SciDAC-2 Project:
Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows Using Advanced Computing
INCITE Project:
Modeling Reactive Flows in Porous Media

Presented by

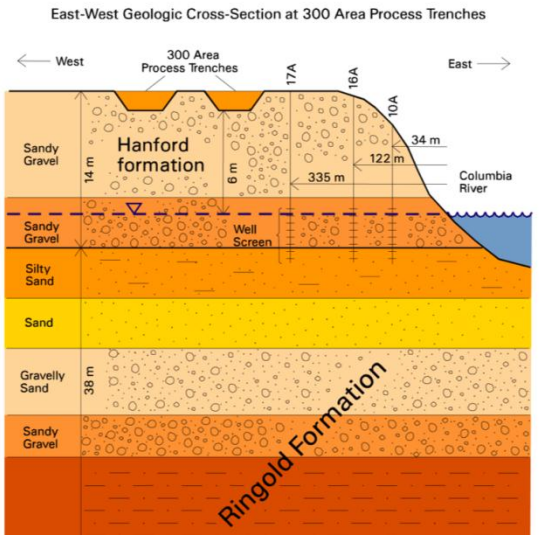
Richard Tran Mills

Computational Earth Sciences Group
Computer Science and Mathematics Division

Introduction

- **Funded by SciDAC-II project, "Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows using Advanced Computing," and sister INCITE project, "Modeling Reactive Flows in Porous Media," involving subsurface scientists, applied mathematicians, and computer scientists at several institutions**
  - **LANL: Peter Lichtner (PI), Daniil Svyatskiy, Scott Painter, David Moulton**
  - **ORNL: Richard Mills, Bobby Philip, Jitendra Kumar, Gautam Bisht**
  - **ANL: Barry Smith**
  - **PNNL: Glenn Hammond, Xingyuan Chen**
  - **U. Illinois: Al Valocchi**
  - **Additional collaborators**
    - **U. Utah: Chuan Lu**
    - **N.C. State: G. Mahinthakumar, Vamsi Sripathi (SciDAC PERI)**
- **Project goals**
  - **Develop a next-generation code (PFLOTRAN) for continuum-scale simulation of multiscale, multiphase, multicomponent flow and reactive transport in porous media**
  - **Apply it to field-scale studies of geologic CO_2 sequestration, contaminant migration**

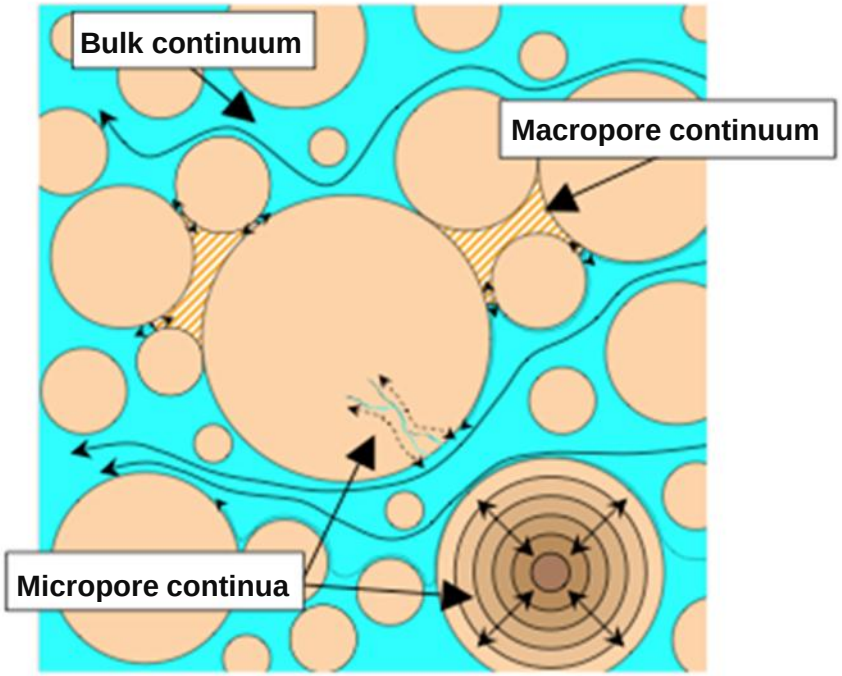
Motivating example—Hanford 300 Area

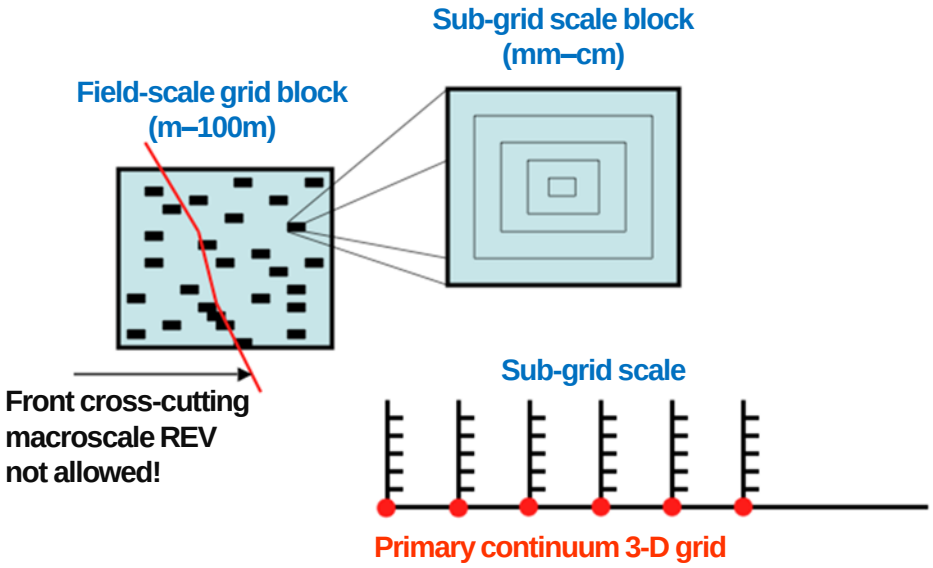


- At the Hanford 300 Area, U(VI) plumes continue to exceed drinking standards
- Calculations predicted cleanup by natural attenuation years ago!
- Because of long in-ground residence times, U(VI) is present in complex, microscopic intergrain fractures, secondary grain coatings, and microporous aggregates (J. Zacharia et al., Uranium Geochemistry in Vadose Zone and Aquifer Sediments from the 300 Area Uranium Plume, Tech. Rep. PNNL-15121, Pacific Northwest National Laboratory, Richland, WA, 2005)
- Models assuming constant Kd (ratio of sorbed mass to mass in solution) do not account for slow release of U(VI) from sediment grain interiors through mineral dissolution and diffusion along tortuous pathways
- In fact, the Kd approach implies behavior contrary to observations
- We must accurately incorporate millimeter-scale effects over a domain measuring approximately 2000 × 1200 × 50 meters

Modeling multiscale processes

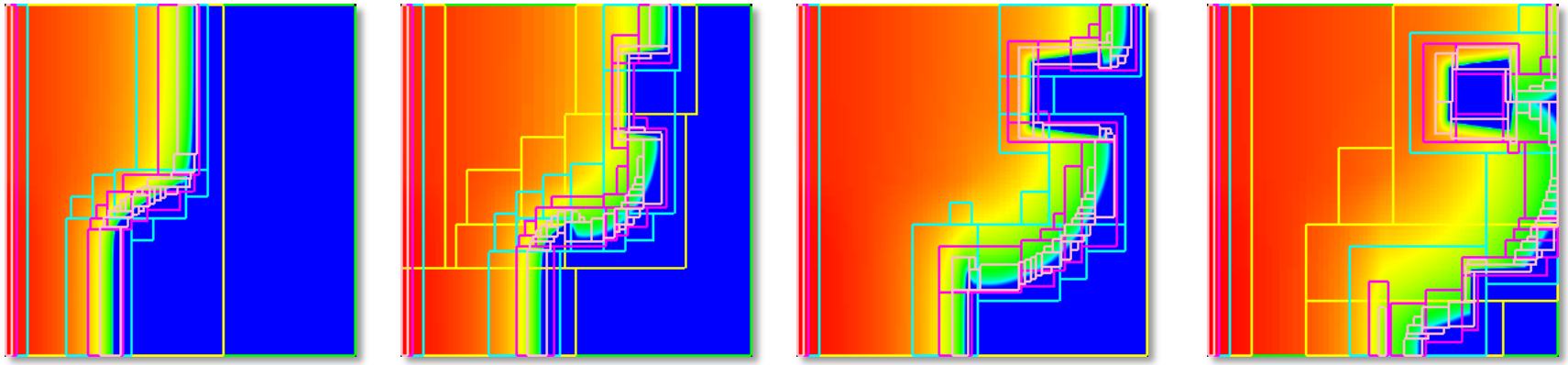
- Represent system through multiple interacting continua with a single primary continuum coupled to sub-grid scale continua
- Associate sub-grid scale model with node in primary continuum
  - 1-dimensional computational domain
  - Multiple sub-grid models can be associated with primary continuum nodes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





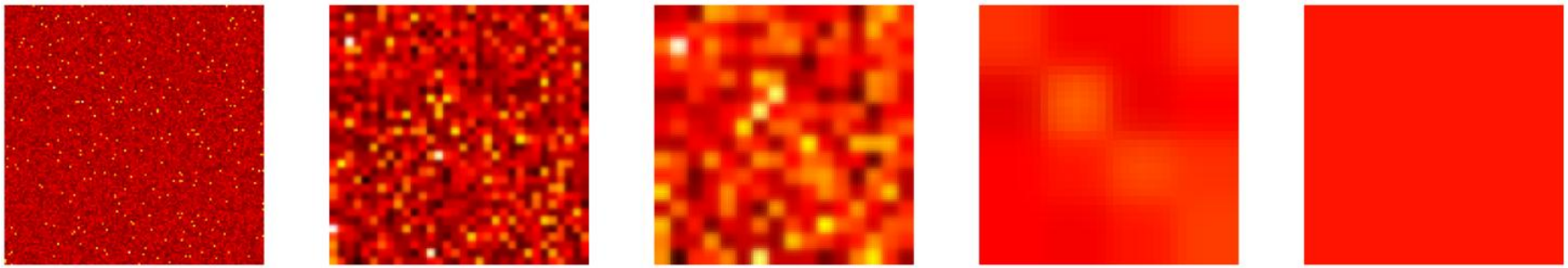
Adaptive mesh refinement (AMR)

- 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-dimensional 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

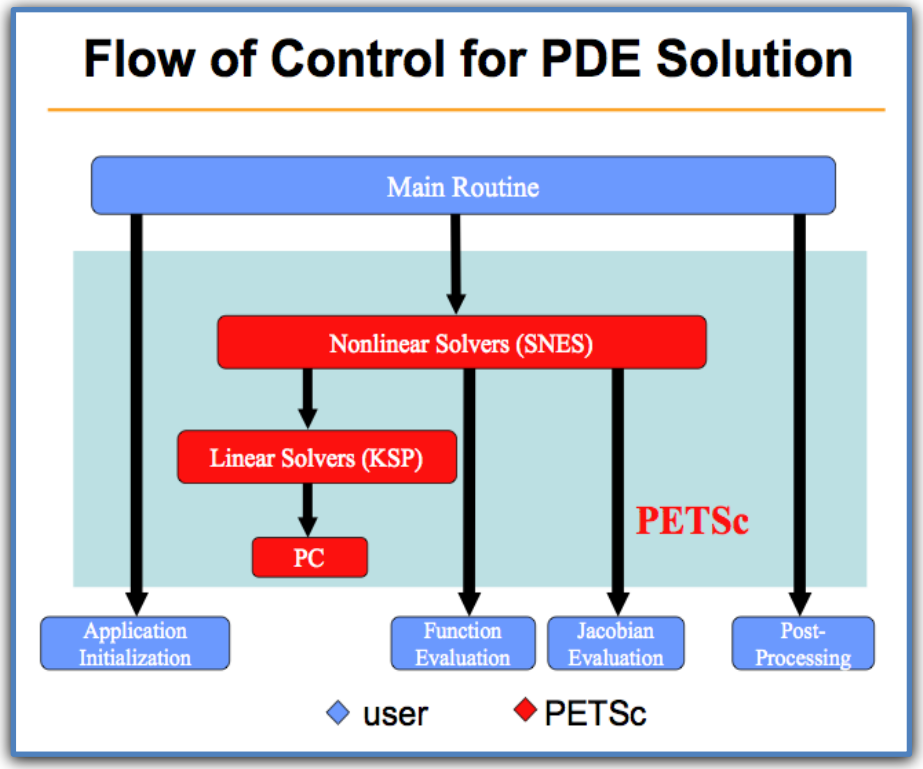
- Governing equations depend on averages of highly variable properties (e.g., permeability) averaged over a sampling window (REV)
- Upscaling and ARM go hand-in-hand: as the grid is refined/coarsened, material properties such as permeability must be calculated at the new scale in a self-consistent manner



Above: A fine-scale realization (128 × 128) of a random permeability field, $\kappa(x,y) = \zeta^{-\ln(\alpha)}$, ζ uniformly distributed in $(0,1)$, $\alpha = 5$ followed by successively upscaled fields ($N \times N$, N = 32, 16, 4, 1) obtained with multigrid homogenization

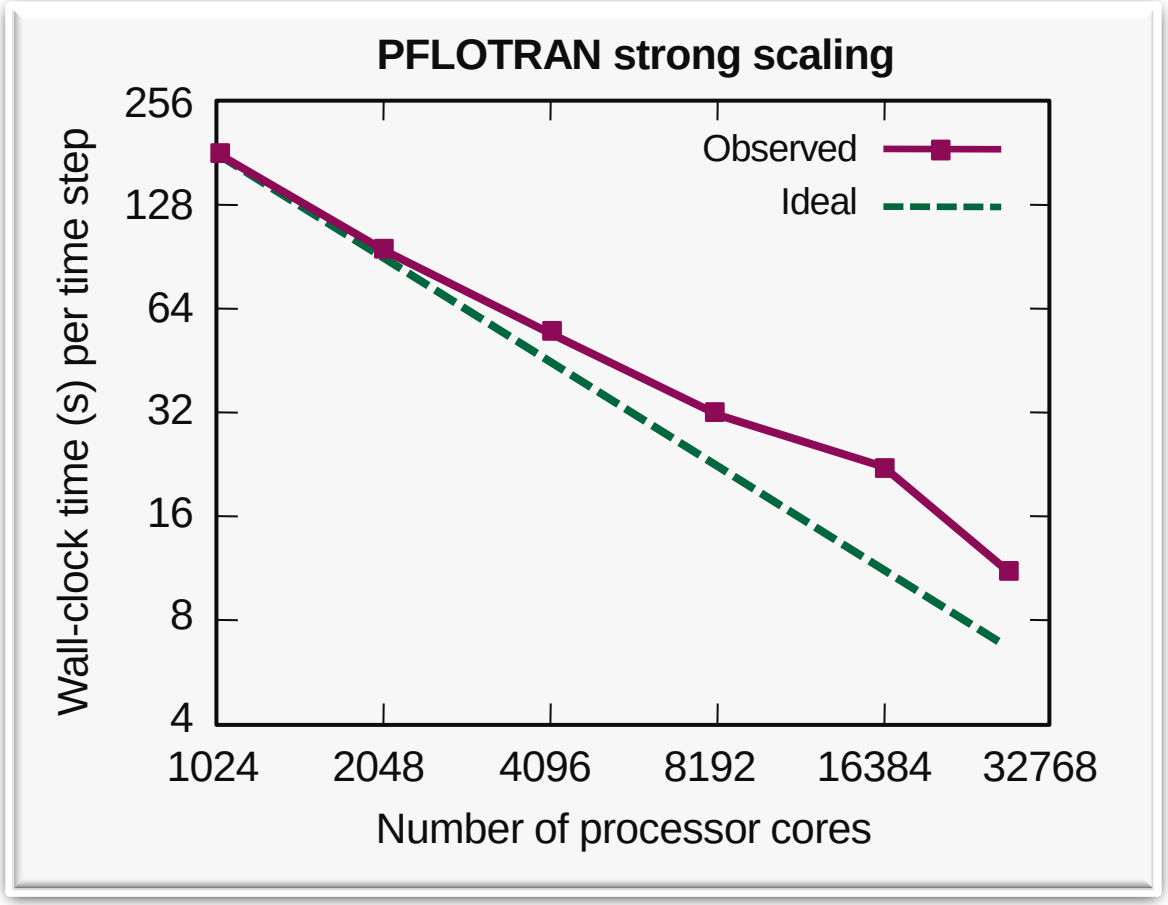
PFLOTRAN architecture

- Built on top of PETSc, which provides
  - Object-oriented management of parallel data structures
    - Create parallel objects (e.g., matrices and vectors) over a set of processors
    - Methods (e.g., MatMult()) called on those objects handle parallel coordination
  - Parallel solvers and preconditioners
  - Efficient parallel construction of Jacobians and residuals
- We provide
  - Initialization, time-stepping, equations of state, post-processing
  - Functions to form residuals (and, optionally, Jacobians) on a local patch (PETSc routines help us with patch formation by setting up scatter/gather contexts)



Parallel scalability

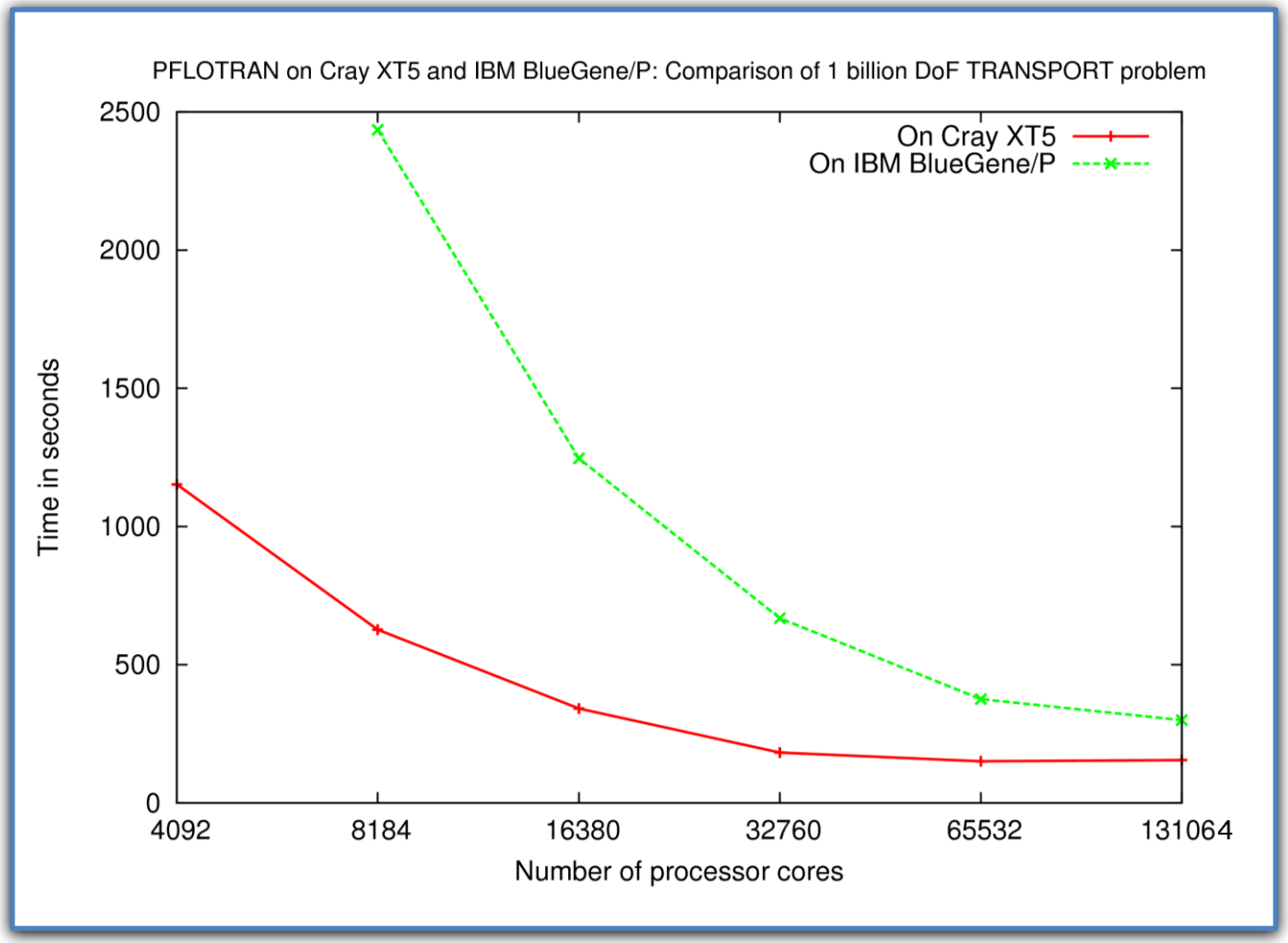
So far, PFLOTRAN has exhibited excellent strong scaling on Jaguar



Strong scaling performance for a variably saturated flow simulation of the Hanford 300 Area with 270 million total degrees of freedom

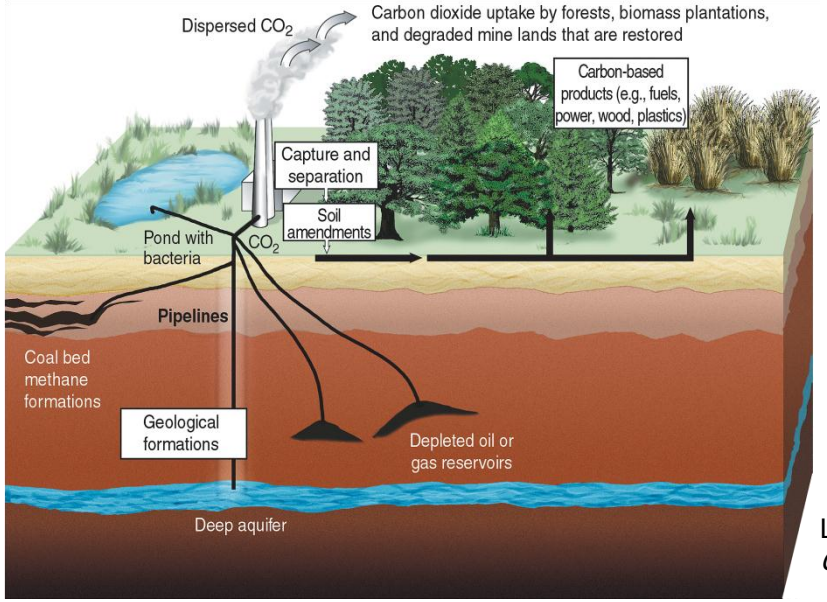
1B DoF reactive transport

1 billion degrees of freedom (850 × 1000 × 80 grid, 15 species)



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.

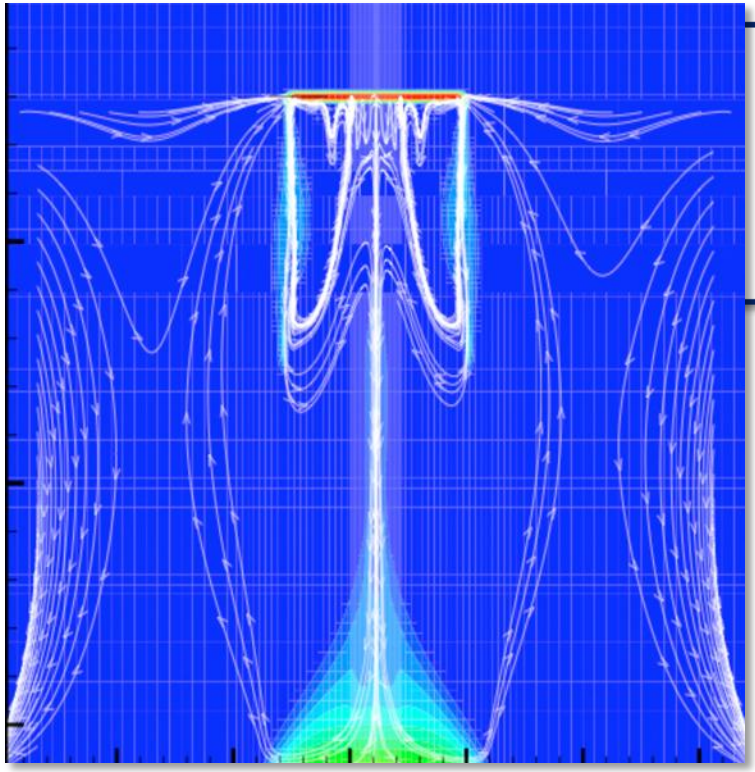


LeJean Hardin and Jamie Payne, *ORNL Review*, v.33.3.

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

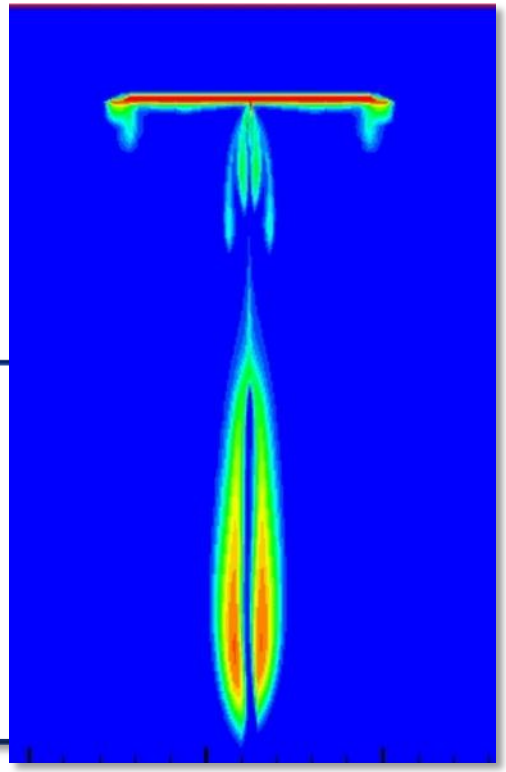
Application: Geologic CO_2 sequestration

- 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



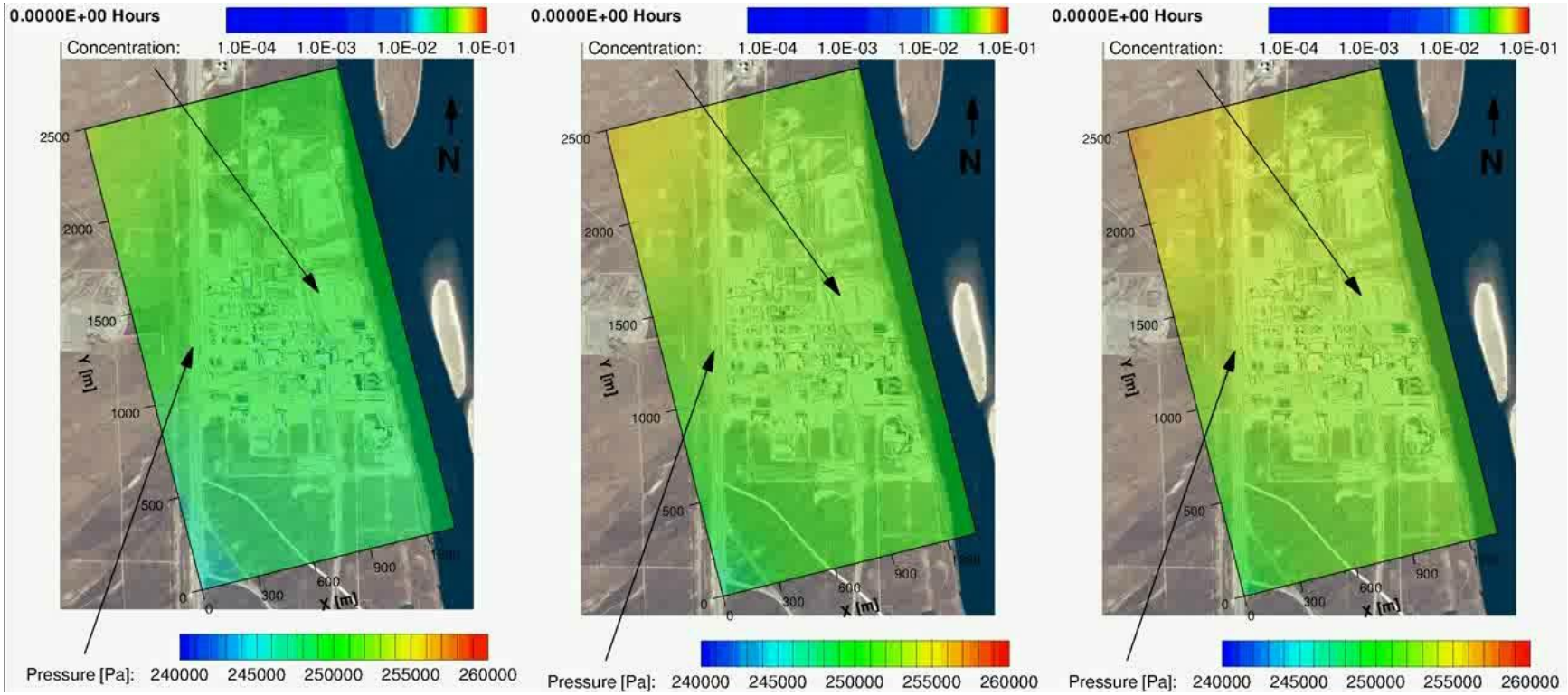
Density-driven vortex made the fluid with higher CO_2 concentration "snap off" from the source—the supercritical CO_2 plume

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 behaviors are under investigation



Application: Hanford 300 Area

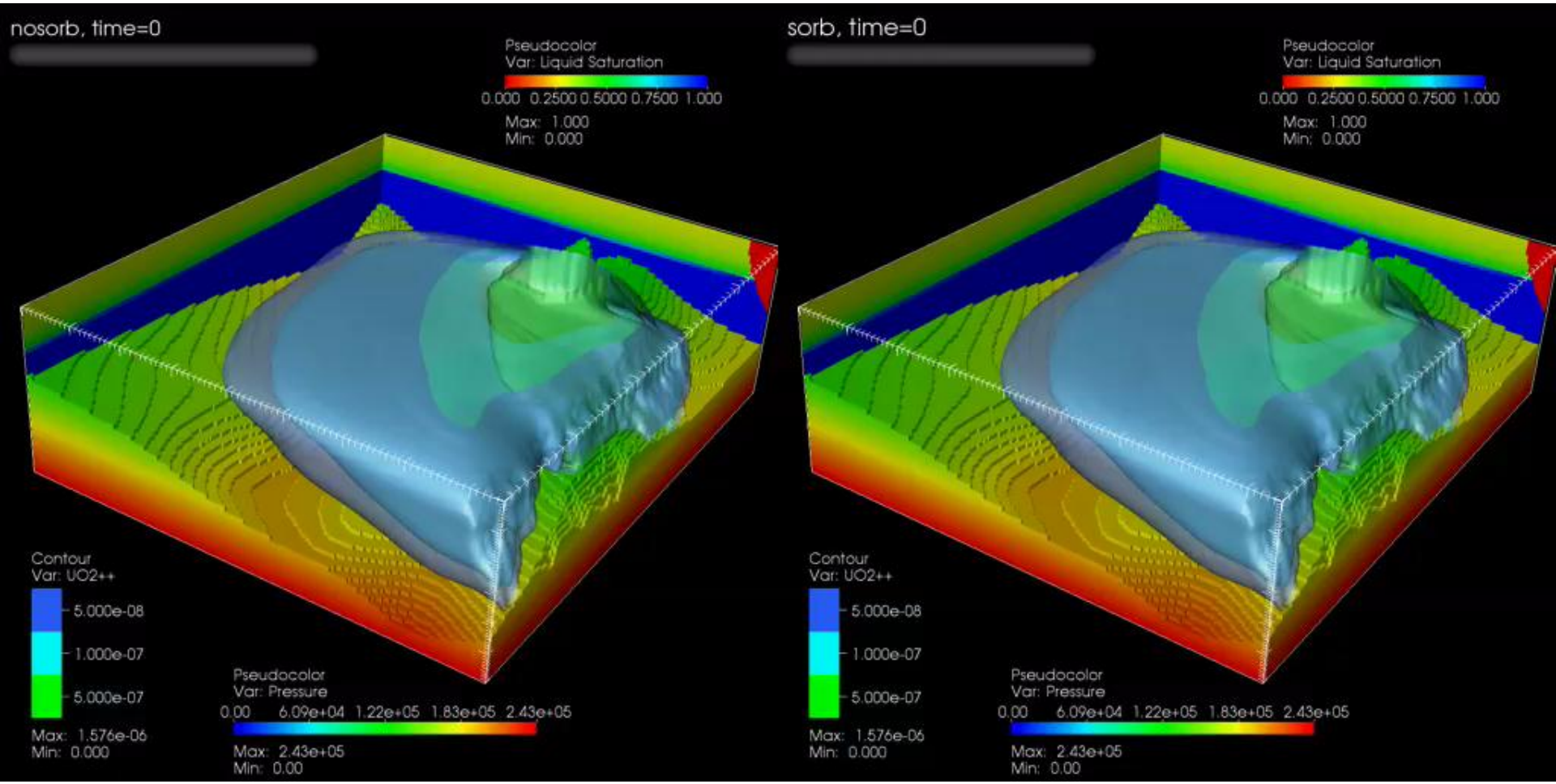
Recent simulations on Jaguar have provided the highest-resolution simulations to date of flow at the Hanford 300 Area in Washington. These simulations will help to determine appropriate remediation strategies



20 m x 20 m x 1 m **10 m x 10 m x 0.5 m** **5 m x 5 m x 0.25 m**

Pressure field and concentration of tracer plume 7500 hours after release at the Hanford 300 Area. Simulations using three different resolutions (with fidelity increasing from left to right) are shown. Velocities do not show convergence at the coarser resolutions, demonstrating the need for the high-resolution simulations that supercomputing enables

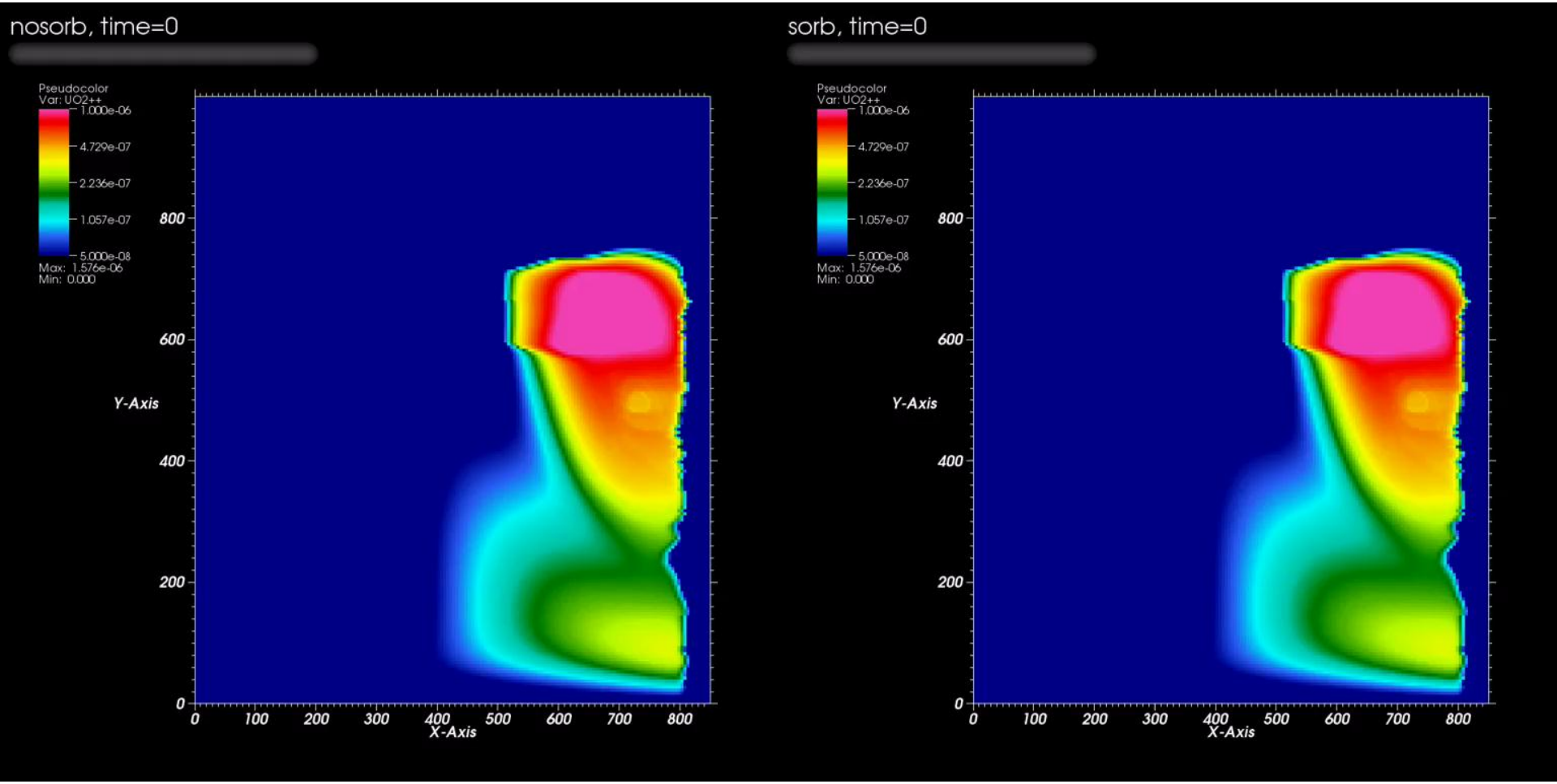
Hypothetical uranium plume migration



Without sorption

With sorption

Hypothetical uranium plume migration



Without sorption

With sorption

Where now?

- Using PETSc, we have developed a code, PFLOTRAN, that is now
- Highly modular, object oriented, extensible
- Can scale all the way from laptop computers to the largest scale computers in the world
  - Not nearly as efficient as we might like…
  - …but capable of solving leadership-class simulation problems NOW
- Current focus is on
  - Unstructured grid implementation. Critical for several problems we want to run on Jaguar
  - Multiple-continuum support
  - Making structured adaptive mesh refinement really work
  - Developing better solvers/preconditioners
    - Multilevel (geometric and algebraic approaches)
    - Physics based
    - For flow solver, able to deal with phase transitions
- Also need to think about
  - Exotic and emerging architectures (e.g., GPGPUs, Cell, many cores)
  - How to visualize simulations with billions of DoFs?

Contact

Richard Tran Mills

Computational Earth Sciences Group
Computer Science and Mathematics Division
(865) 241-3198
rmills@ornl.gov