SciDAC-2 project:
Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows Using Advance Computing

INCITE project:
Modeling Reactive Flows in Porous Media

Presented by

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SC07

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Introduction

- SciDAC-II project "Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows Using Advanced Computing" involves several institutions:
  - LANL: Peter Lichtner (PI), Chuan Lu, Bobby Philip, David Moulton
  - ORNL: Richard Mills
  - ANL: Barry Smith
  - PNNL: Glenn Hammond, Steve Yabusaki
  - U. Illinois: Al Valocchi
- Sister INCITE project, "Modeling Reactive Flows in Porous Media"

Project goals:

- Develop a next-generation code (PFLOTRAN) for simulation of multiscale, multiphase, multicomponent flow and reactive transport in porous media
- Apply it to field-scale studies of
  - Geologic CO_2 sequestration,
  - Radionuclide migration at Hanford site, Nevada Test Site,
  - Others…

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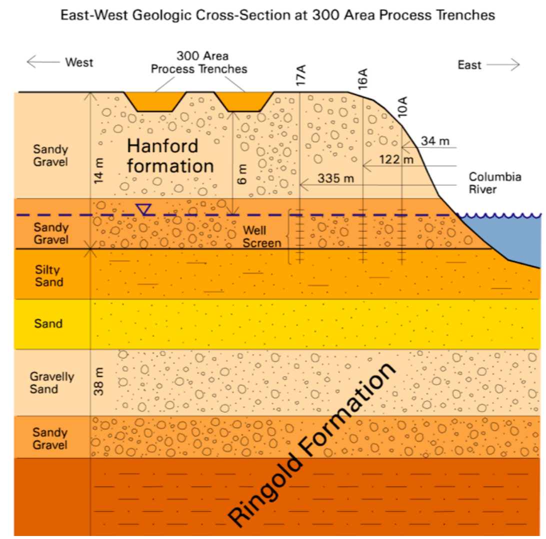
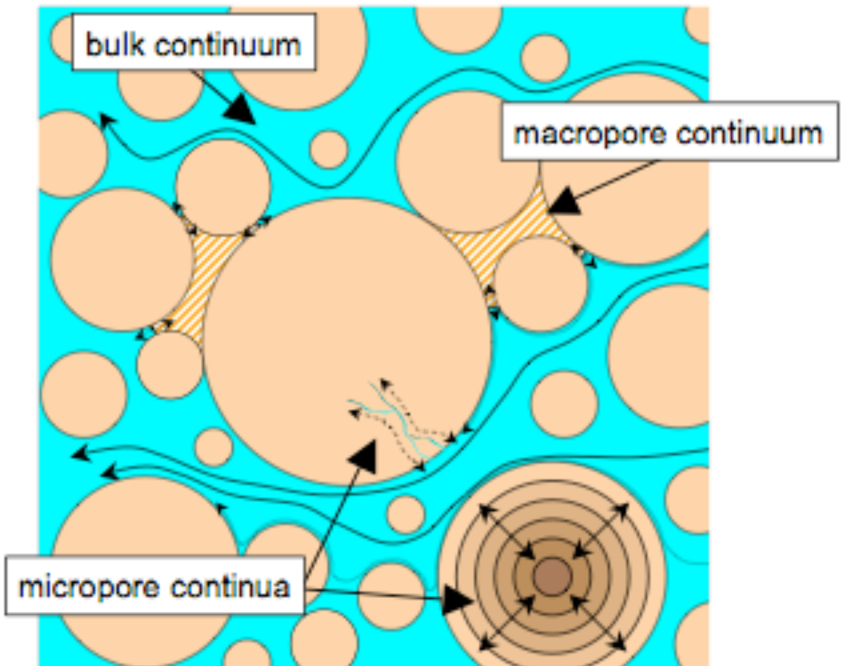
Motivating example—Hanford 300 area

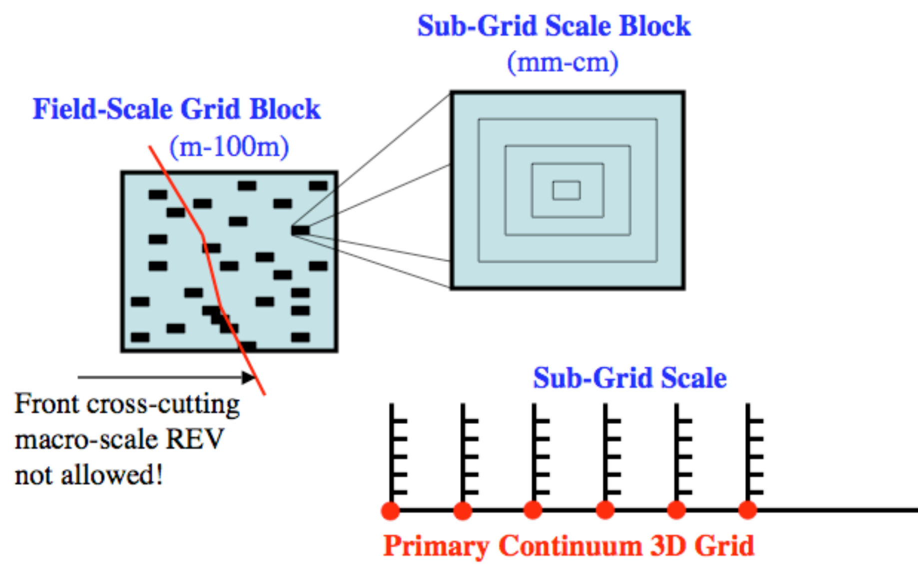


- At the 300 area, U(VI) plumes continue to exceed drinking standards.
- Calculations predicted cleanup by natural attenuation years ago!
- Because of long in-ground residence times, U(VI) is present in complex, microscopic inter-grain fractures, secondary grain coatings, and micro-porous aggregates. (Zachara et al., 2005).
- Constant K_d models do not account for slow release of U(VI) from sediment grain interiors through mineral dissolution and diffusion along tortuous pathways.
- In fact, the K_d approach implies behavior opposite to observations!
- We must accurately incorporate millimeter-scale effects over a domain measuring approximately 2000 x 1200 x 50 meters!

Modeling multiscale processes

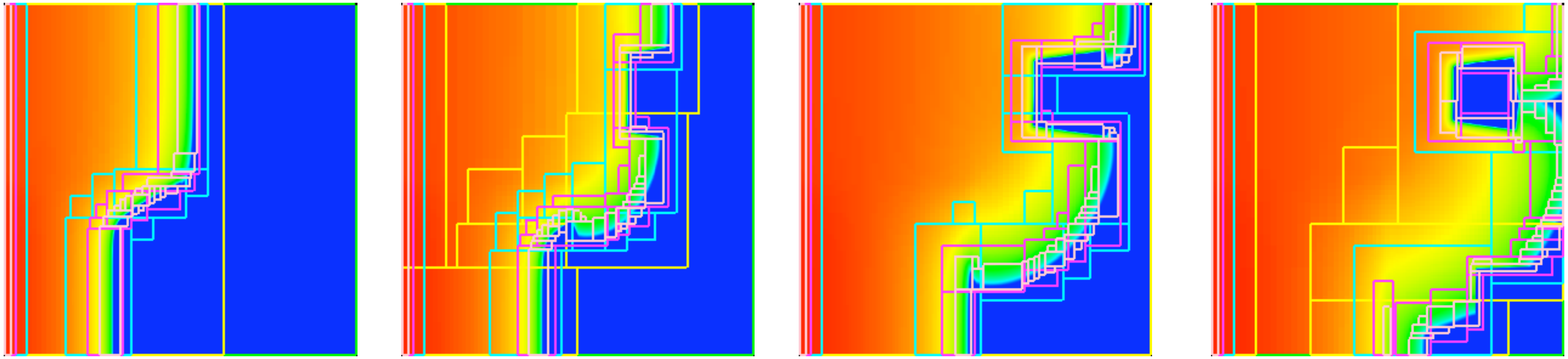
- Represent system through multiple interacting continua with a single primary continuum coupled to sub-grid scale continua.
- Associate sub-grid scale model with node in primary continuum
  - 1-D computational domain.
  - Multiple sub-grid models can be associated w/ primary continuum nodes.
  - Degrees of freedom: $N \times N_K \times N_{\mathrm{DCM}} \times N_c$.





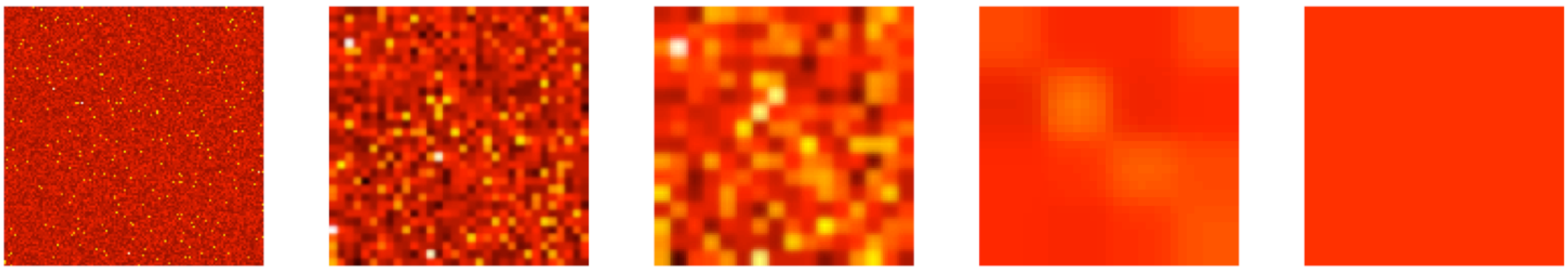
Adaptive mesh refinement (AMR)

- AMR introduces local fine resolution only in regions where needed.
- Significant reduction in memory and computational costs for simulating complex physical processes exhibiting localized fine scale features.
- AMR provides front tracking capability in the primary grid that can range from a centimeter to tens of meters.
- Sub-grid scale models can be introduced in regions of significant activity and not at every node within the 3-D domain.
- It is not necessary to include the sub-grid model equations in the primary continuum Jacobian even though these equations are solved in a fully coupled manner.



Upscaling

- Governing equations depend on averages of highly variable properties (e.g., permeability) averaged over a sampling window (REV).
- Upscaling and ARM go hand-in-hand: as the grid is refined/coarsened, material properties such as permeability must be calculated at the new scale in a self-consistent manner.



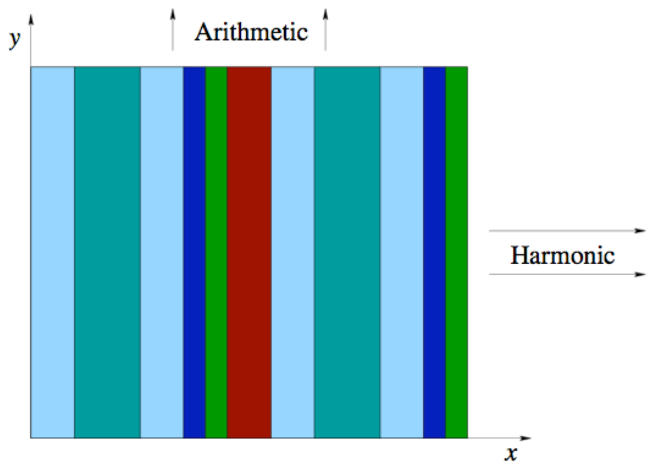
Above: A fine-scale realization (128 x 128) of a random permeability field,

$$\kappa(x,y) = \zeta^{-\ln(\alpha)},\ \zeta \text{ uniformly distributed in } (0,1),\ \alpha = 5$$

followed by successively upscaled fields (*N* x *N*, *N* = 32, 16, 4, 1) obtained with multigrid homogenization.

Upscaling

- Coarse-scale anisotropy: permeability must, in general, be considered as a tensor at larger scales even if it is a scalar (i.e., isotropic) at the finest scale.
- A single multidimensional average is inadequate for modeling



- Uniform flow from left to right governed by harmonic mean.
- Uniform flow from bottom to top governed by arithmetic mean.
- Suggests a diagonal permability tensor; HOWEVER, if stripes not aligned with coordinate axes, equivalent permeability must be described by a full tensor.

- Upscaling that captures full-tensor permeability includes multigrid homogenization and asymptotic theory for periodic media.
- Theory is limited to periodic two-scale media (well separated scales).
- Upscaling reactions poses a significant challenge as well. In some aspects of this work, volume averaging will suffice; while in others, new multiscale models will be required.

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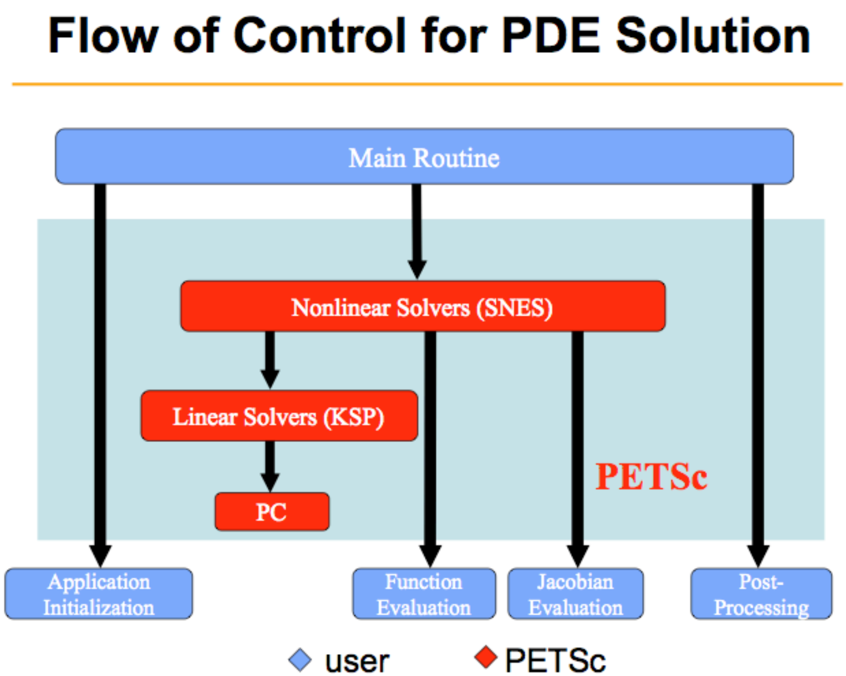
PFLOTRAN architecture

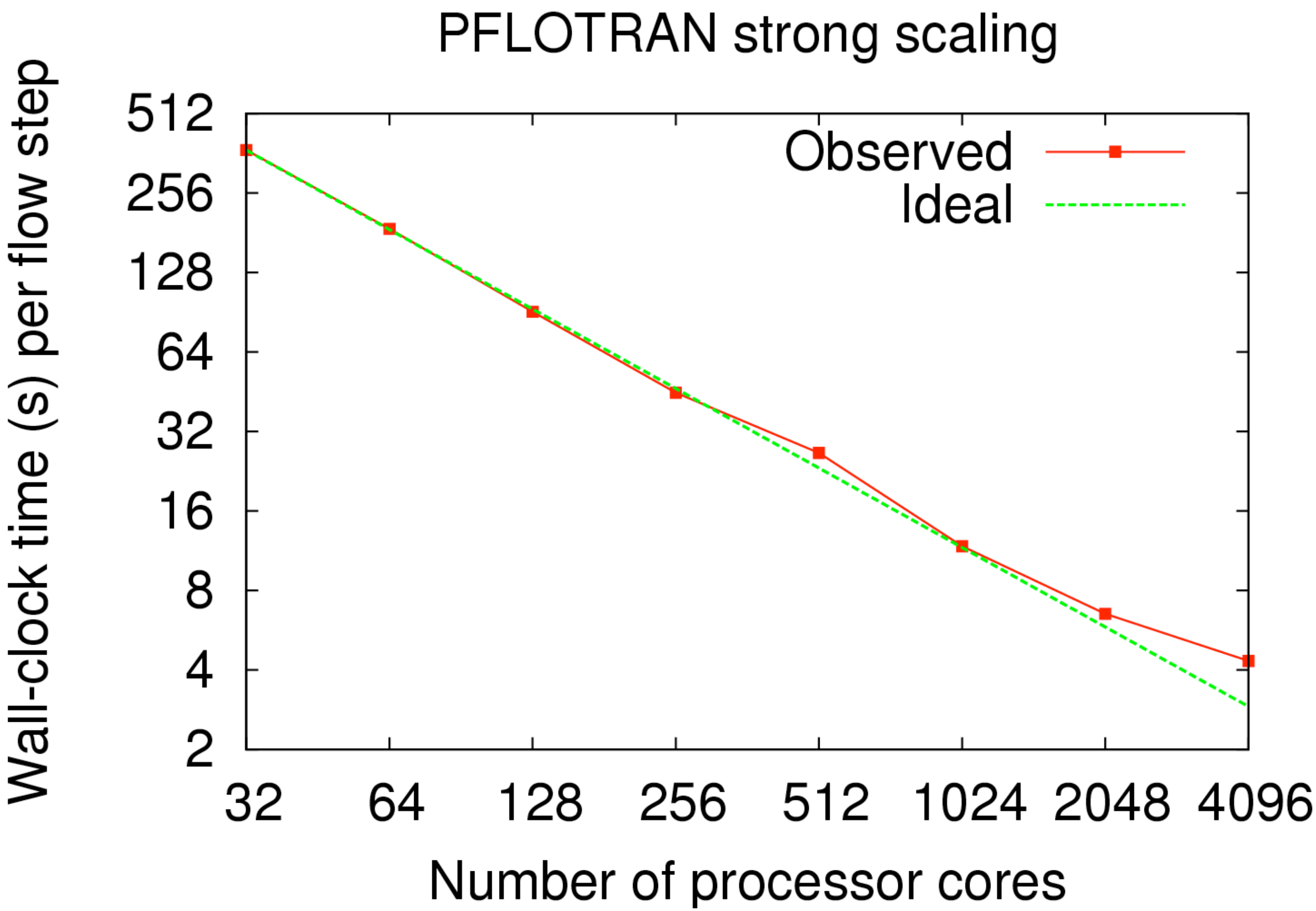
- PFLOTRAN is designed from the ground up for parallel scalability.
- Built on top of PETSc, which provides
  - management of parallel data structures,
  - parallel solvers and preconditioners,
  - efficient parallel construction of Jacobian and residuals



- AMR capability being built on top of SAMRAI.

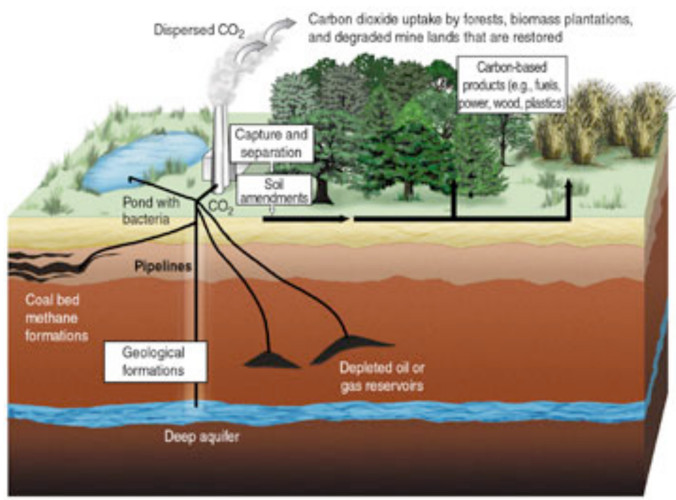
Parallel scalability

So far, PFLOTRAN has exhibited excellent strong scaling on Jaguar:



Application: Geologic CO_2 sequestration

- Capture CO_2 from power production plants and inject it as supercritical liquid in abandoned oil wells, saline aquifers, etc.



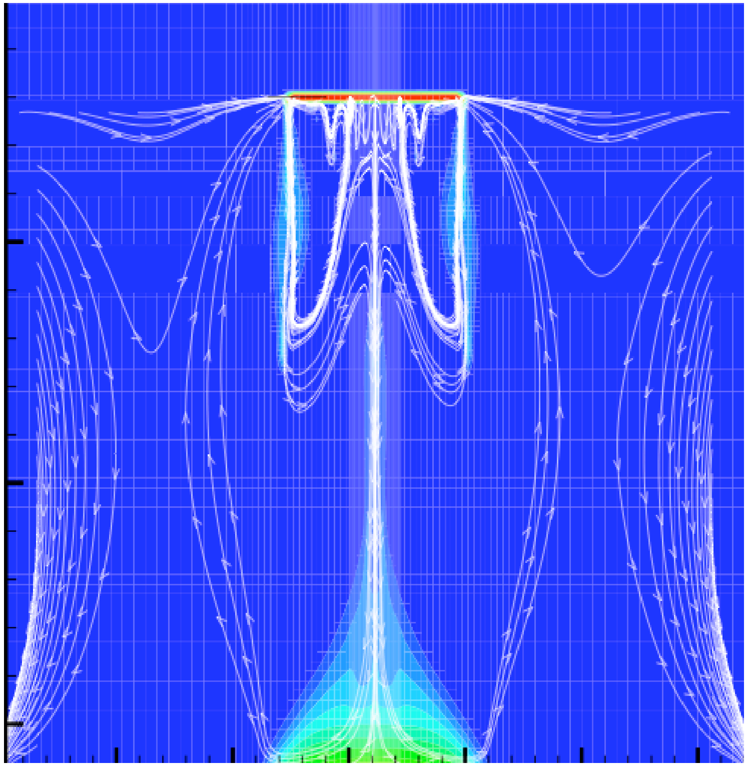
LeJean Hardin and Jamie Payne, ORNL Review, v.33.3.

- Must be able to predict long-term fate:
  - Slow leakage defeats the point.
  - Fast leakage could kill people!
- Many associated phenomena are very poorly understood.

Application: Geologic CO_2 sequestration

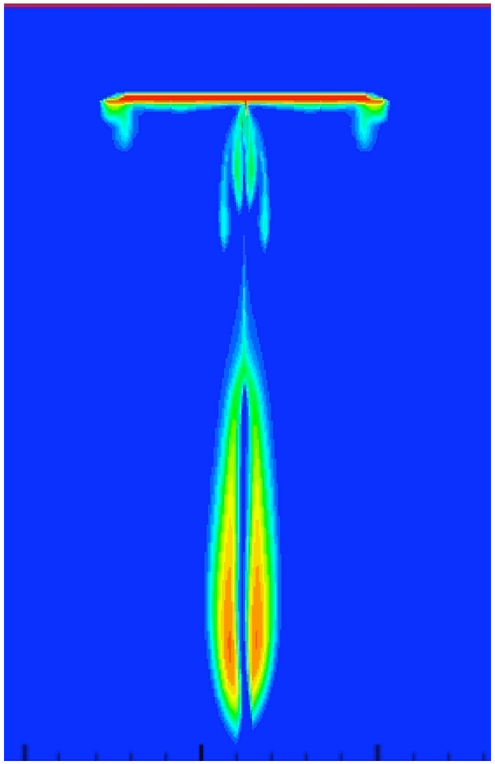
Density-driven fingering is one feature of interest:

- Density increases as supercritical CO_2 dissolves into formation brine.
- Buoyancy effects result in fingering.
- Widths may be on the order of meters or smaller.

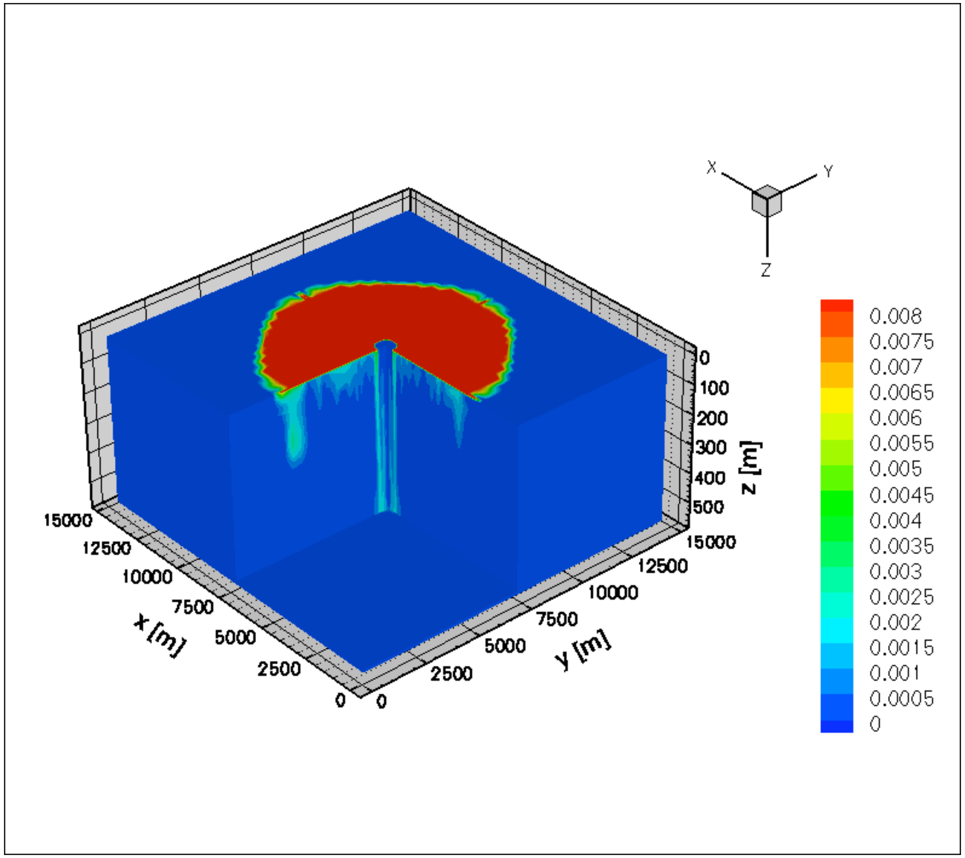


Left: Density-driven vortex made the fluid with higher CO_2 concentration "snap-off" from the source—the supercritical CO_2 plume.

Right: Enlarged center part of this domain at earlier time, illustrating two sequential snap-offs; the secondary is much weaker than the first one. The detailed mechanisms behind these behavior are under investigation.



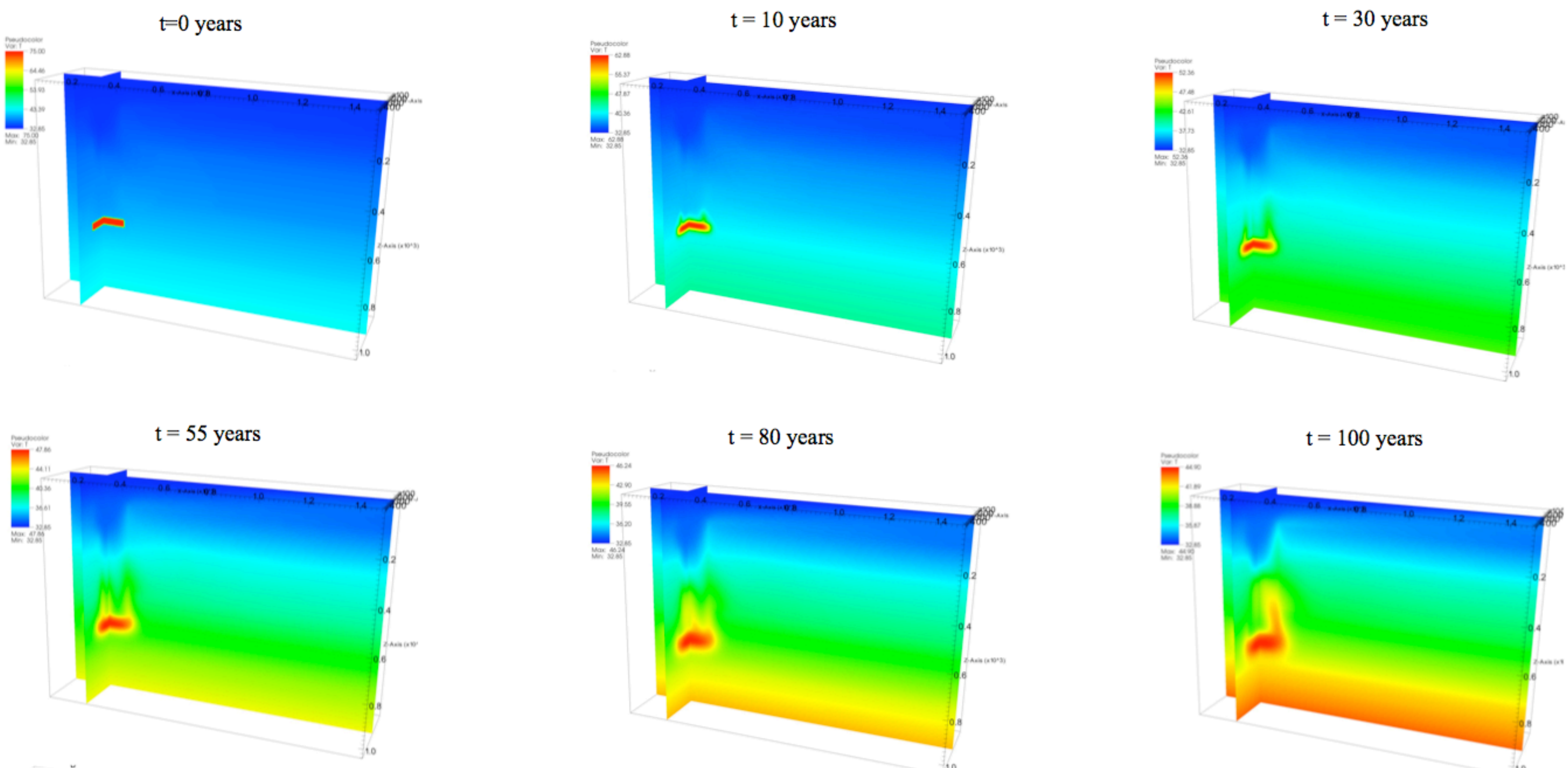
Application: Geologic CO_2 sequestration



Dissolved CO_2 after an elapsed time of 500 years following steady injection of supercritical CO_2 for 25 years. The figure illustrates instability caused by fingering as CO_2 dissolves into the formation brine. The calculation was performed on a grid 100x100x64 with 3 degrees of freedom per cell using Jaguar. Resolution of fingers is important because of its effect on the rate of plume dissipation, but difficult to model: fingers may range from centimeters to meters over a domain size of kilometers. The two-phase nature of the problem causes stability issues as the supercritical phase (not shown) spreads and eventually disappears with time.

Application: Radionuclide migration at NTS

Below: Simulation of near-field temperature distribution for an underground nuclear test at the Nevada Test Site. Heat from the melt glass causes convection plumes to develop, advecting radionuclides up into aquifers where lateral flow fields result in long-distance transport.



Summary

- Aim is to develop a next-generation, open-source code, PFLOTRAN, for simulation of subsurface reactive flows on machines ranging from workstations to ultrascale machines.

- Algorithmic and software developments include
  - multiple interacting continua,
  - structured adaptive mesh refinement,
  - fully unstructured meshes,
  - upscaling approaches to capture full-tensor permeability.

- PFLOTRAN will be applied to a variety of important problems:
  - geologic CO_2 sequestation,
  - radionuclide migration,
  - Others.

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