Pore scale modeling and simulation of geosystems

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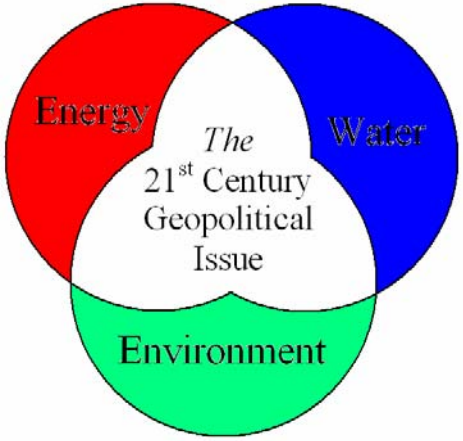
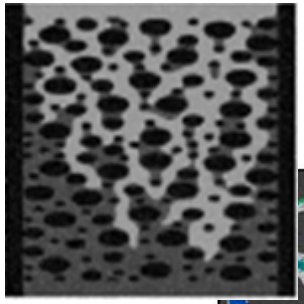
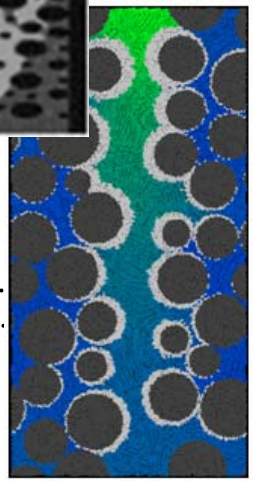
Scientific Impacts and Opportunities for Computing, Jan 10-13, 2008, Maui

Pore scale modeling and simulation of geosystems

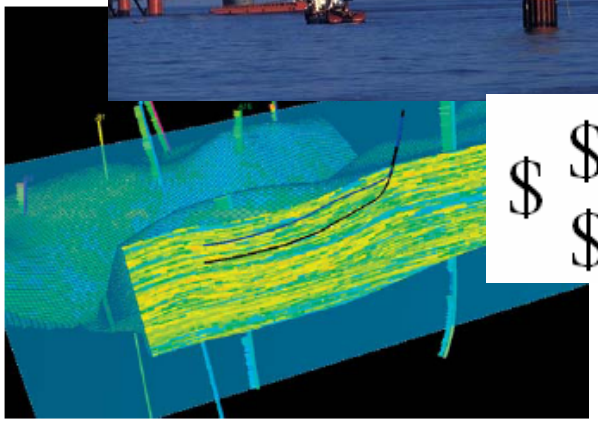




Tartakovsky *et al.*, WRR, **43**: W05437 (2007), Physics of Fluids, **19**:103301 (2007)



www.statoil.com



$ $ $ $

Transfer of information across scales – coupled models

10^4 m, 10^9 sec

www.slb.com

Oil will remain the most available and economic transportation fuel for decades

Van Duin and Larter, Geochemical Transactions, **2**: 35 (2001)

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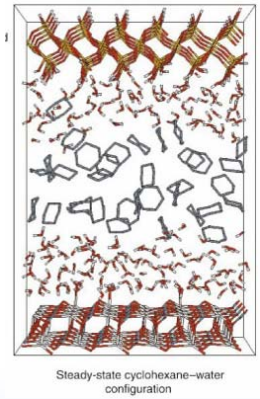

10^{-7} m, 10^{-9} sec

Transfer of information across scales – coupled models

10^{-3} m, 10^2 sec

Assuming 4 trillion barrels of oil (including unconventional) still recoverable, 40.00% recovery → 40.01% is worth $100 billion at $100/barrel. 4 trillion barrels → 5 → 6 ····· with better technology?

Incremental improvements in economic CO_2 sequestration would be worth at least as much

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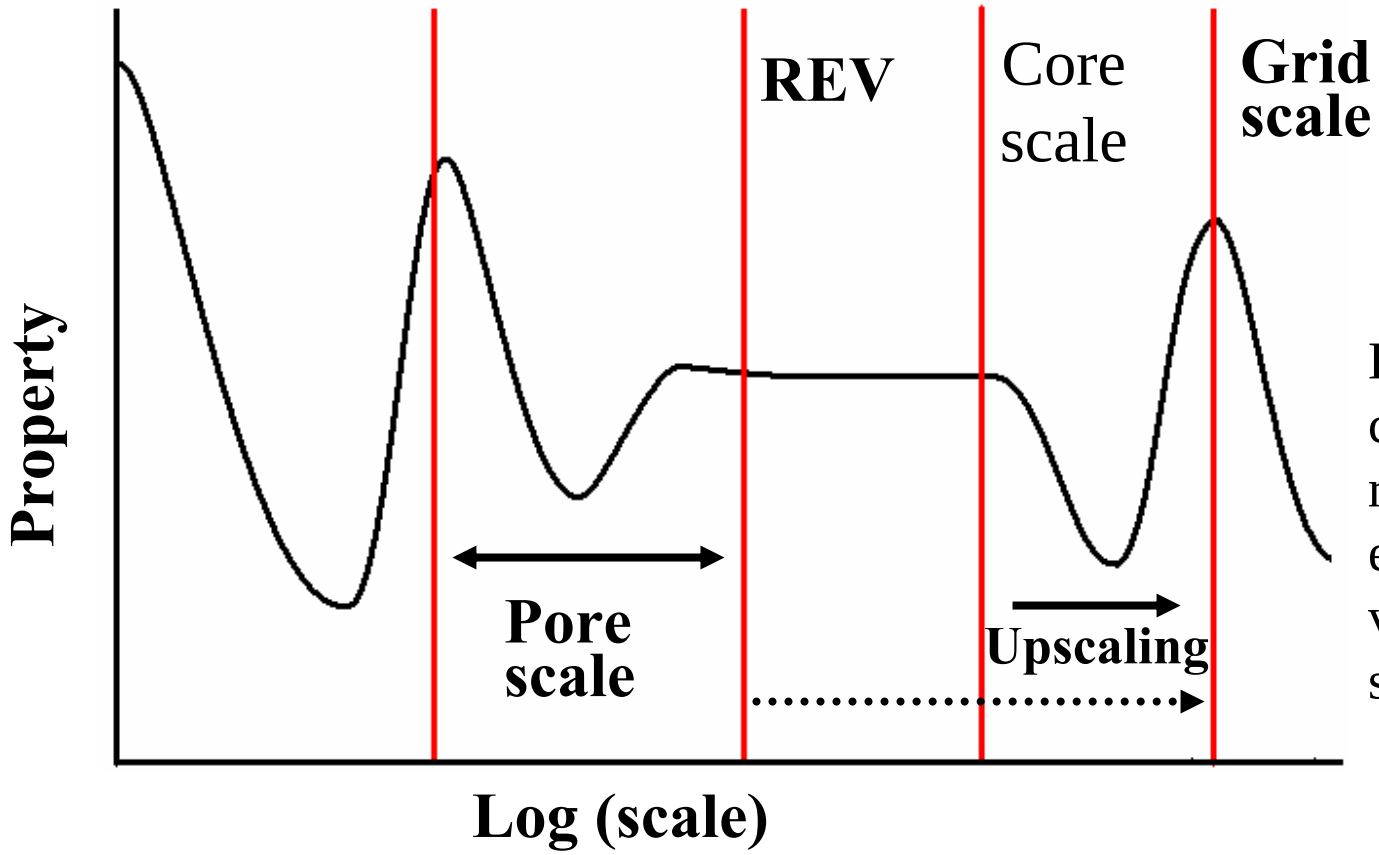
Pore scale modeling and simulation of geosystems

Use large pore scale simulations to obtain constitutive relationships needed by reservoir/field scale models



However, the concept of a representative elementary volume is suspect at best

Use pore scale simulations to develop conceptual models for reservoir/field scale models

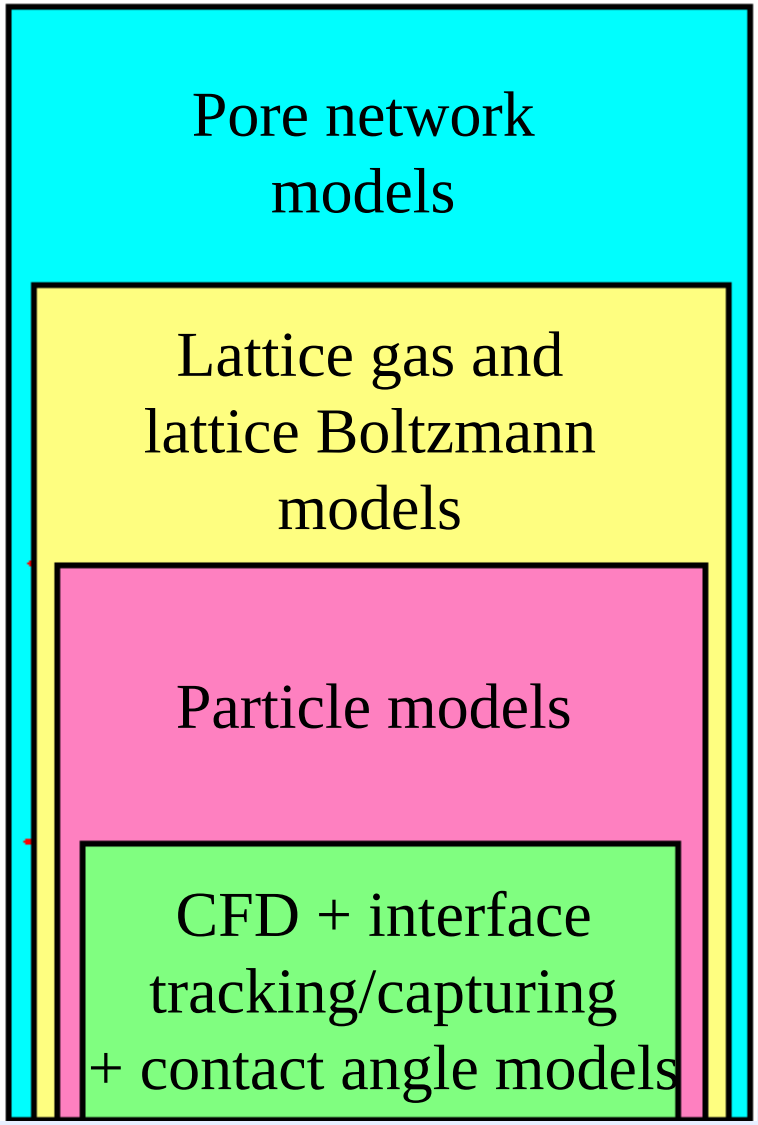
Pore scale modeling and simulation of geosystems

Objective: Accurately simulate pore scale coupled subsurface physical chemical and biological processes with the complexity typical of natural and experimental systems

- Single- and multi-phase fluid flow
- Reactive transport (dissolution/precipitation adsorption/desorption)
- Geomechanical phenomena: pressure solution, fracturing
- Biological phenomena: Biofilm growth, enhanced dissolution, particle and polymer formation, redox chemistry
- Formation transport and aggregation/deposition of inorganic and biological colloids

Pore scale modeling and simulation of geosystems

Historical development →



+ Speed
- Approximate pore geometry and physics, lack of generality

+ Simplicity → speed, rigorous mass and momentum conservation
- Poor numerical stability → limited range of application

+ Simplicity, stability, rigorous mass and momentum conservation, flexibility
- Slow relative to other methods, must be calibrated

+ Fast, works well for wide range of fluid properties
- Complexity, needs interface tracking and contact line/angle model

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Complementary strengths and weaknesses: No one model, in it's current state of development meets all our research needs

Pore scale modeling and simulation of multiphase fluid flow

1. Create model pore space and/or fracture apertures

Tomography/microscopy→ geometric/statistical models

Direct application of three-dimensional tomographic “maps”

Process based morphology

2. Formulate model and perform simulation

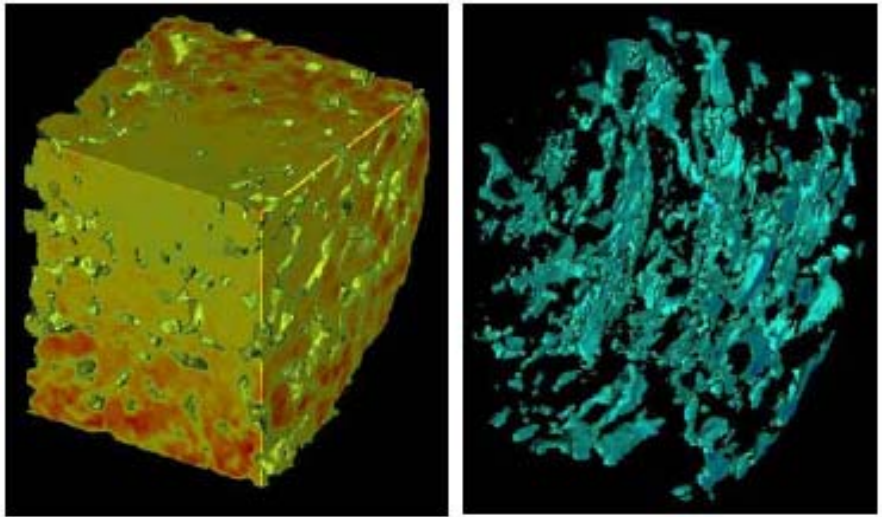
Challenges:

Complex highly dynamic fluid-fluid interfaces (topological changes)

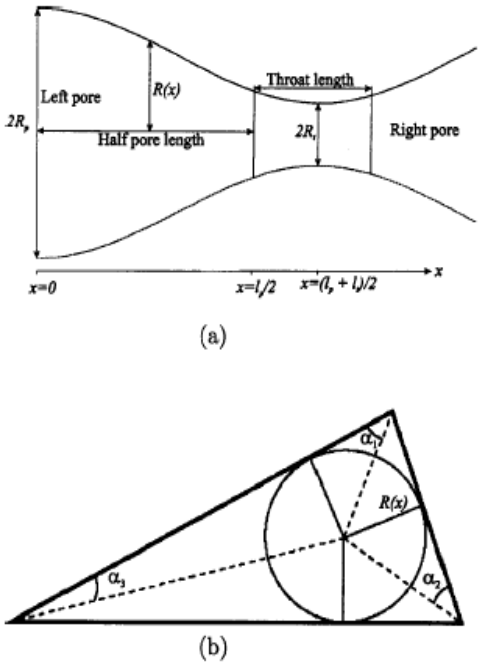
Inherently complex fluid-fluid-solid contact line dynamics

We do not have models that work well for all geologically relevant fluids under a wide range of geologically important conditions

Pore network models



Halverson *et al*., Mid-Continent Transportation Research Symposium, 2005



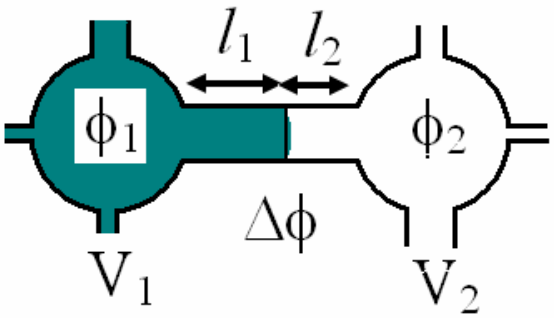
Al Gharbi and Blunt

Phys Rev **E71:**016308 (2005)

Network of pore volumes (nodes) connected by channels

Flow rate in each channel depends on potential in pore volumes (nodes) fluid viscosities, surface tension and position of meniscus in channel

Pore network models



$$Q_{12} = S_\eta(\phi_1 - \phi_2 - \Delta P_{12}^c) r_{12}^4 / (l_{12}^{(1)}\eta_1 + l_{12}^{(2)}\eta_2)$$

$$Q_{12} = G_{12}(\phi_1 - \phi_2 - \Delta P_{12}^c)$$

- (over) Simplified pore space geometry and fluid flow physics
- Requires repeated solution of Kirchoff equations

- Flow rate boundary conditions

$$\sum_j G_{ij}(\Phi_j - \Phi_i) = 0 \quad \mathbf{G}''\mathbf{\Phi} = -\mathbf{Q}_B \quad \mathbf{G}''_{ii} - \sum_{j \neq i} G_{ij} \quad \mathbf{G}'' = G_{ij}$$

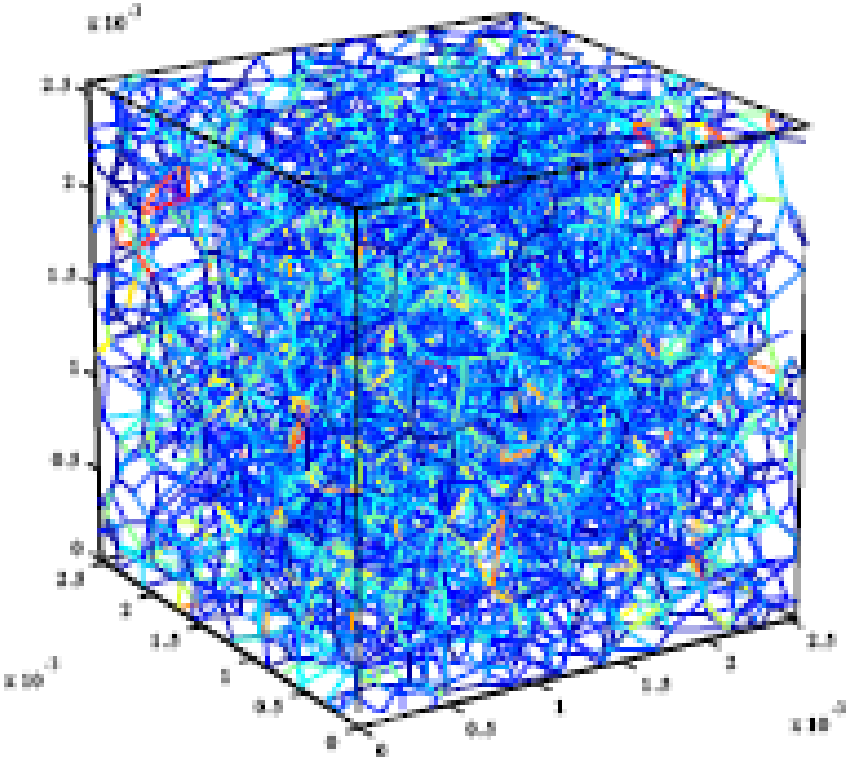
- Potential boundary conditions

$$\mathbf{\Lambda\Phi}_I = \mathbf{G}_B\mathbf{B} + \mathbf{G}_I\mathbf{\Phi}_I \quad \mathbf{\Phi}_I = (\mathbf{\Lambda} - \mathbf{G})^{-1}\mathbf{G}_B\mathbf{B} \quad \Lambda_{ii} = \sum_{j \neq i} G_{ij}\Phi_i$$

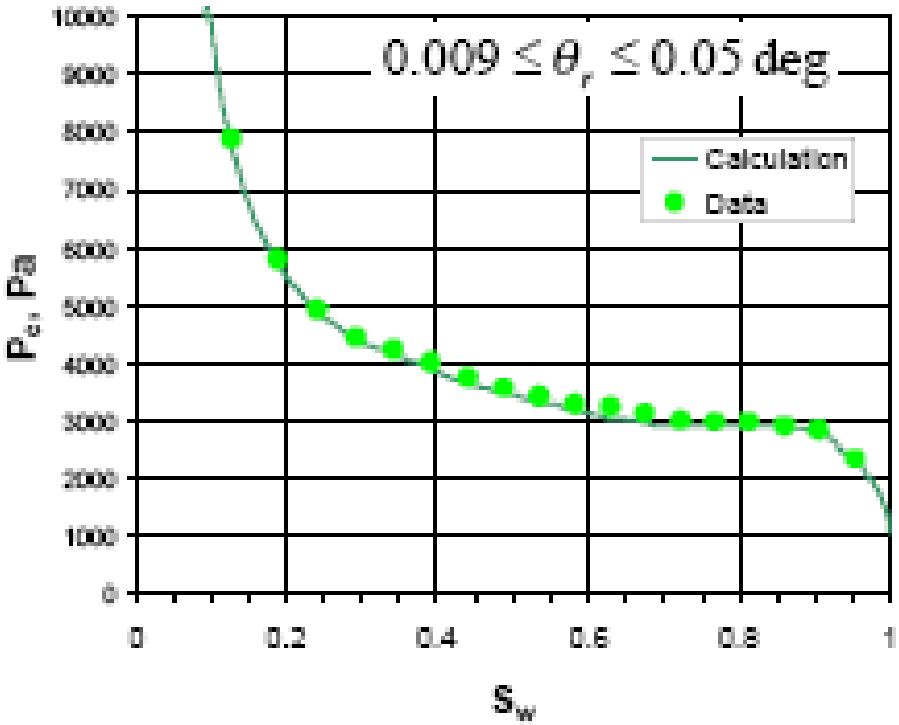
- Most simulations carried out using simple SOR and conjugate gradient algorithms

- Fast parallel linear equation solvers

Pore network models



Patzek, SPE 59312, (2000)/Statoil



Primary drainage

Principles of particle and particle based models for multiphase fluid dynamics

- Particle microdynamics → continuum fluid dynamics

Essential ingredients:

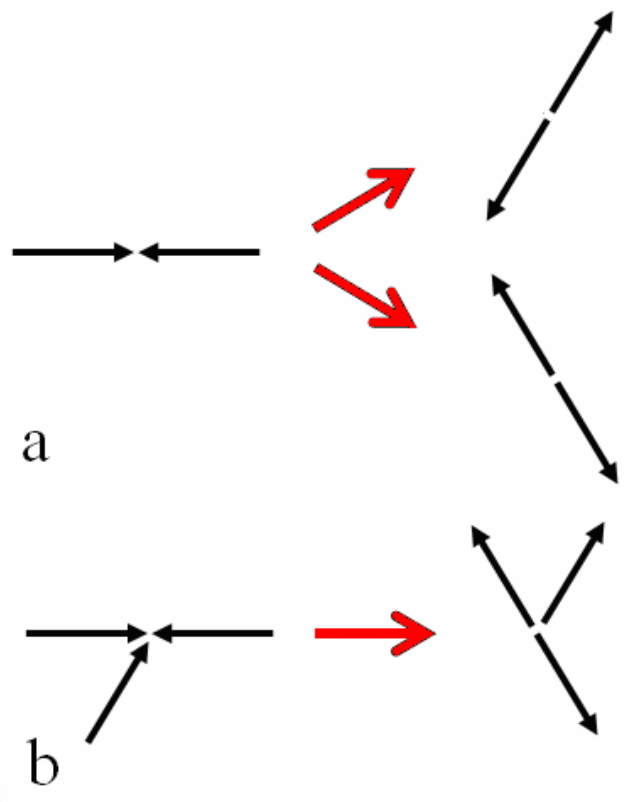
- ➢Conservation of mass
- ➢Conservation of momentum
- ➢Conservation of energy (implicit in most models)
- ➢Galilean Invariance
- ➢Isotropy
- ➢Knudsen number (mean free path/system) size <<1

Any model that that includes these conservation principles, symmetries and contraints is virtually guaranteed to be a valid fluid dynamics model in the continuum limit ⇒ many models with different strengths and weaknesses and fertile ground for innovation

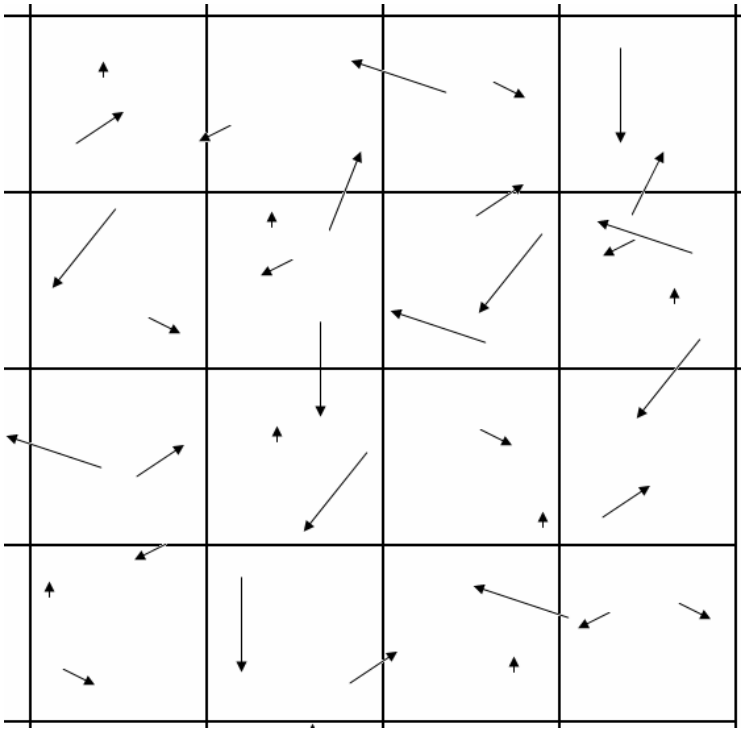
Particle methods obviate interface tracking

Lattice gas and Monte Carlo models

Conventional lattice gas



Real coded lattice gas



$$\mathbf{r}_i(t+\Delta t) \rightarrow \mathbf{r}_i(t) + \mathbf{v}_i \Delta t$$

$$\mathbf{v}_i(t^+) \rightarrow \langle \mathbf{v} \rangle + \mathcal{R}\left(\mathbf{v}_i(t) - \langle \mathbf{v} \rangle\right)$$

Randomly shift grid to ensure Galilean invariance

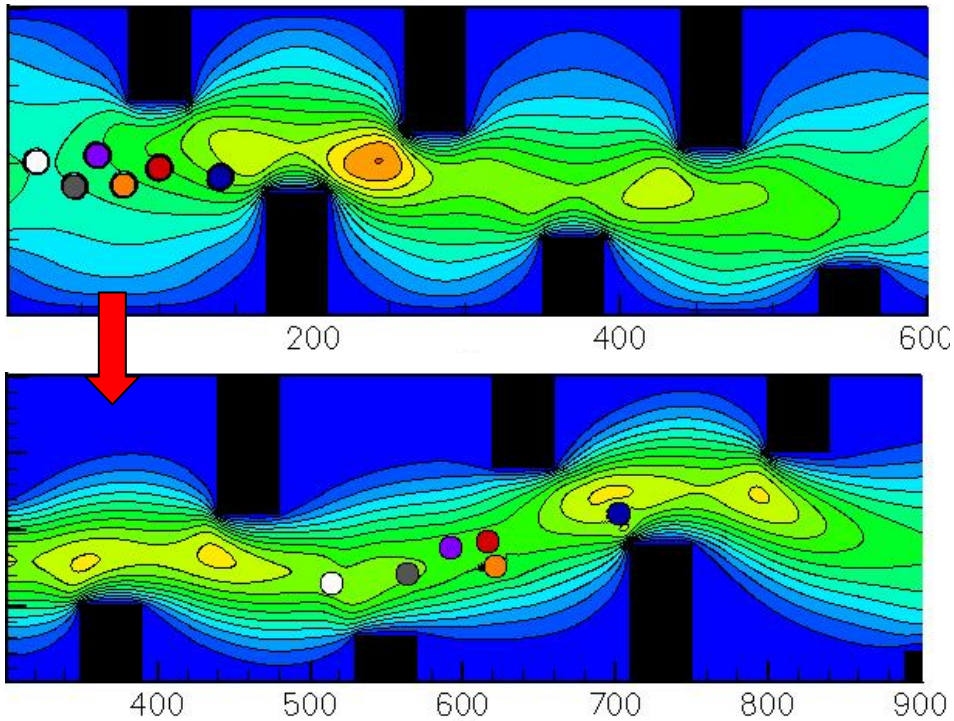
Lattice Boltzmann models

- Two theoretical origins: 1. “average” lattice gas to eliminate fluctuations; 2. discretize classical Boltzmann equation
- Computationally efficient and widely applied – but there are significant deficiencies. The most important are:

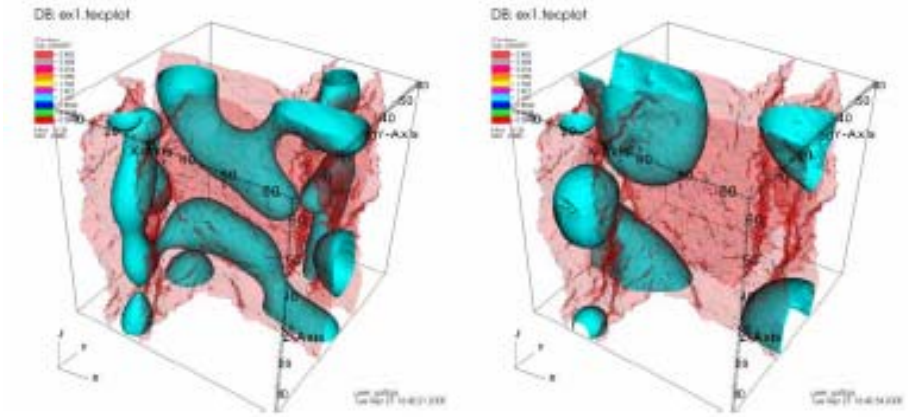
1. Poor numerical stability limits density ratios, viscosity ratio and dimensionless diffusion coefficient
2. Schmidt number (ratio between momentum diffusion and molecular diffusion) is O(1) vs. $O(10^3)$ for typical liquids
3. Compressibility effects are too large for some applications

Progress is being made on these issues. Advanced parallel lattice Boltzmann code will probably be available in 5 years, but not in 12-18 months.

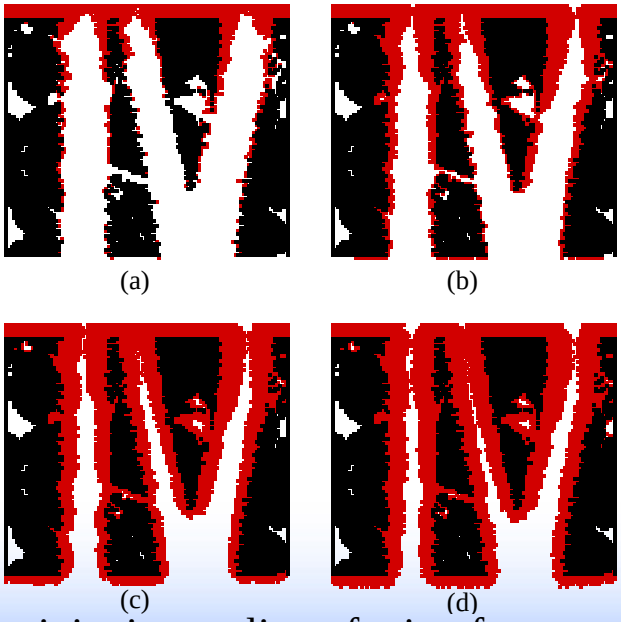
Lattice Boltzmann simulations



Colloid transport



Flow in 3-dimensional fracture junction - with Hakan Basagaoglu



Precipitation sealing of microfractures - Kang, *et al*, Fuel Processing Technology, **86:** 1647-1665 (2005).

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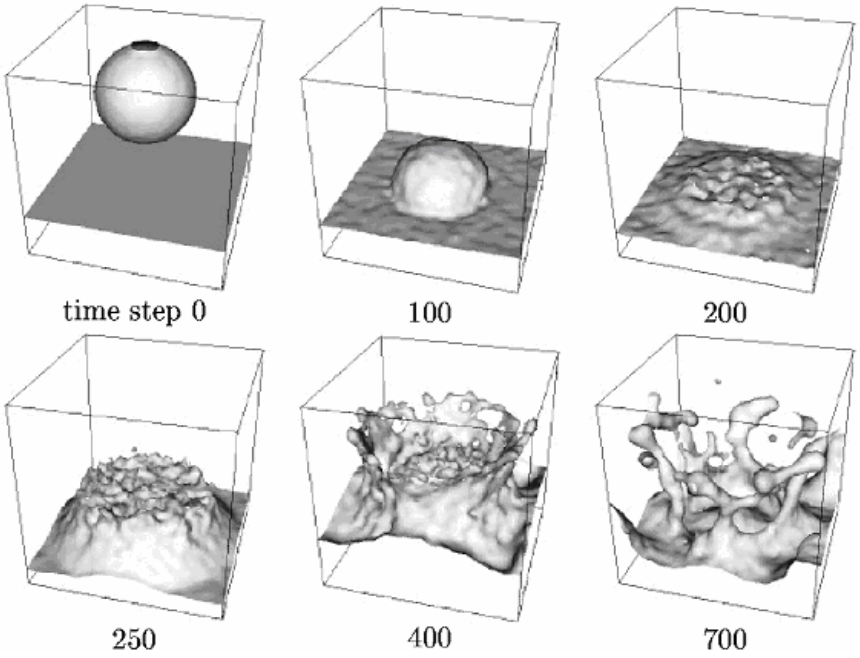
Lattice gas and Monte Carlo models

Conventional lattice gas:

Simple and stable, but noisy and violates Galilean invariance, superseded by lattice Boltzmann, can use fast logical operations

Real coded lattice gas:

Stable and Galilean invariant, has not been applied to multiphase fluid flow in fractured and porous media.



Hashimoto *et al*. Computer Physics Communications **129**: 56-62 (2000).

Particle methods for multiphase fluid flow

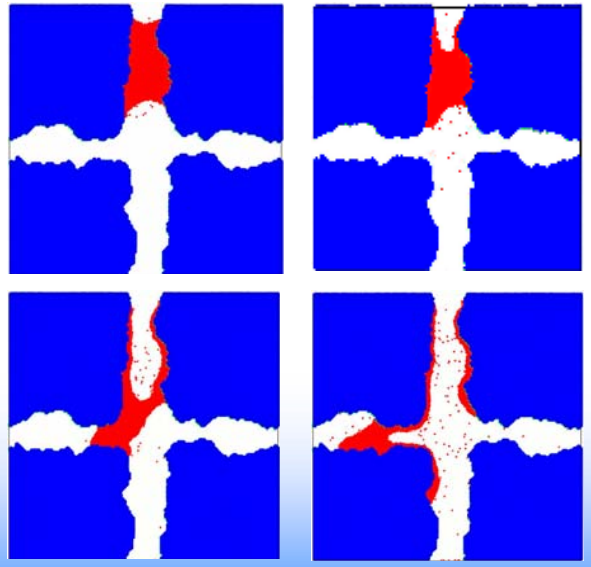
- Non-equilibrium molecular dynamics (MD): time step $O(10^{-15})$ sec, particle size < 1*nm*. Very large strain rates, cannot be used as scale model for pore scale fluid flow

- Dissipative particle dynamics (DPD): time step $O(10^{-12})$ sec, particle size O(1nm). Can be used as scale model for pore scale fluid flow. Well suited to simulation of colloids, polymers and soft condensed matter (biofilm). Equivalent to non-equilibrium MD with very soft particle-particle interactions

- Smoothed particle hydrodynamics (SPH): macroscopic model: includes dissipative but not fluctuating forces.

Dissipative particle dynamics models

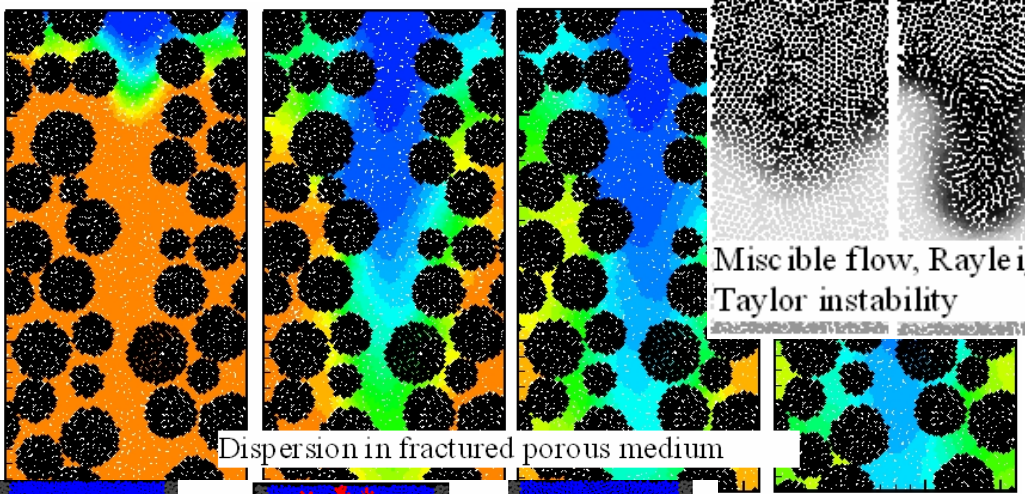
- Particles represent cluster of atoms or molecules (soft conservative interactions + fluctuating and dissipative interactions related by fluctuation-dissipation theorem
- Equivalent to thermostatted (nonequilibrium) molecular dynamics with soft interaction
- Well suited to simulation of colloids, polymers and soft condensed matter (biofilm)



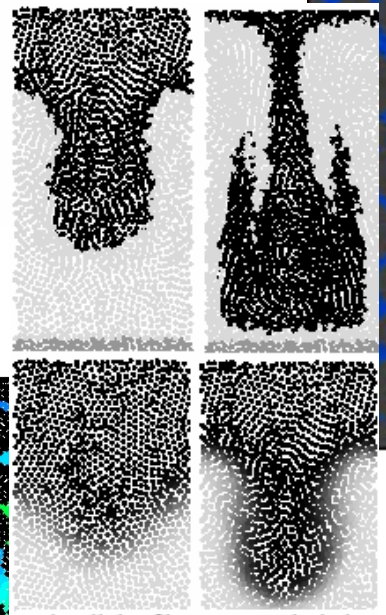
With Moubin Liu and Hai Huang

Smoothed particle hydrodynamics simulations

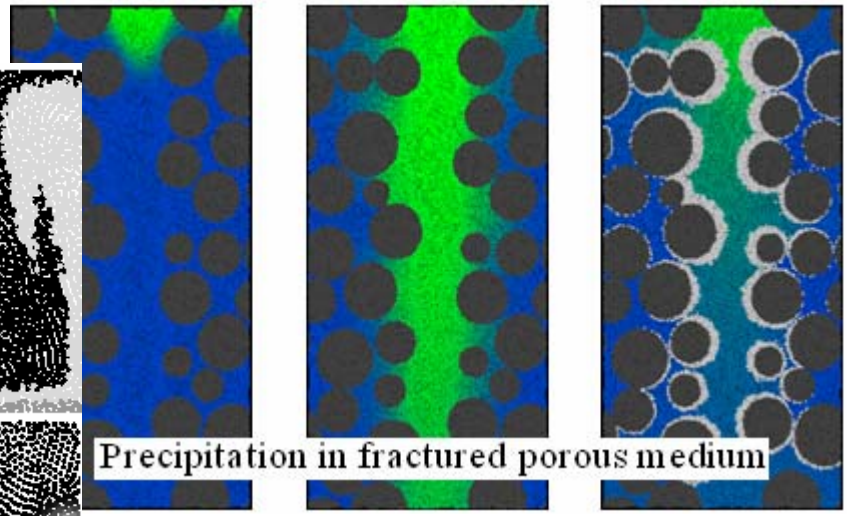
Diffusion – limited/ reaction - limited growth transition



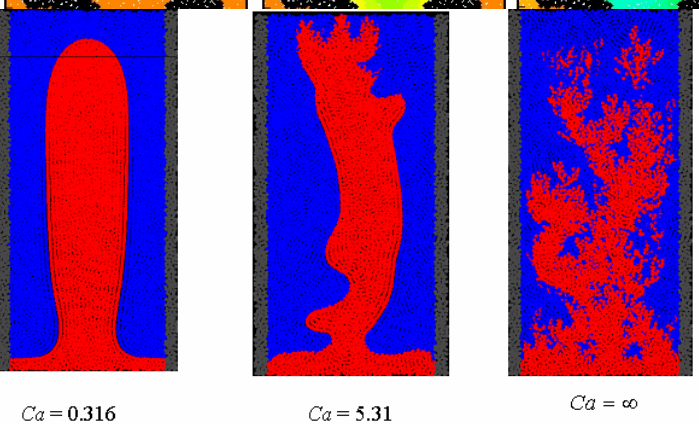
Dispersion in fractured porous medium

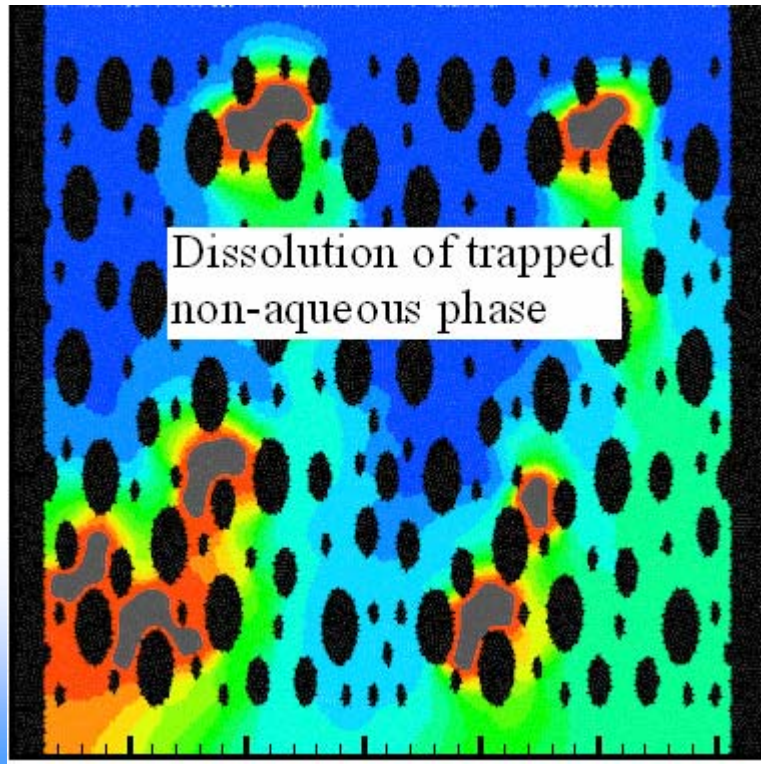


Miscible flow, Rayleigh-Taylor instability



Precipitation in fractured porous medium





Dissolution of trapped non-aqueous phase

With Alexandre Tartakovsky, Tim Scheibe & Andy Ward - PNNL

Computational fluid dynamics + interface tracking + contact angle dynamics model

Interface tracking models:

- Particle methods
- Moving grid
- Fixed grid + indicator function (indicator function identifies phase and is advected with flow)
  - ➢Volume of fluid (VOF)
  - ➢Level set method (LS)
  - ➢Phase field (PP)
- Hybrid methods

Fixed grid + indicator function methods

Relatively easy to implement and provide subgrid scale interface location, handle topological changes well

➢Volume of fluid (VOF)

• Good mass conservation

• Interface represented by disconnected line segments in each cell

➢Level set method (LS)

• Poor mass conservation without adaptive mesh refinement

➢Phase field (PP)

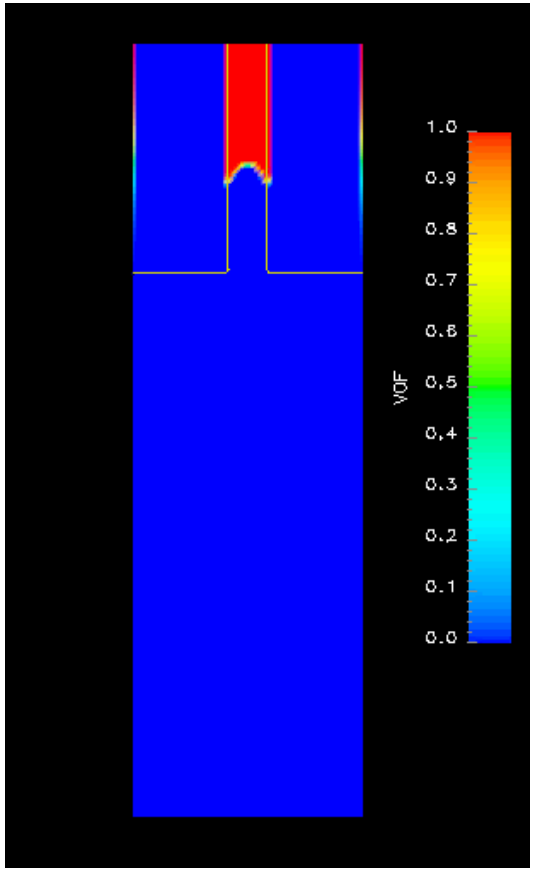
• Closely related to LS method – diffusional (Cahn-Hilliard) or relaxational (Allen-Cahn) indicator function "reinitialization" vs level set function reinitialization

• Phase field can be used as interface tracking algorithm or phase filed physics can be coupled with Navier Stokes equation (Navier Stokes – Cahn Hilliard equation)

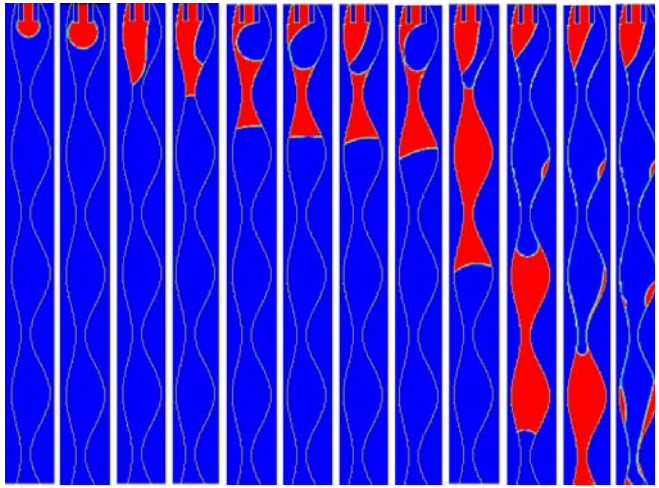
• Contact line dynamics can be included within consistent phase field framework

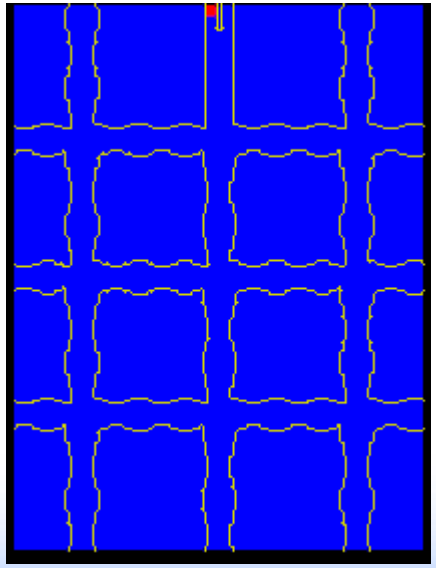
CFD + interface tracking + contact angle model

With Hai Huang, INL,
VOF interface tracking

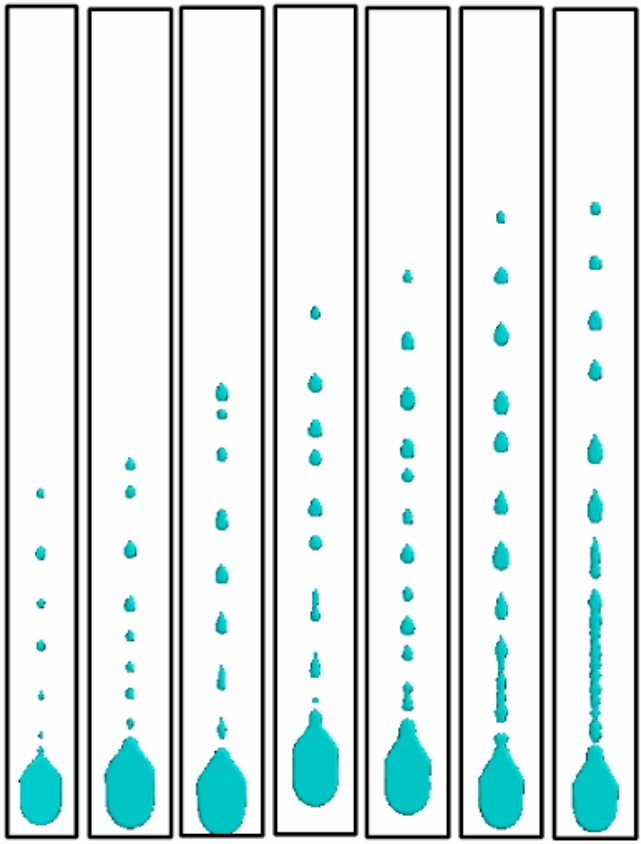


Video: 3-dimensional dripping faucet





Video – multiphase fluid flow in 2-d-mensional fracture network



Drop sliding in vertical Hele-Shaw cell

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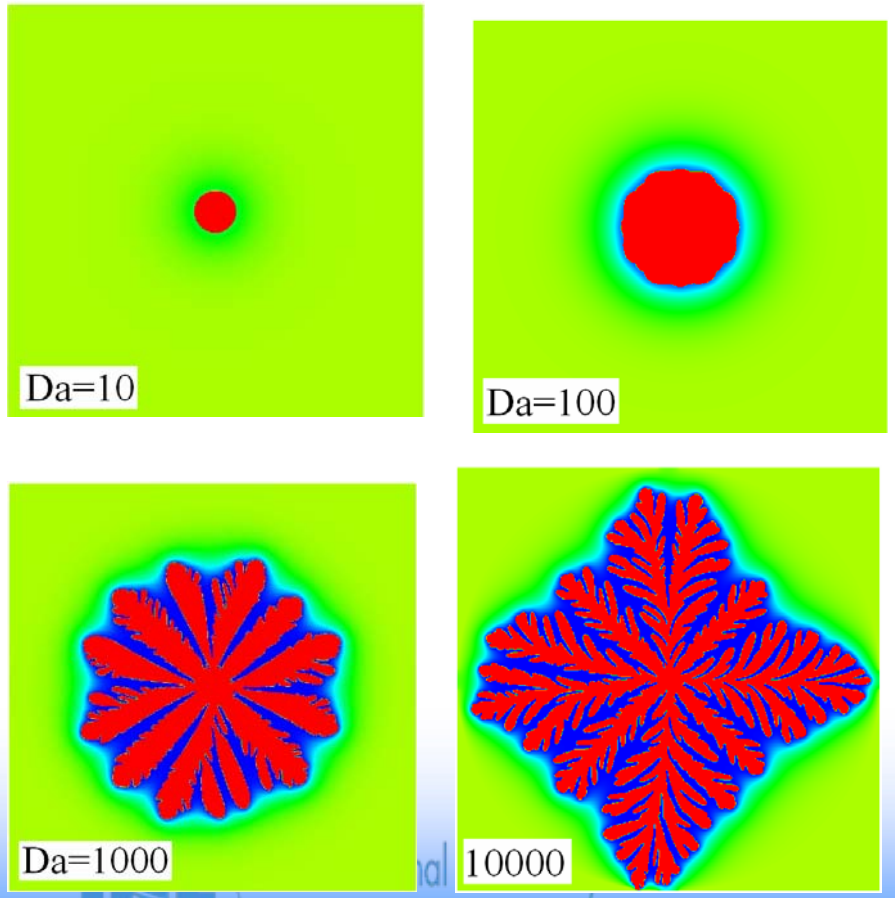
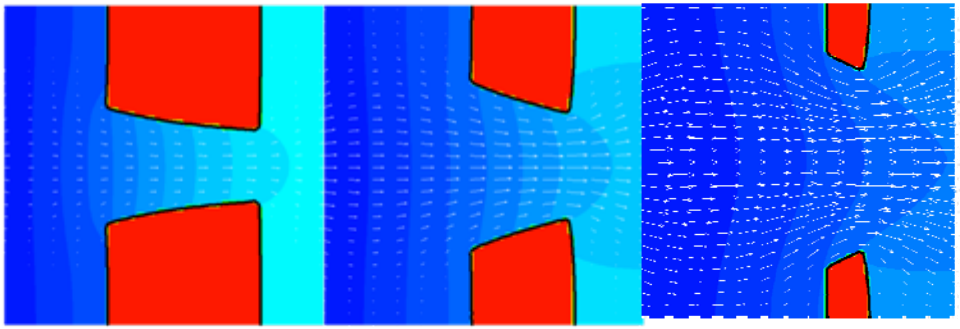
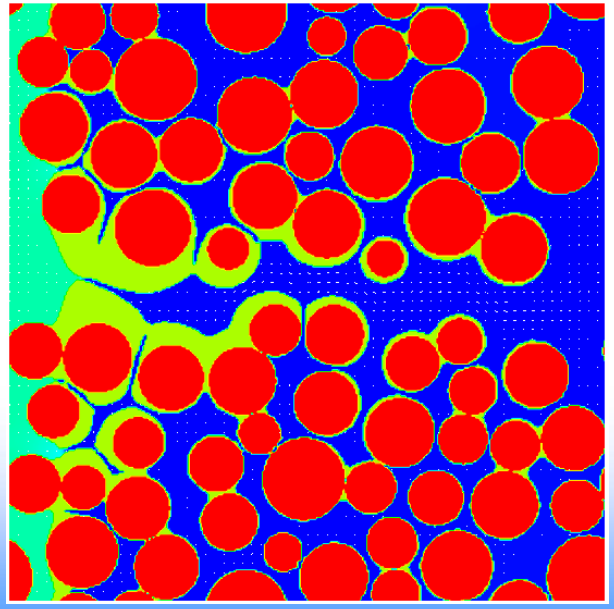
Interface tracking/capturing for dissolution/precipitation

- VOF, LS and PP methods can be used to locate solid fluid interface with subgrid scale resolution
- Interface curvature can be calculated at interface to include Gibbs Thompson effect



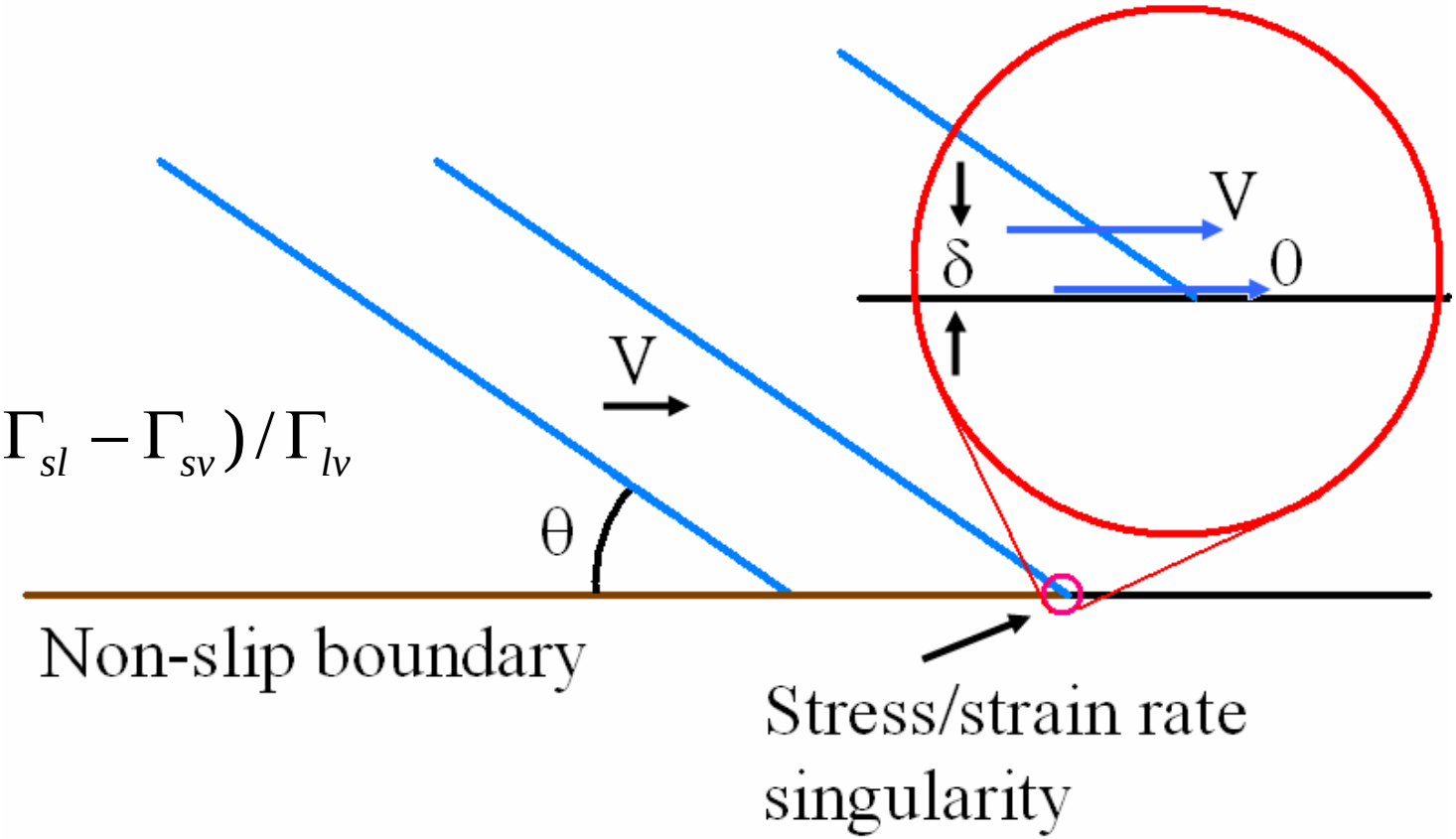




With Xiaoyi Li and Hai Huang

Contact line dynamics: Classical continuum fluid mechanics contact line problem

$$\cos(\theta) = (\Gamma_{sl} - \Gamma_{sv}) / \Gamma_{lv}$$

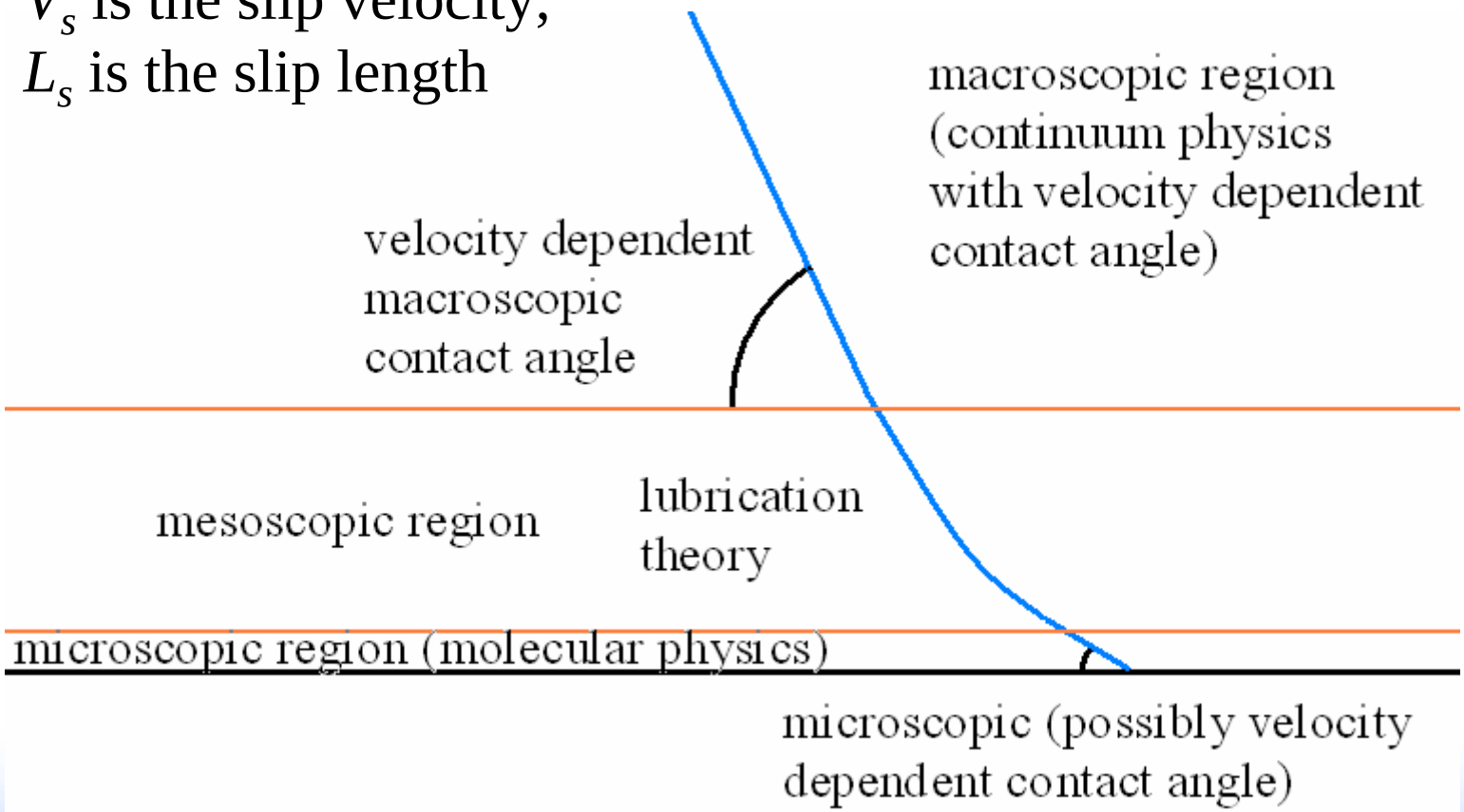


Non-physical stress singularity at fluid-fluid-solid contact line

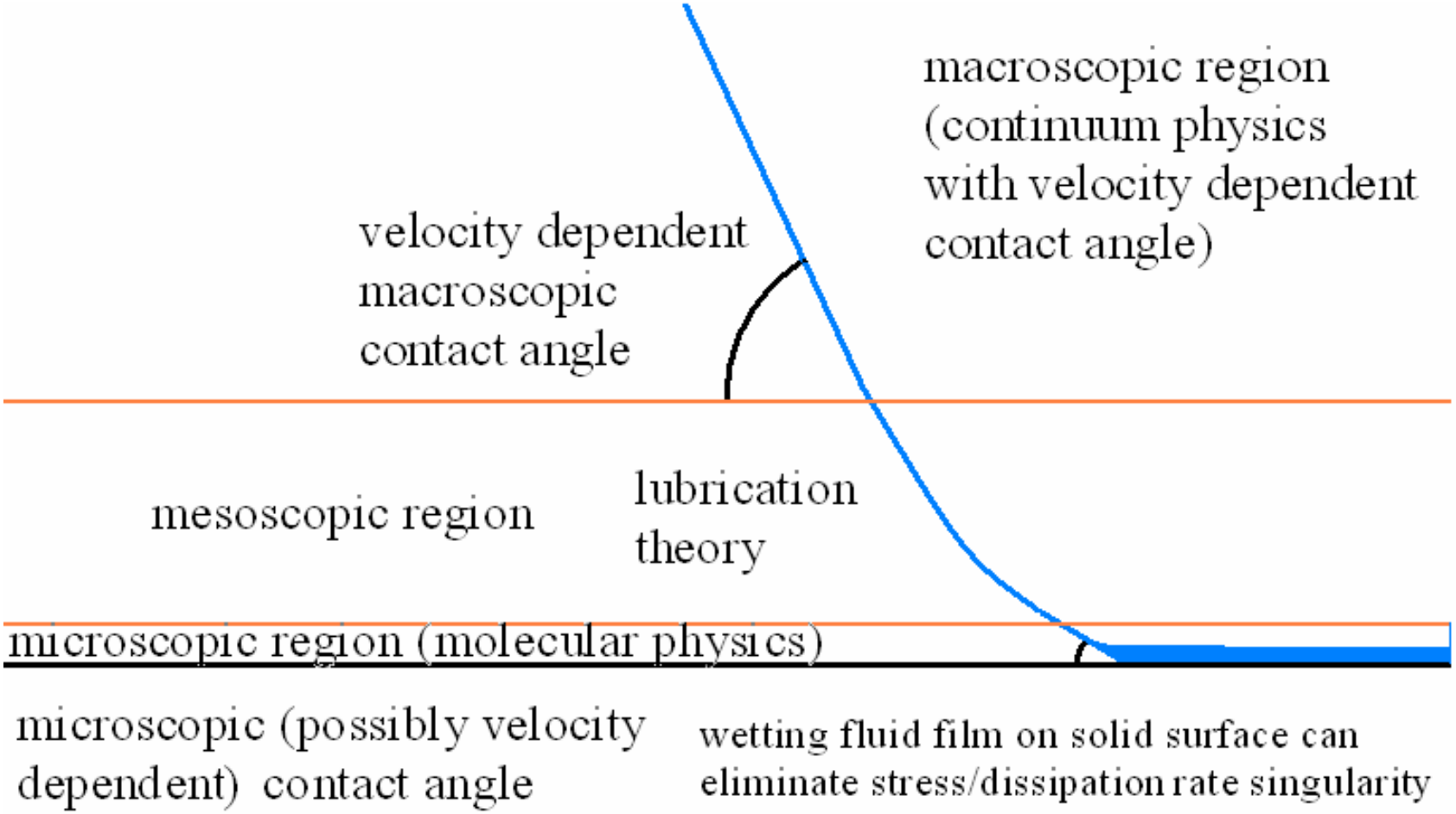
Contact line dynamics: Classical continuum fluid mechanics contact line problem

Simple fix: Use Navier slip boundary condition $V_s = L_s \dot{\varepsilon}$

V_s is the slip velocity,
L_s is the slip length

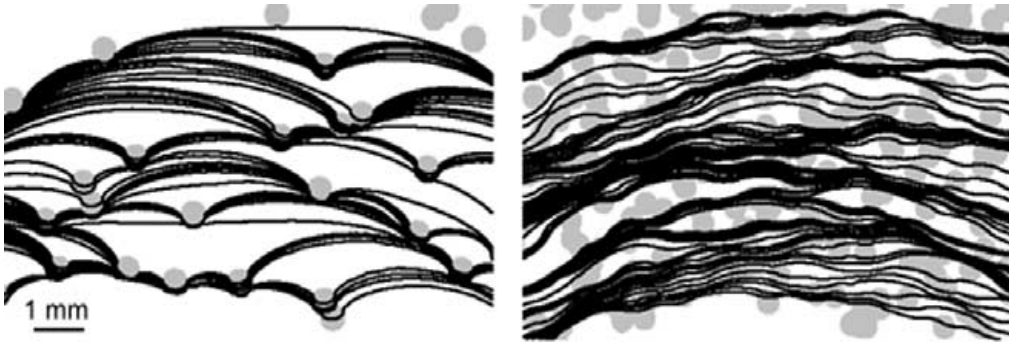


Contact line dynamics: eliminate stress/dissipation rate singularity by assuming that there is a liquid film on the solid surface.

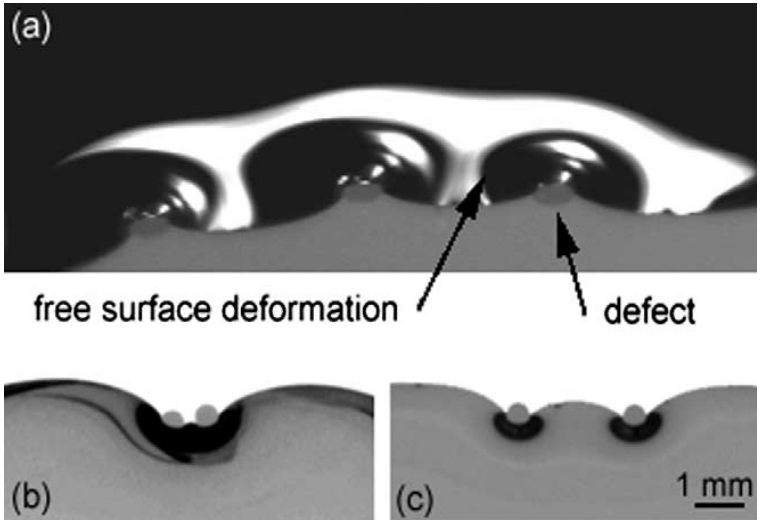


Wetting films are often observed, but very thin wetting films may be more like solids than liquids

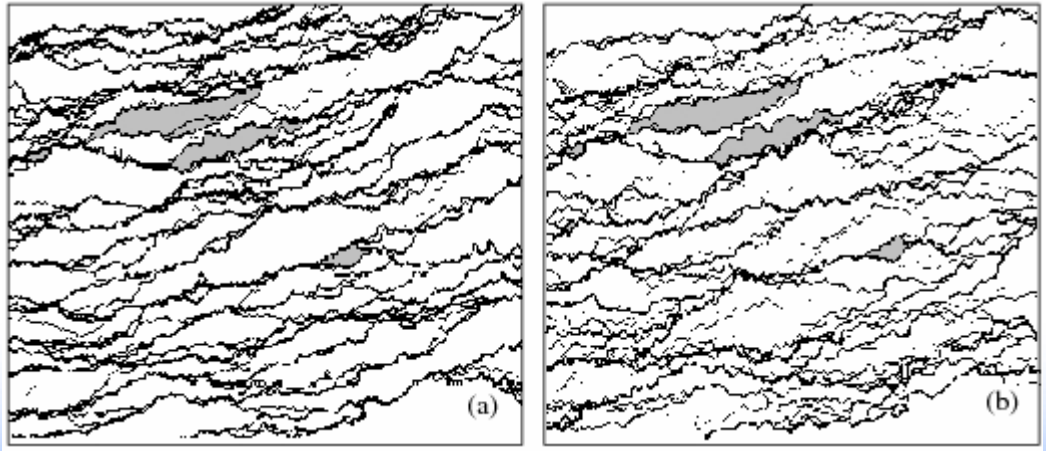
Contact line/contact angle dynamics



T. Cubaud and M. Fermigier, J. Colloid and Int. Sci. **269**: 171-177 (2004)



In subsurface applications heterogeneity is important at all scales



^{4}He on Cs, Prevost *et al*., Phys. Rev., B**65**: 064517 (2006).

Moving contact line dynamics and wetting behavior: inherently complex multiscale processes

- Contact line behavior is still not well understood
- Experiments are difficult because of sensitivity to trace impurities (change in chemical heterogeneity due to adsorption/desorption) and reactivity of geologically relevant materials (change in chemical and physical heterogeneity)
- Molecular processes near to contact line are coupled with mesoscale and continuum
- The surfaces of geologically relevant materials are often physically and chemically complex

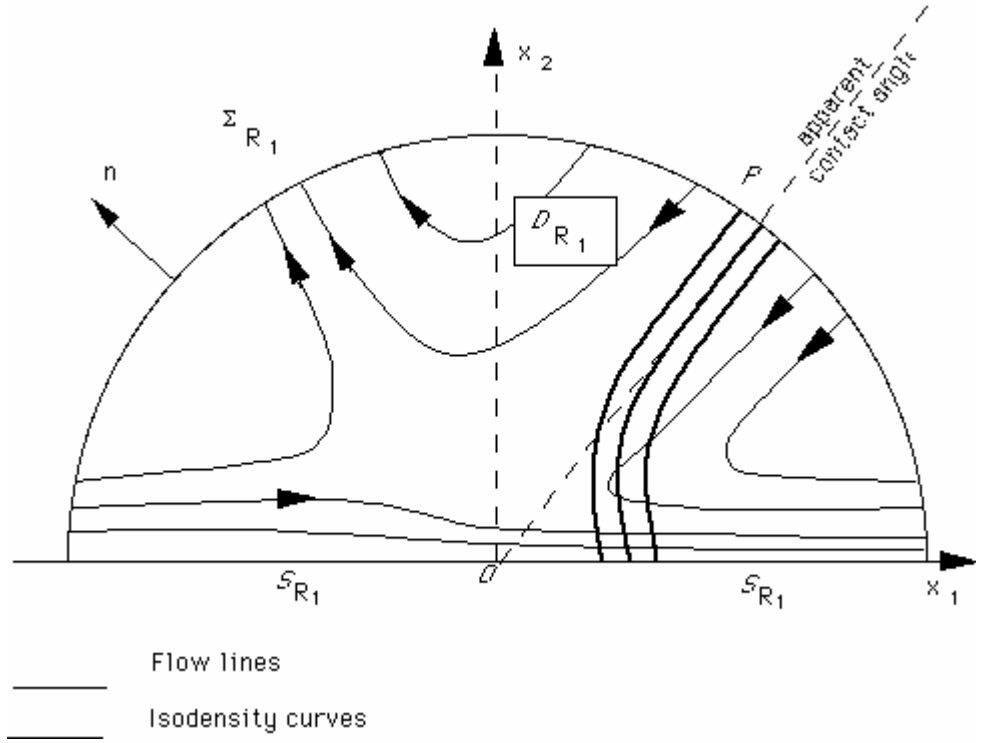
Moving contact line dynamics and wetting behavior: modeling and simulation

- Molecular dynamics: Provides detailed information on very small time and length scales
- Dissipative particle dynamics, smoothed particle hydrodynamics lattice Boltzmann ….: Realistic, but not necessarily correct behavior
- Stochastic differential equations (Langevin equation) with quenched and/or temporally fluctuating disorder coupled to flow simulation: needs theoretical development
- Simplified velocity dependent contact angle models: semi empirical
- Phase field models: does not include molecular level details
- Hybrid models (MD/continuum): not practical because of 10^{-15} sec. MD time scale

Moving contact line dynamics and wetting behavior: modeling and simulation

Seppecher, Internationa Journal of Engineering Mechanics, 34: 977 (1996)

Phase filed model for contact line. Phase field model for contact line. Mass transfer across interface eliminates stress singularity at contact line

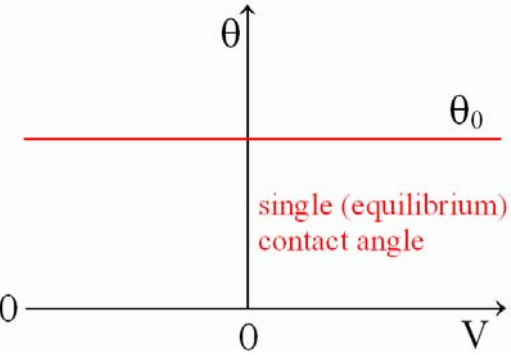


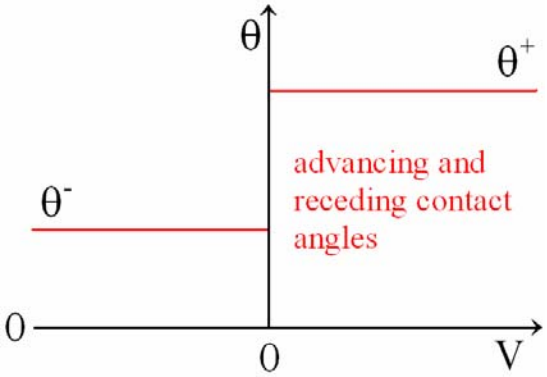
$$\partial h(\mathbf{x},t)/\partial t = a\nabla^2 h(\mathbf{x},t) + c[\mathcal{F} + \eta_q(\mathbf{x},h(\mathbf{x},t))],$$

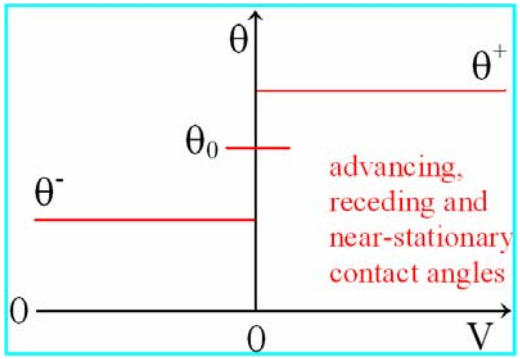
$$\partial h(\mathbf{x},t)/\partial t = a\nabla^2 h(\mathbf{x},t) + b(\nabla h(x,t))^2 + c[\mathcal{F} + \eta_q(\mathbf{x},h(\mathbf{x},t))],$$

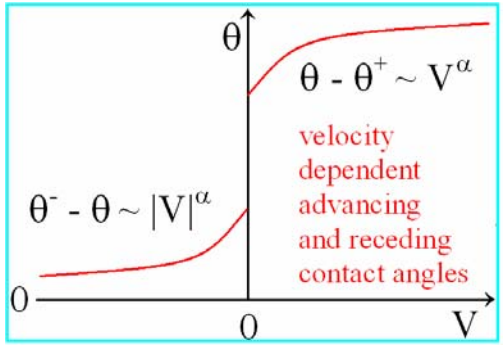
Quenched Edwards-Wilkinson and Quenched Kardar-Parisi-Zhang equations. Simplified Langevin equations for contact line dynamics

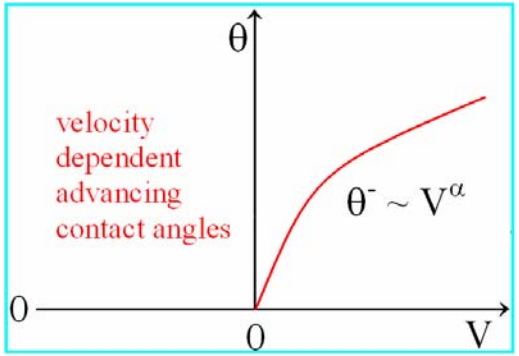
Contact angle/contact line dynamics models

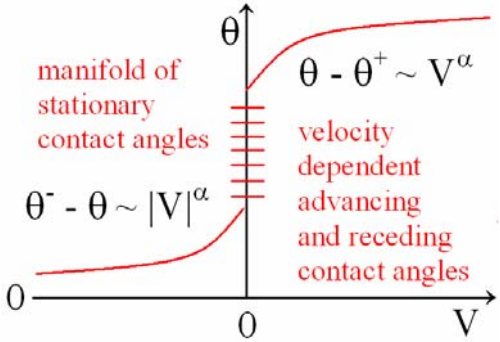






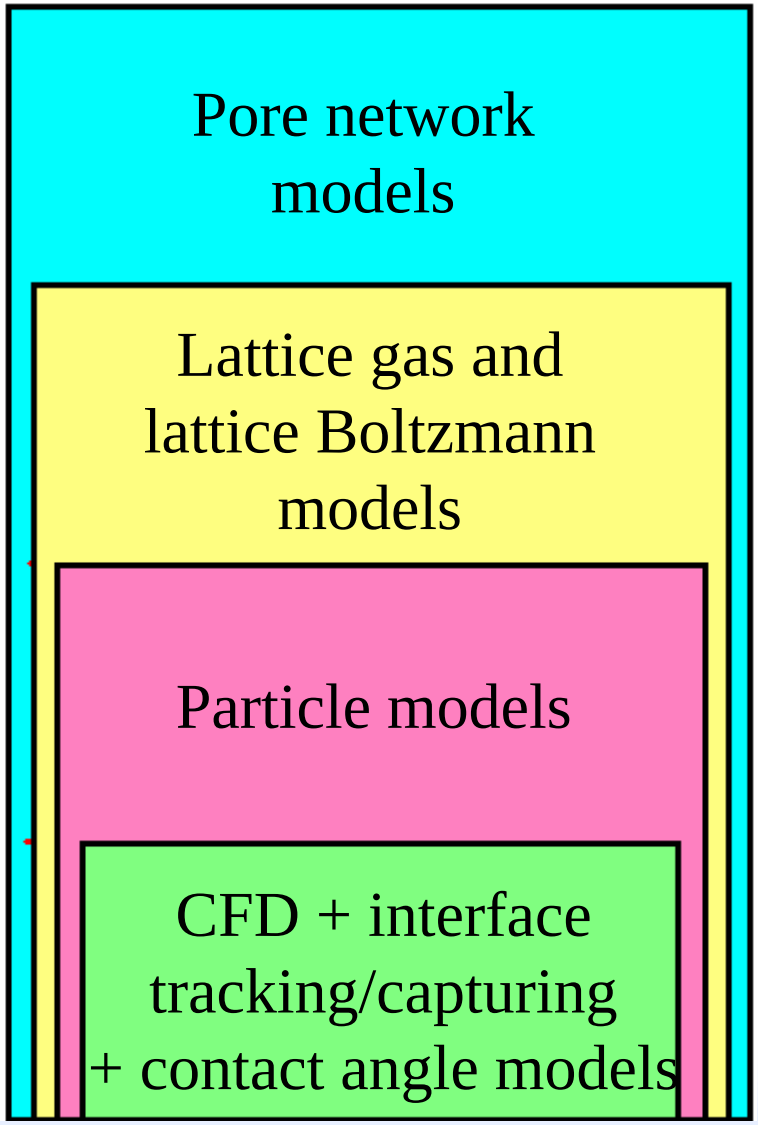






- Couple to Langevin dynamics model for contact line
- Couple to mesoscale model (dissipative particle dynamics, for example)
- Couple to molecular dynamics – but time scale is MUCH too short

Pore scale modeling and simulation of geosystems – numerical methods



Linear equation (Kirchoff equation) solver: Successive over relaxation, conjugate gradient, fast sparse linear equation solvers

Local updating (exchange of information between nearest neighbors)

Integration of Newton's second law (velocity Verlet, Gear predictor corrector). Local interactions → underlying grid with linked list or neighborhood list/tree search.

Pressure Poisson equation solver for incompressible solver (alternating direction implicit) → multigrid
Compressible Navier Stokes – implicit multigrid

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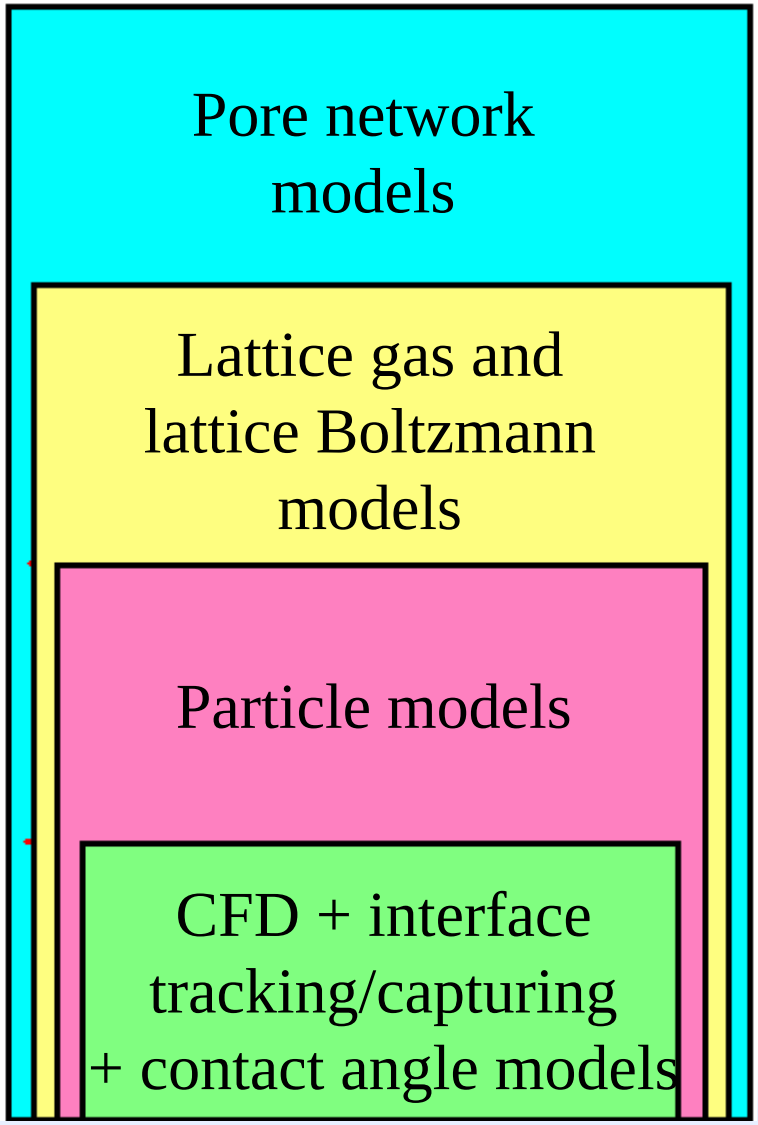
All these methods scale well on large computing systems

Pore scale modeling and simulation of geosystems: petascale computing



1,000,000 hours for 1,000,000,000 pore simulation. 100,000,000 hours + to investigate different pore geometries, wetting conditions, Bond numbers and capillary numbers

1,000,000 hours for 2048 × 2048 × 2048 multiphase fluid flow simulation
100,000,000 hours + to investigate different pore geometries, wetting conditions, Bond numbers and capillary numbers

1,000,000 hours for 10,000 pore 3-dimensional simulation. 100,000,000 hours
100,000,000 hours + to investigate different pore geometries, wetting conditions, Bond numbers and capillary numbers

1,000,000 hours for 100-1000 fracture 3-dimensional network
100,000,000 hours + to investigate different pore geometries, wetting conditions, Bond numbers and capillary numbers

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With current methods or incremental improvements + efficient parallel code

Pore scale modeling and simulation of geosystems: path forward

- Better models to cover all geologically relevant materials and conditions
- Better algorithms + implementation on petascale computing
- Access to very large computing systems
- More manpower and/or collaborations

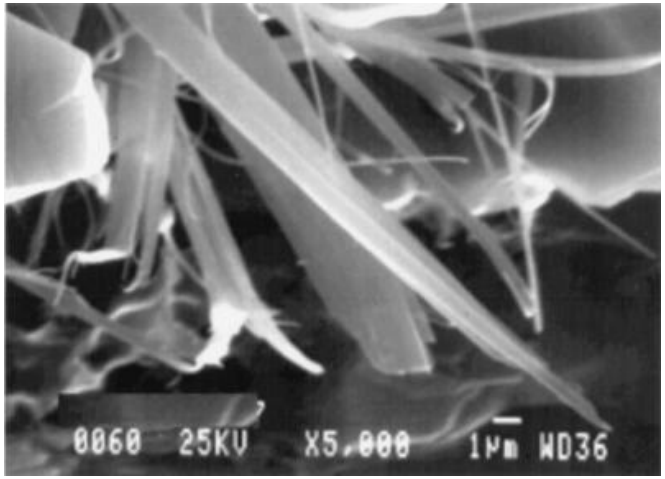
So far, we have focused on model development and implementation on workstations. We have parallel particle codes, but we have not tested scaling to more than O(100) processor cores. Others have performed large scale ($1024 \times 1024 \times 1024$) lattice Boltzmann simulations

Pore scale modeling and simulation of geosystems: path forward

- More robust lattice Boltzmann models applicable to wider range of conditions
- Adaptive particle refinement
- Adaptive mesh refinement + interface capturing for CFD in confined systems
- Coupling with better contact line dynamics models
- Particle and/or continuum (soft condensed matter) models for biofilm growth/decay and coupling with fluid flow and solute transport. Dissipative particle dynamics is promising.

Pore scale modeling and simulation of geosystems: path forward

- It is important to focus more on scales between the molecular and pore scale (microfractures, rough mineral grain surfaces, diagenetic morphologies ···)
- It is important to focus more on scales between the pore scale and the field scale (fracture networks ···)
- Need tight integration with experiments on natural and synthetic materials – synergy, validation, relevance

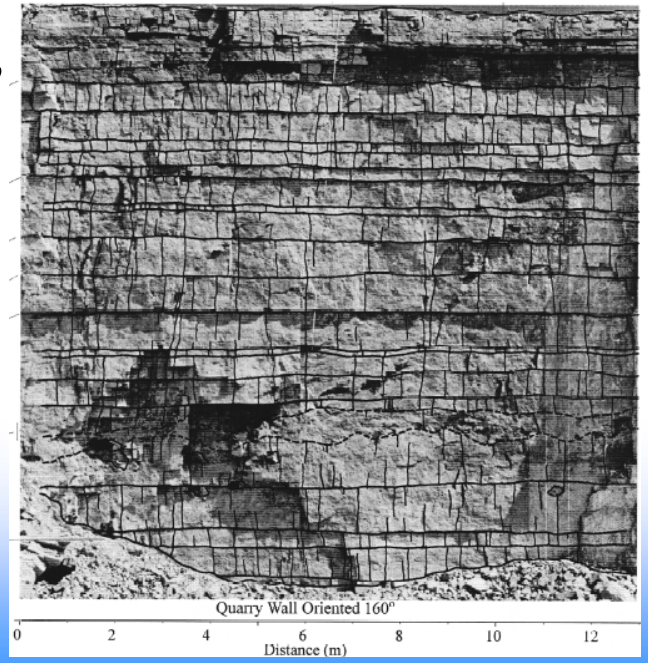


Illite in sandstone, Revear, Proc. US Natl. Acad Sci., 94: 3440-3446 (1999)

In the future, rheologically complex fluids (heavy oil etc.) will become more important

Fractures in Silurian dolomite, Underwood *et al*. AAPG Bulletin, 87: 121-142 (2003): Caveat – exposure can create new fractures

2m



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