An Adaptive Embedded Boundary Method for Pore Scale Reactive Transport

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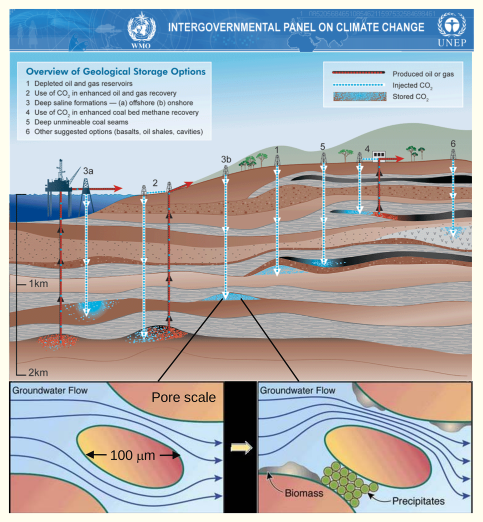
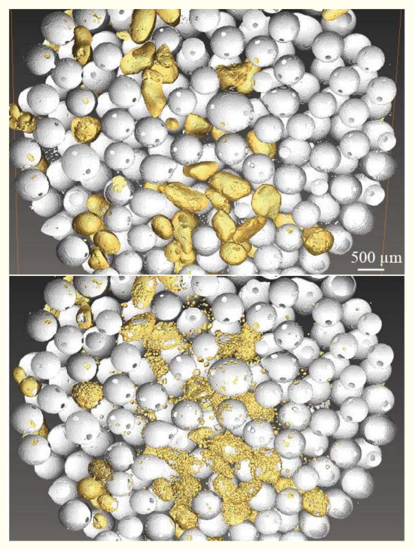
MOTIVATION

Subsurface Carbon Sequestration

Geochemical transport modeling using continuum-scale models has served as a valuable predictive tool in evaluating fate of CO_2 in geologic sequestration scenarios. However,

- Spatial variation of chemical concentrations due to mass-transport limitations leads to phenomena far from equilibrium.
- Pore structure can evolve due to mineral reactions.
- Reactions rates are based on lab-measured rates at the fluid-mineral pore scale, leading to field-laboratory disparity.
- Pore-scale modeling may be used to inform continuum-scale (Darcy) models and achieve more accurate upscaling.





Before calcite precipitation experiment

After calcite precipitation experiment

Noiriel et al., *AGU* (2010)

MODELING APPROACH

Adaptive Finite Volume Methods

We have developed a high performance simulation capability for incompressible Navier-Stokes (INS) and scalar advection-diffusion-reaction (ADR) equations:

$$\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\,\mathbf{u} + \nabla p = \nu\Delta\mathbf{u}$$
$$\nabla\cdot\mathbf{u} = 0$$
$$\frac{\partial c_k}{\partial t} + (\mathbf{u}\cdot\nabla)\,c_k = \nabla\cdot D_k\nabla c_k + R$$

- Embedded Boundary (EB) method for complex geometry
- Adaptive mesh refinement (AMR)
- Direct simulation from image / X-ray Microtomography (XMT) data using level sets and implicit functions
- Efficient predictor-corrector projection scheme
- 2^{nd}-order accurate advection scheme with new stable hybridization of advective derivative
- Novel multigrid solver for elliptic problems in very complex geometry (multiply-connected domains)
- Time-dependent fluid-solid boundary
- Fluid-fluid interface tracking
- Amenable to multi-component reaction networks
- Scalable to 100,000s processors

ALGORITHMS

Embedded Boundary Advection Discretization

We have developed a new higher-order upwinding advection scheme with new treatment of small cell problem for embedded boundary methods that hybridizes a linear combination of the conservative estimate of the advective derivative from the divergence theorem with a normalized by volume fraction estimate of the same:

$$\vec{u}\cdot\nabla\vec{u}^{n+1/2} = \kappa_i(\nabla\cdot(\vec{u}\vec{u}))_i + (1-\kappa_i)(\vec{u}\cdot\nabla\vec{u})_i^{NC}$$
$$\vec{u}\cdot\nabla\vec{u}_i^{NC} = \frac{\sum_i(\kappa_i\nabla\cdot(\vec{u}\vec{u})_i)}{\sum_i\kappa_i}$$

Unlimited transverse upwind slopes in the advection algorithm can lead to out of bounds updated scalar values. We redistribute the under/over shoot in a cell to its neighbors by mass:

if $c_i < 0$, $\delta m_i = \kappa_i c_i$, $w_i = \max(0, c_i)$, $c_i = 0$;

if $c_i > 1$, $\delta m_i = \kappa_i(c_i - 1)$, $w_i = \max(0, 1 - c_i)$, $c_i = 1$;

$\longrightarrow$

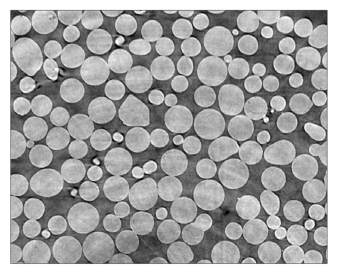
$$c_{i'} = c_{i'} + \delta m_{i,i'},\ \ i' \in N(i)$$
$$\delta m_{i,i'} = (w_{i'}\delta m_i)\left(\sum_{i'\in N(i)}\kappa_{i'}w_{i'}\right)^{-1}$$

Hybrid Multigrid Preconditioner for Poisson

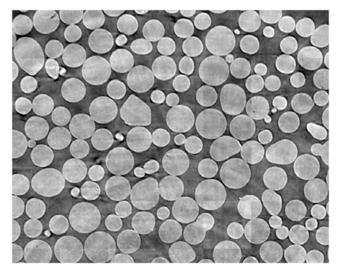
Realistic pore space can lead to very complex geometry made up of multiply-connected domains leading to unrepresented geometry at the coarsest levels of geometric multigrid (GMG) and subsequent pitfalls in restriction and prolongation. Instead, when solving pressure-Poisson we proceed directly to algebraic multigrid (AMG) as the preconditioner. AMG convergence rates improve by 3-4 orders of magnitude compared to GMG V-cycles.

Image Data Pre-Processing for Simulation

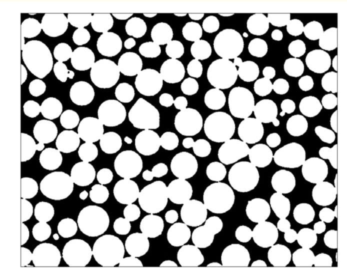
X-ray microtomography image data must be pre-processed due to noise, illumination, streaks and other artifacts:



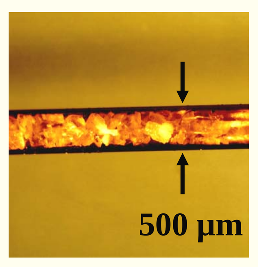
Original XMT image courtesy of J. Ajo-Franklin



De-noised and regionally corrected by wavelet

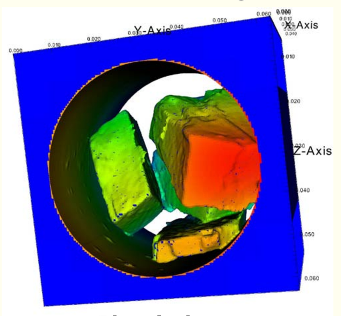


Bi-Gaussian mode identification and 3D flood fill algorithm



Crushed calcite experiment Li Yang

XMT image Jonathan Ajo-Franklin



Simulation

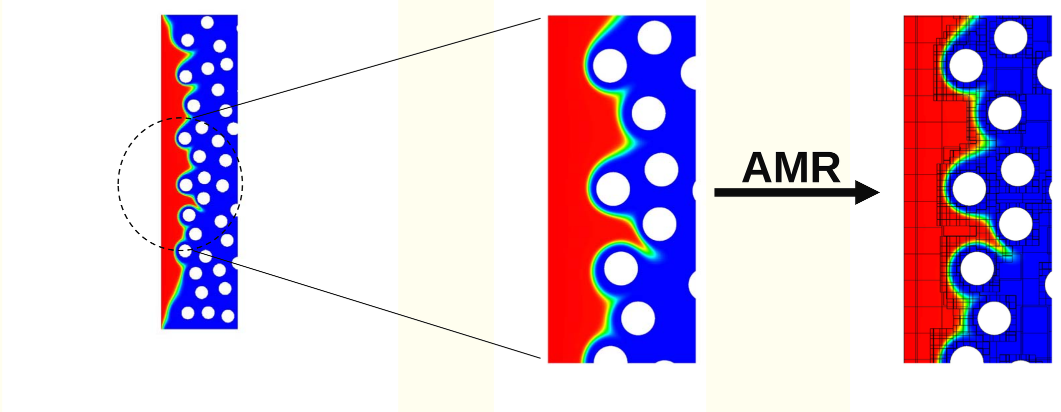
Fluid-Fluid / Fluid-Solid Interfaces

We have developed algorithmically consistent methods for time-dependent solid boundaries and fluid-fluid interfaces using level set representation of the interface and space-time discretization of the divergence theorem.

RESULTS

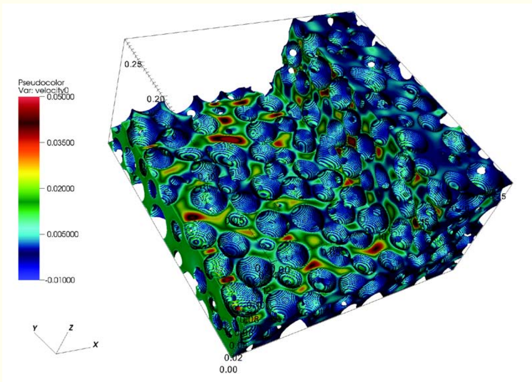
EB AMR in Packed Bed Systems

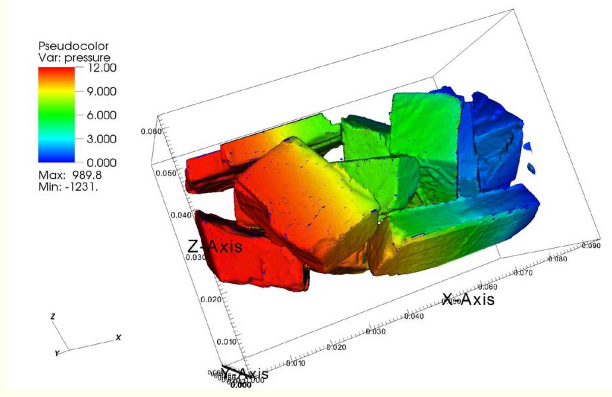
2D scalar ADR with first-order decay reaction.



Direct Numerical Simulation from Image Data

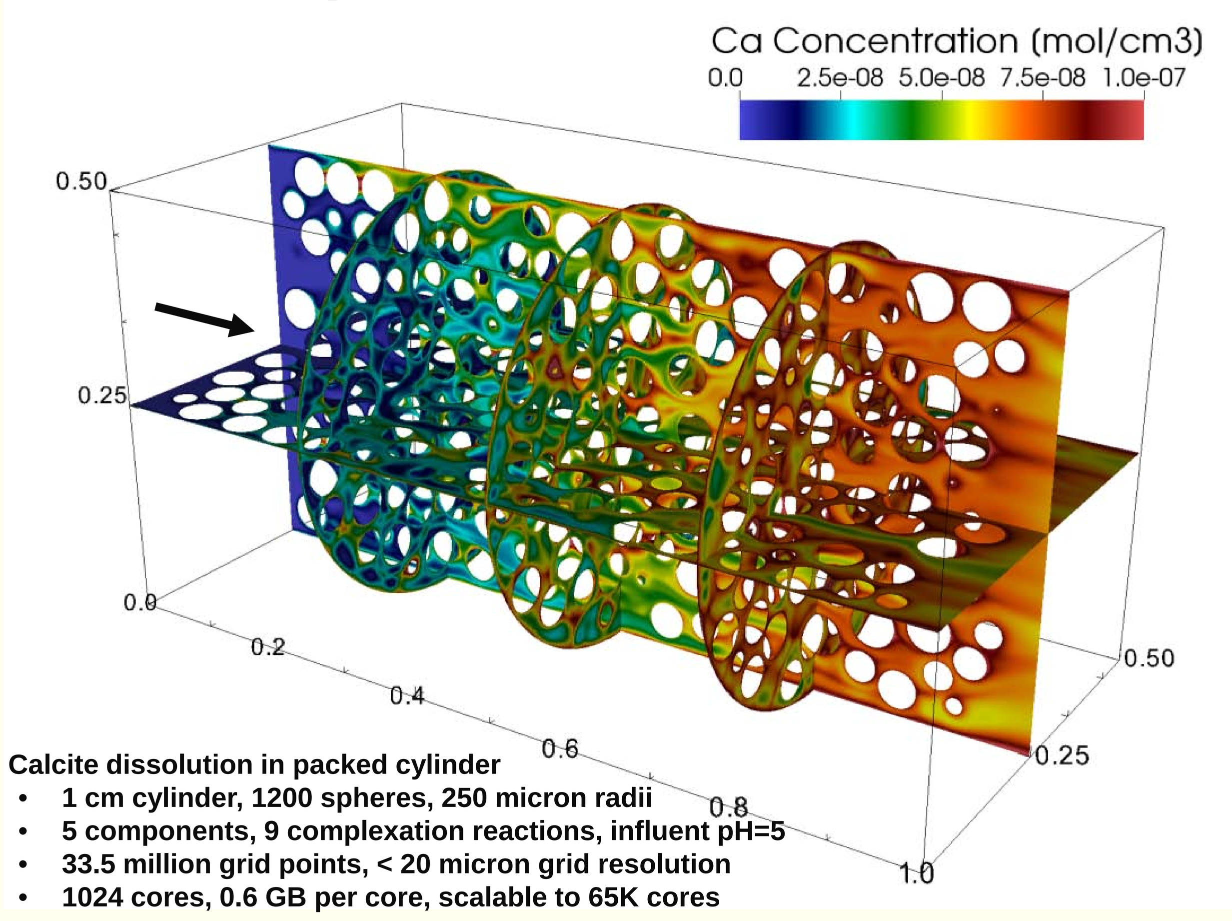
(L) Sintered glass bead pack (R) crushed calcite capillary tube





“World’s Largest Pore Scale Reactive Transport Simulation”

Using operator splitting, we interfaced the multi-component geochemistry module of CrunchFlow with the Chombo INS-ADR framework and simulated 5 components, 9 complexation reactions in a cylinder packed with 1200 reactive microspheres at < 20 micron grid resolution:



Calcite dissolution in packed cylinder

- **1 cm cylinder, 1200 spheres, 250 micron radii**
- **5 components, 9 complexation reactions, influent pH=5**
- **33.5 million grid points, < 20 micron grid resolution**
- **1024 cores, 0.6 GB per core, scalable to 65K cores**

References

- D. Trebotich and D. T. Graves (2011), “An Adaptive Finite Volume Method for Incompressible Flow and Transport in Complex Geometry”, in preparation
- G. H. Miller and D. Trebotich (2011), “An embedded boundary method for the Navier-Stokes equations on a time-dependent domain”, in press *Communications in Applied Math and Computational Science.*
- S. Molins, D. Trebotich, C. I. Steefel and C. Shen (2011) “An Investigation of the Effect of Pore Scale Flow on Average Geochemical Reaction Rates Using Direct Numerical Simulation”, submitted *Water Resources Research*
- C. Shen et al. (2011) “High Performance Computations of Subsurface Reactive Transport Processes at the Pore Scale”, SciDAC 2011

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