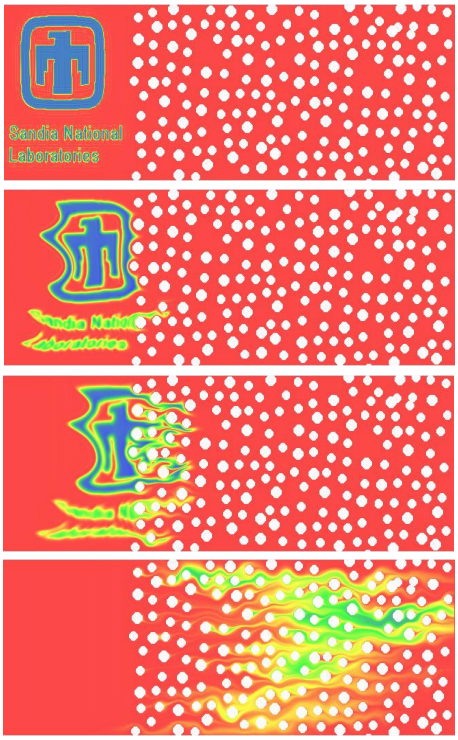
Sandia National Laboratories

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.



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

Needs

Fracture network models

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

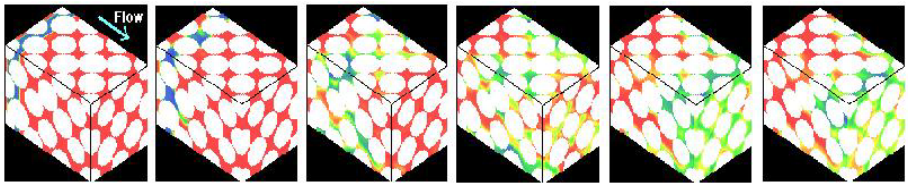
Single fracture / Hele-Shaw models

- 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 $(Pu,U)O_2$ in molten salts, near-field corrosion of glass and metal waste forms, ^{90}Sr and actinide exchange in carbonate rocks.

3D LB: Dispersion in Sandstone



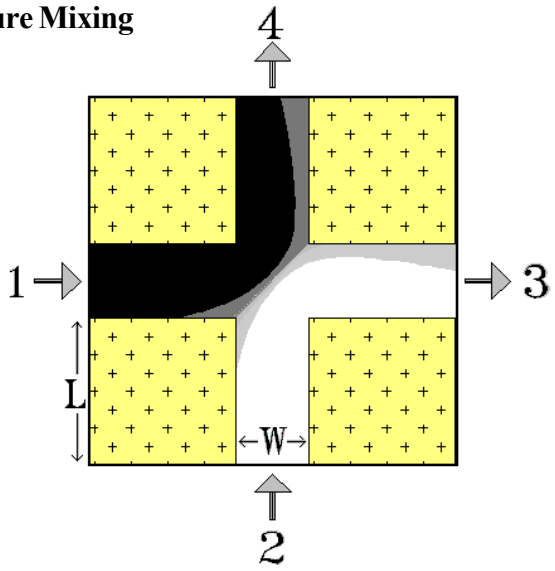
The idealized "sandstone" is an array of cubic closest-packed spheres, with the sphere centers and radii randomized by 10%. A slug of blue solute is injected into the left back face, and is dispersed by the flow. The slight variations from ideal geometry create inhomogeneities in the flow field, enhancing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

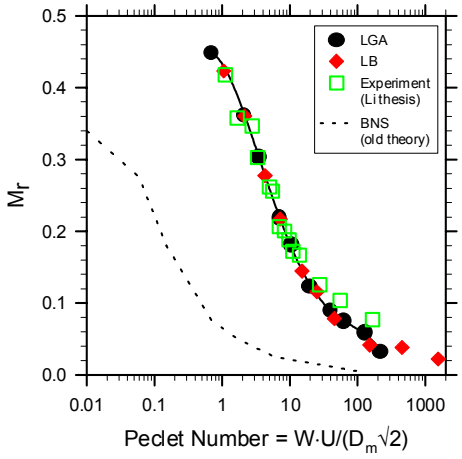
Sandia is a multiprogram laboratory operated by Sandia corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Sandia National Laboratories

Applications

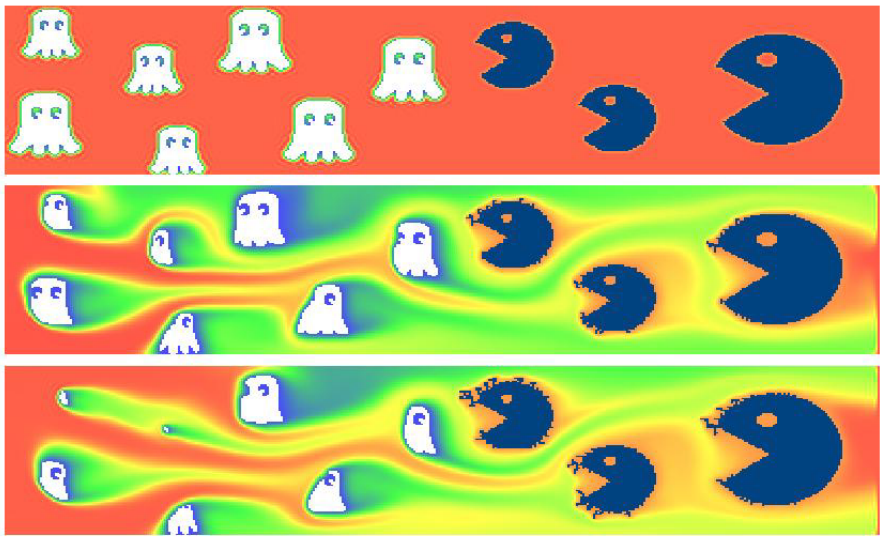
Fracture Mixing





Fluid flows in through inlets 1&2 with speed U; fluid stream 1 caries a "black" tracer. The mixing ratio M_r = C3/C1 » C3/(C3 + C4).

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.

Contact

Harlan W. Stockman
Geochemistry Department
Sandia National Laboratories
P.O. Box 5800, MS 1399
Albuquerque, New Mexico 87185-1399
Phone: (702) 363-8552
Fax: (702) 295-4438
Email: stockman3@earthlink. net

Sponsors

- Sandia LDRD Office
- DOE Office of Basic Energy Sciences