

# High Resolution Simulation and Characterization of Density-Driven Flow in CO<sub>2</sub> Storage in Saline Aquifers

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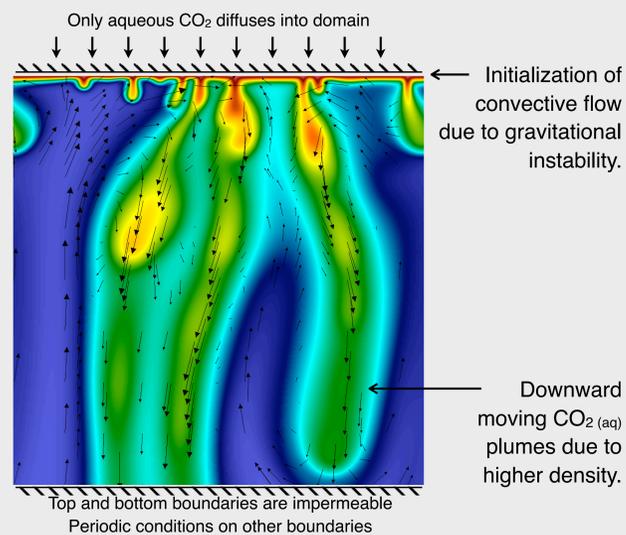
## The Approach

### Motivation

The dissolution-diffusion-convective process removes CO<sub>2</sub> from a highly mobile and buoyant gas phase and puts it into a less mobile and negatively buoyant aqueous phase. We study the short term and long term behaviors of the process through high resolution simulations using a second-order accurate sequential algorithm, implemented within a block structured adaptive mesh refinement framework.

### Problem Setup

Variable-density single-phase incompressible model to efficiently capture the transport mechanisms.



- Equation of states:  $\frac{1}{\rho} = \sum_{i=1}^2 \frac{X_i}{\rho_i}$   
 $\rho_i, X_i$ : component density, mass fraction
- Density increase due to CO<sub>2</sub> dissolution = 10.45 kgm<sup>-3</sup>.
- Convective flow is induced by random permeability or porosity.

### Governing Equations

Based on a total velocity splitting approach:

- Velocity divergence constraint reflects dependence of fluid density on the mass fraction of dissolved CO<sub>2</sub>:

$$\nabla \cdot \mathbf{u} = \sum_{i=1}^2 \frac{1}{\rho_i} \nabla \cdot \phi \rho \tau D \nabla X_i, \quad i = 1(\text{CO}_2), 2(\text{H}_2\text{O})$$

$\phi$ : porosity  $D$ : diffusion coefficient

- Darcy flow.

$$\mathbf{u} = -\frac{\kappa}{\mu} (\nabla p - \rho \mathbf{g})$$

$\kappa$ : permeability  $\mu$ : viscosity  $p$ : pressure

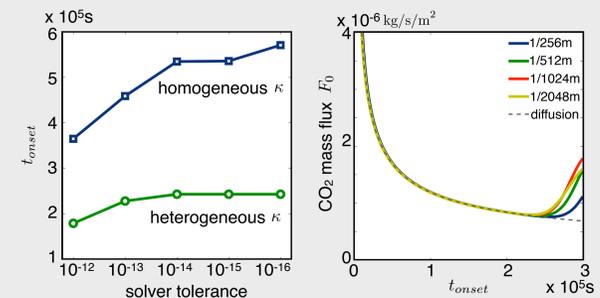
- Mass conservation.

$$\frac{\partial \phi \rho X_i}{\partial t} + \nabla \cdot (\rho X_i \mathbf{u}) = \nabla \cdot \phi \rho \tau D \nabla X_i, \quad i = 1, 2$$

## Numerical Method

### Second-order IMPES Algorithm

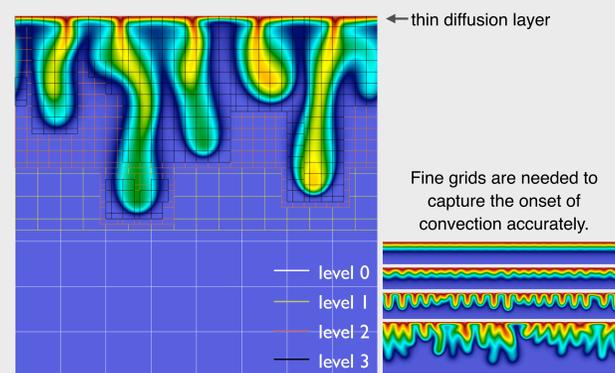
- Discretization
  - pressure equation → elliptic
    - finite difference, solved implicitly.
  - mass conservation equation → parabolic
    - advection term: 2nd order Godunov method;
    - diffusion term: Crank-Nicolson implicit scheme.
- Time stepping: time-centered.
- Advantages
  - minimizes numerical dispersion.
  - amenable to simple parallelization.



Accurate solver ensures the onset of convection is solely due to heterogeneity in rock properties and the onset time converges as grid spacing → 0.

### Adaptive Mesh Refinement (AMR) Framework

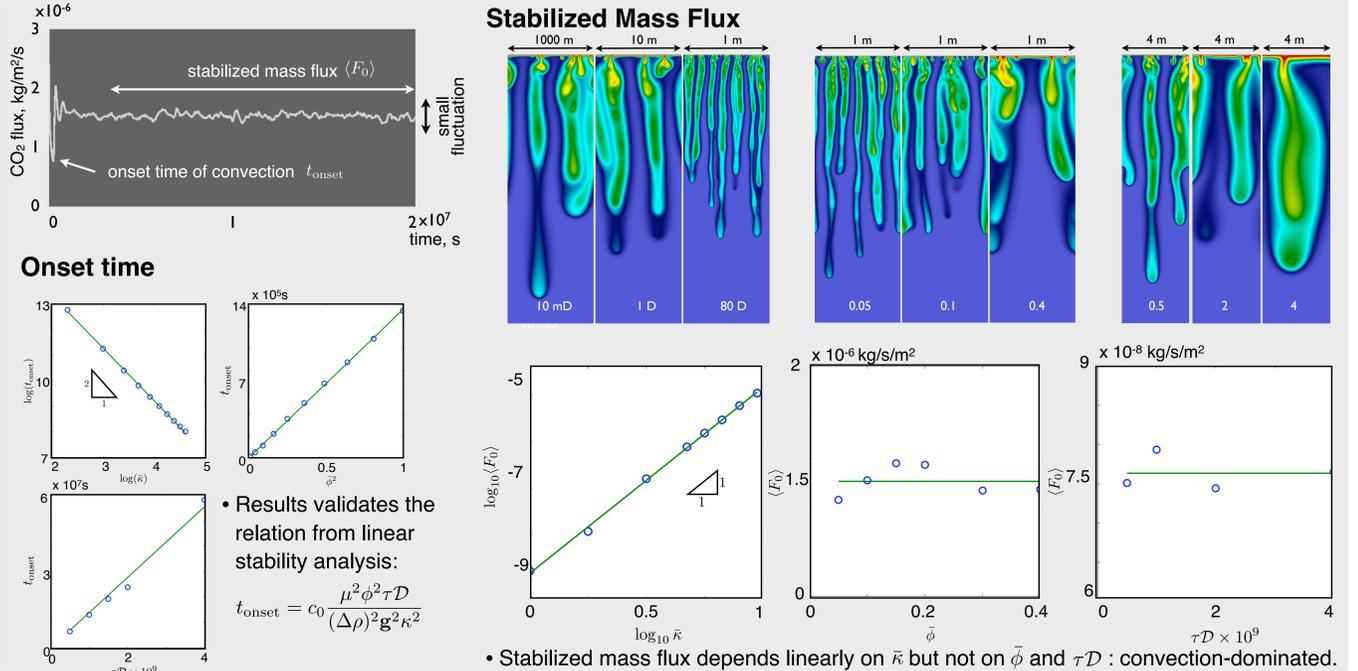
- Multiscale: resolves difference in length scales between flow regimes and time scales between flow and reaction.
- Parallelized codes: good scaling behavior up to several thousands CPUs, allowing large 3D simulation.
- Improved resolution: significant gain compared to existing codes, e.g. TOUGH family of codes.



### Relevant Publications

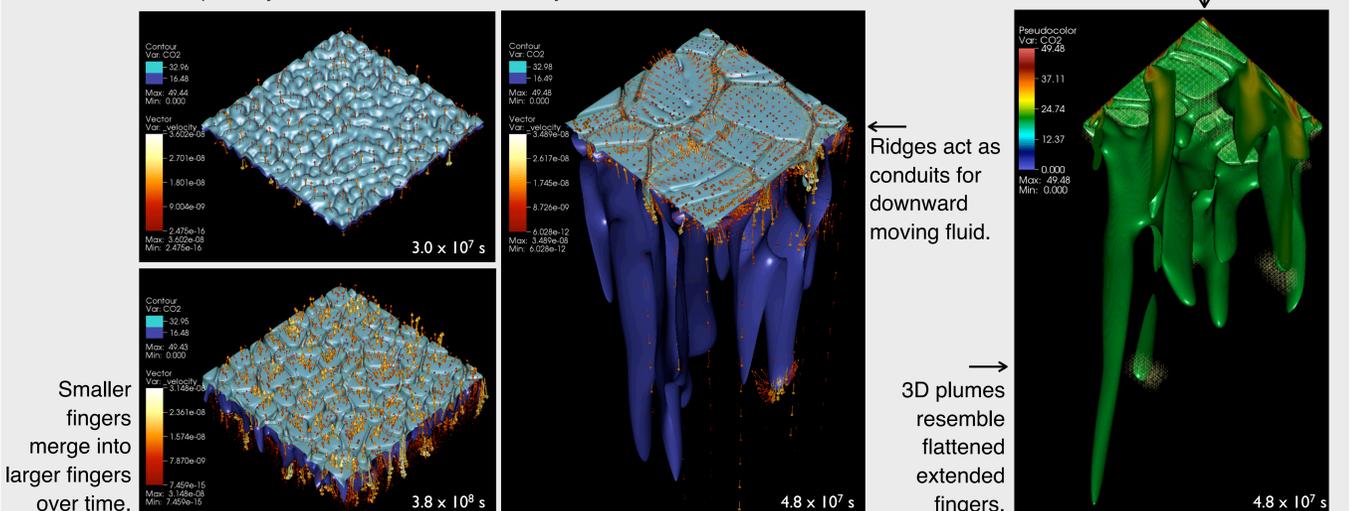
G. S. H. Pau, J. B. Bell, K. Pruess, A. S. Almgren, M. J. Lijewski and K. Zhang, "High resolution simulation and characterization of density-driven flow in CO<sub>2</sub> storage in saline aquifers", submitted, 2009.  
G. S. H. Pau, A. S. Almgren, J. B. Bell, and M. J. Lijewski, "A parallel second-order adaptive mesh algorithm for incompressible flow in porous media", *Phil. Trans. R. Soc. A* 367, 4633-4654, 2009.  
K. Pruess and K. Zhang, "Numerical modeling studies of the dissolution-diffusion-convective process during CO<sub>2</sub> storage in saline aquifers", Technical Report LBNL-1243E, LBNL, 2008.

## Results



### 3D Simulation

- Based on the Carrizo-Wilcox aquifer modeled by a mean permeability of 500 mD, uniform porosity of 0.15 and uniform diffusivity of  $2 \times 10^{-9}$  m<sup>2</sup>/s.



### Conclusion

- Integral measures (onset time and stabilized mass flux) are robust and insensitive to details of fluctuation.
- The onset time of convection follows the prediction of linear stability analysis.
- At long time, convection is the dominant transport mechanism.

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