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Lattice Boltzmann Calculations of Flow, Dispersion and Reaction

Description

The Lattice Boltzmann (LB) method is a simple numerical technique to calculate fluid flow, dispersion, dissolution, precipitation and melting in multi-component systems. LB solutions obey the *Navier-Stokes* and *Advection-Dispersion* equations, and can model complex interfacial processes without the gridding constraints that plague other numerical methods. Our 3D and 2D codes are principally used for lab- and pore-scale modeling, but there are Darcy flow models, and Hele-Shaw models for fracture paths up to several meters.

Needs

Fracture network models

- Devise mixing rules for fracture junctions
- Analyze lab experiments
- Benchmark continuum codes

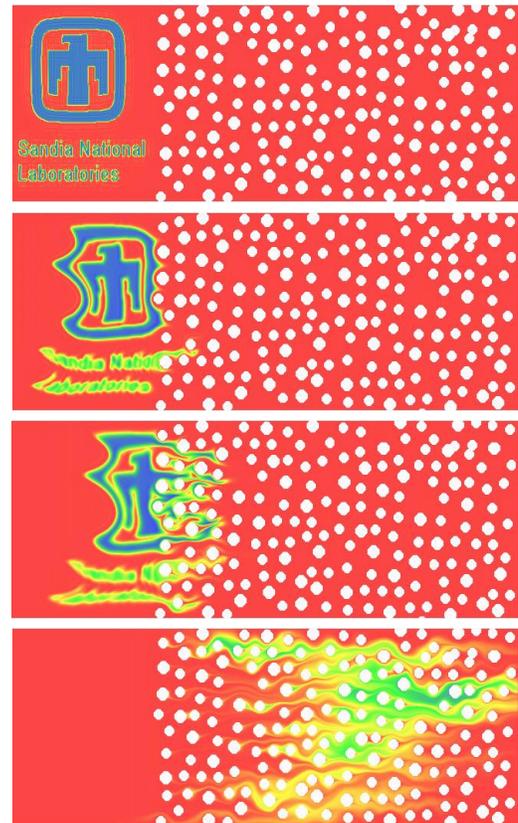
Single fracture / Hele-Shaw models

- Model double-diffusive convection, fingering, effect of "roughness" on dispersion
- Assess scaling errors in lab experiments

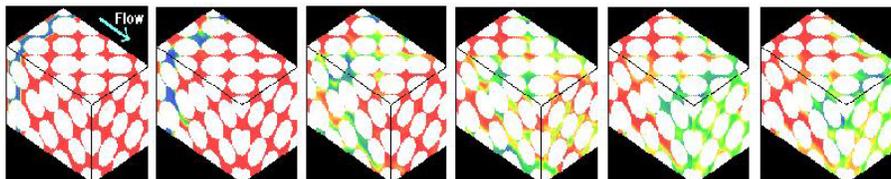
Dissolution-precipitation with coupled flow

- Model silica precipitation in repository rocks, reprocessing of (Pu,U)O₂ in molten salts, near-field corrosion of glass and metal waste forms, ⁹⁰Sr and actinide exchange in carbonate rocks.

3D LB: Dispersion in Sandstone



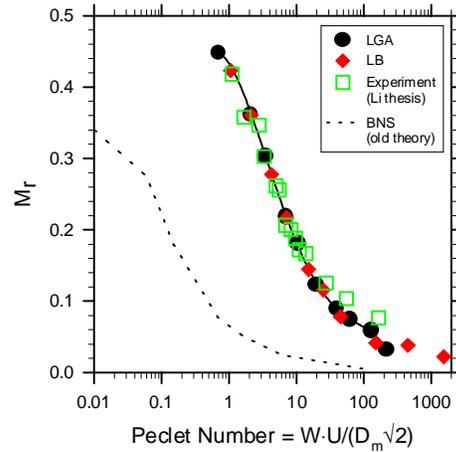
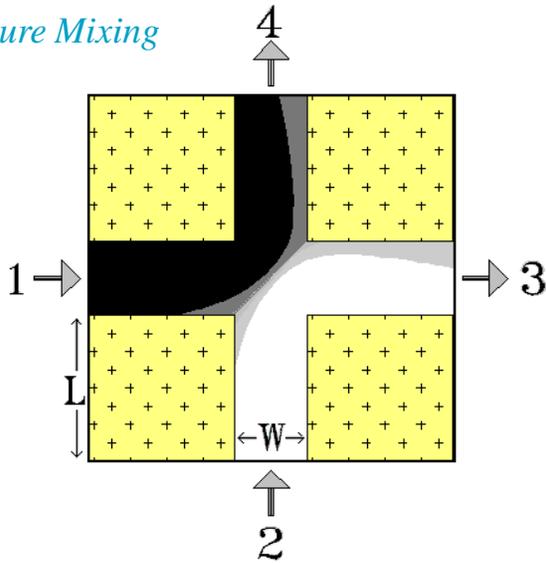
LB Dispersion Calculation: Solids are white; T-bird is tracer injected into flow. $Pe = 800$, 660x240 nodes; 20 minutes on Pentium Pro PC



The idealized "sandstone" is an array of cubic closest-packed spheres, with the sphere centers and radii randomized by 10%. A slug of blue solute is injected into the left back face, and is dispersed by the flow. The slight variations from ideal geometry create inhomogeneities in the flow field, enhancing dispersion.

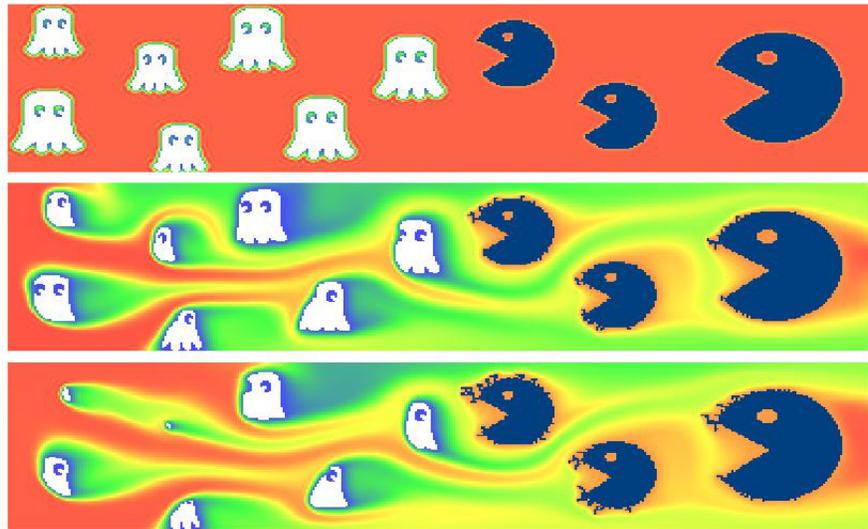
Applications

Fracture Mixing



Fluid flows in through inlets 1&2 with speed U ; fluid stream 1 carries a “black” tracer. The mixing ratio $M_r = C_3/C_1 \gg C_3/(C_3 + C_4)$.

Dissolution and Precipitation (Dendrite Growth)



The “ghosts” and “pacmen” are solids with the same chemical composition, but the ghosts are more soluble (metastable). Colors denote concentration. Left-to-right flow strips the boundary layers from the ghosts, ablating leading edges. Dendrites growing on the pacmen snouts lift the boundary layer, making dendrite tips the most probable sites for new growth.

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