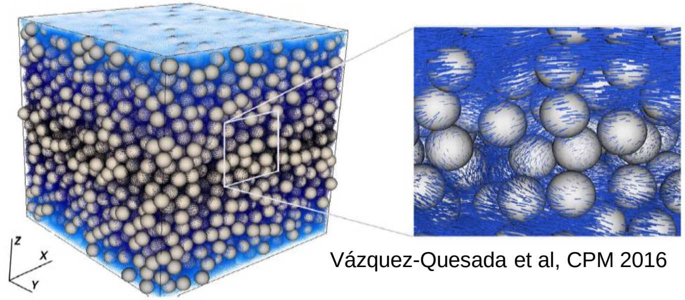


DualSPHysics:





Hydrodynamics in colloidal suspensions

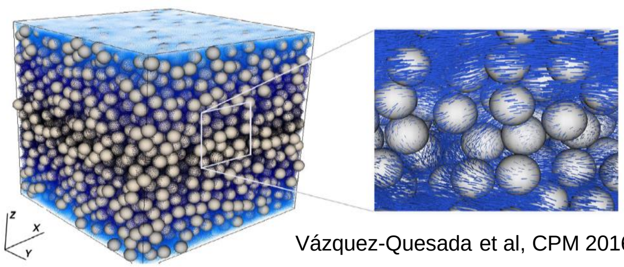


Vázquez-Quesada et al, CPM 2016

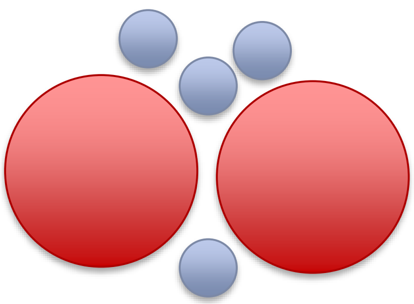
Colloid particles macroscopic ~1 micron: COLLOID package, fix nve/sphere
Solvent: (fluctuating) hydrodynamics!

- Particle methods (DPD, etc.)
- Lattice Boltzmann (USER-LB), stochastic rotation dynamics (SRD)
- FLD: simplified version of Stokesian dynamics
- MANGO-SELM: Atzberger group; solvers of fluctuating hydrodynamics

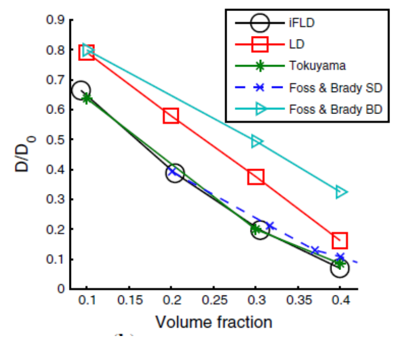
Hydrodynamics in colloidal suspensions



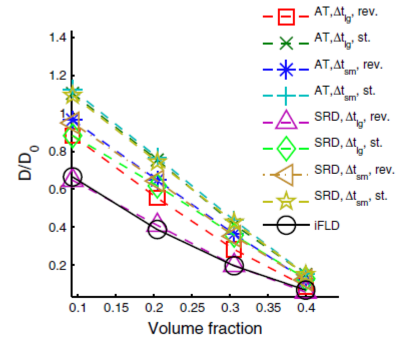
Vázquez-Quesada et al, CPM 2016



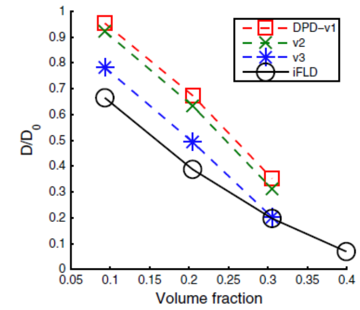
Dynamics



FLD

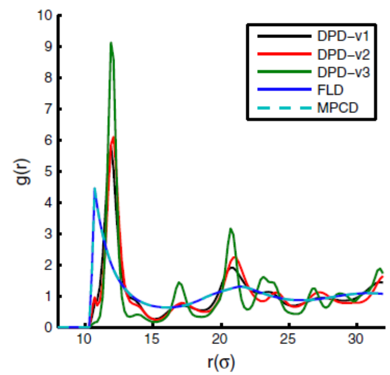


SRD/MPCD



DPD*

Structure



Bolintineanu et al, CPM 2014

All particle methods suffer from:

- Compressibility (not a big deal)
- ‘Lubrication gap’ resolution problems
- Boundary conditions can be tricky

Implicit methods (SD, FLD):

- Limited to simple particle shapes, domain geometries
- Newtonian only

Granular

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pair gran/hertz:
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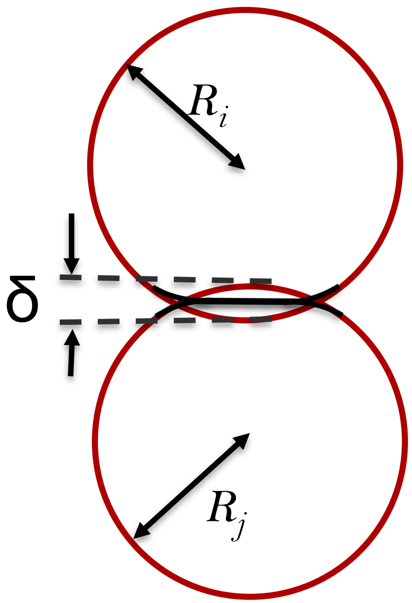
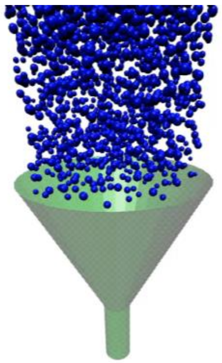
Analytical Hertz solution (1882 for normal contact force:



$$\delta = R_i + R_j - \|\mathbf{r}_i - \mathbf{r}_j\| > 0$$

$$\mathbf{F}_n = k_n \sqrt{R} \delta^{3/2} \mathbf{n} - \sqrt{R\delta} m \gamma_n \mathbf{v}_n$$

Dissipative term;
Many damping models



What about oblique contact/tangential force?
→ friction, with option of accumulated shear

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pair gran/hertz/history
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$$\boldsymbol{F}_S = -k_S \int_{t0}^{t} v_{tR}(\tau) \mathrm{d}\tau - \eta_T v_{tR}$$

Needs to account for rotating frame of reference

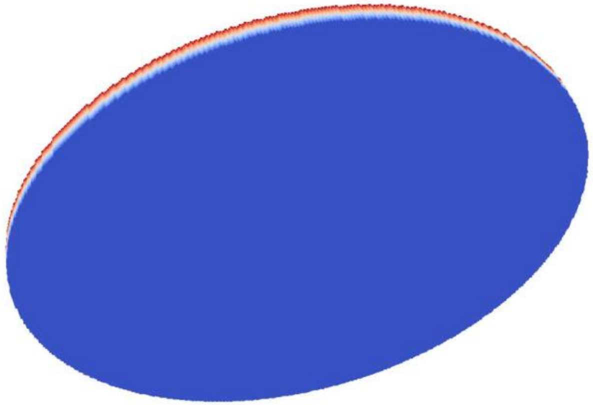
$$v_{tR} = v_t - (R_i \boldsymbol{\Omega}_i + R_j \boldsymbol{\Omega}_j) \times \boldsymbol{n}$$

$$\|\boldsymbol{F}_S\| \leq \mu_S \|\boldsymbol{F}_n\|$$

Also see: LIGGGHTS/CFDEM project

Peridynamics

- Nonlocal formulation of solid mechanics
- Good alternative to e.g. XFEM for modeling fracture/fragmentation
- PERI package in LAMMPS
- Not frequently maintained, much of peridynamics development now in Peridigm



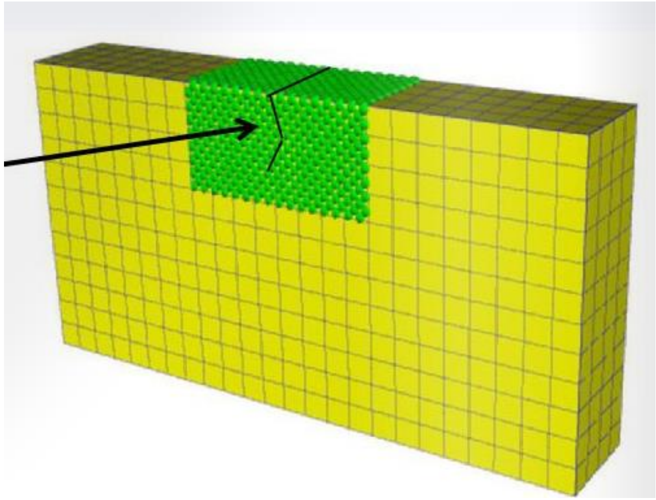
Stewart Silling, Mike Parks, many others (SNL)

Silling, Stewart A. "Reformulation of elasticity theory for discontinuities and long-range forces." *Journal of the Mechanics and Physics of Solids* 48.1 (2000): 175-209.

Molecular and macroscopic

USER-AtC package:

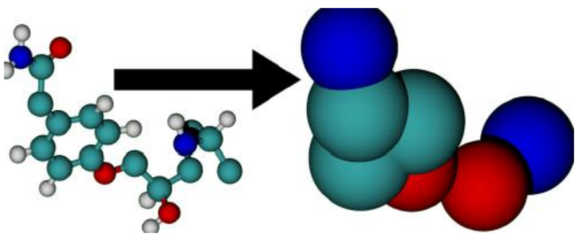
- Molecular simulation in one region coupled to continuum (e.g. FEM)
- Couple continuum equations throughout domain to molecular system
- On-the-fly analysis of MD to extract continuum quantities



Reese Jones, Jeremy Templeton (both SNL)

‘Detailed’ MD to coarse-grained MD

Basic idea: access larger length/time scales by using less detailed representations



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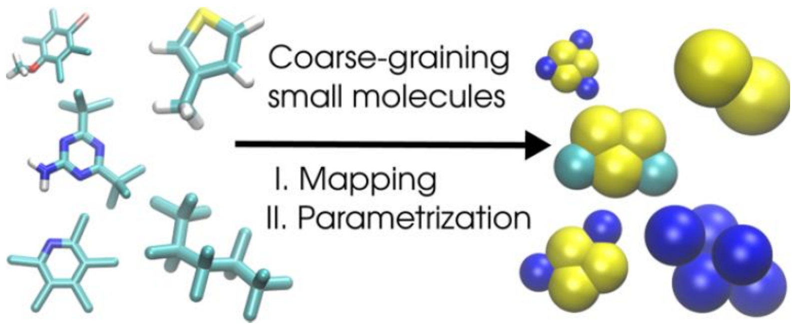

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This works because:

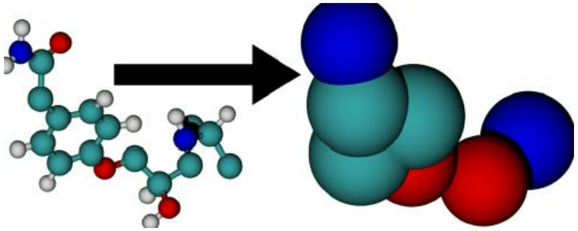
1. Fewer particles!
2. ‘Softer’, sometimes simpler potentials → enables larger time step

- Not limited to atomistic→bead-spring; hierarchical also possible

1. Graham et al, J Chem Info Modeling 2017; 2. Bereau and Kramer, JCTC 2015

Methods

Need to:
1.) Select chemical groups to coarse-grain
2.) Obtain parameters



'DIY' coarse-graining, e.g.
- Force matching
- (Iterative) Boltzmann inversion

Tools:
VOTCA, fix mscg, PyCGTOOL, Auto_MARTINI

$$U_{\alpha\beta,0}(r) = -k_B T \ln\left(g_{\alpha\beta}(r)\right)$$

$$U_{\alpha\beta,i+1}(r) = U_{\alpha\beta,i}(r) + k_B T \ln\left(\frac{g_{\alpha\beta,i}(r)}{g_{\alpha\beta}(r)}\right)$$

Note: all of these map only static properties, dynamics may be way off!

'Pre-packaged' CG force fields:
MARTINI, ELBA, USER-CGDNA, various UA (e.g. OLPS-UA)