Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows using Advanced Computing

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Scientific Impacts and Opportunities in Computing

Maui Prince Hotel, Hawaii

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Outline

- Modeling Subsurface Reactive Transport
- CO_2 Sequestration
- Hanford 300 Area

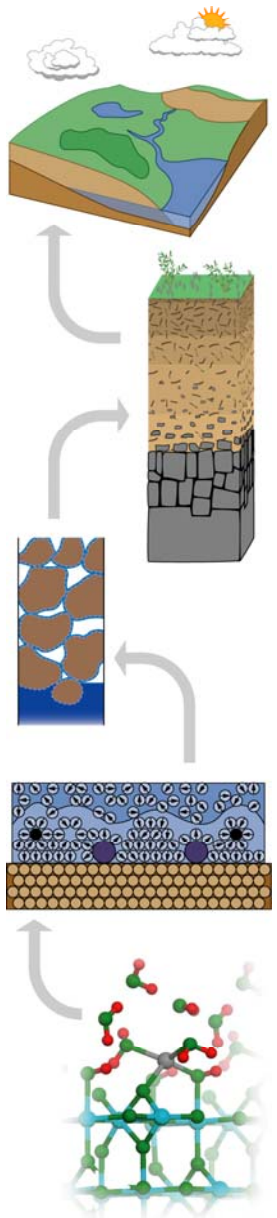
Modeling Subsurface Processes

- Mass & energy conservation equations in porous and fractured media:
  - multiphase
  - multicomponent
  - Multiscale

- Challenges
  - Inability to fully characterize system
    - How accurate is accurate enough?

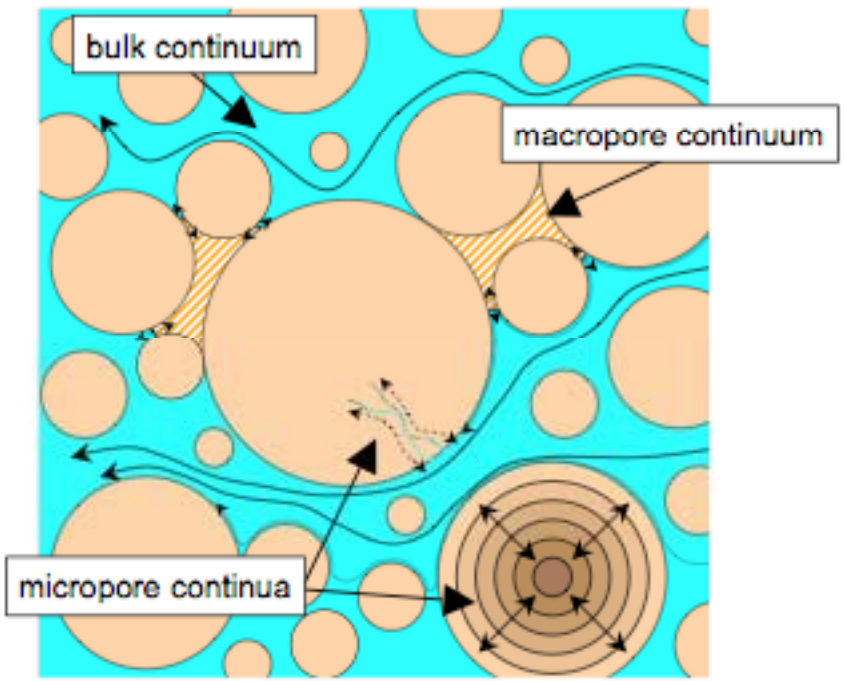
  - Upscaling: pore $\Rightarrow$ lab $\Rightarrow$ field
    - Is volume averaging sufficient?
    - In general a multiscale model is required at lab and field scales (subgrid scale)

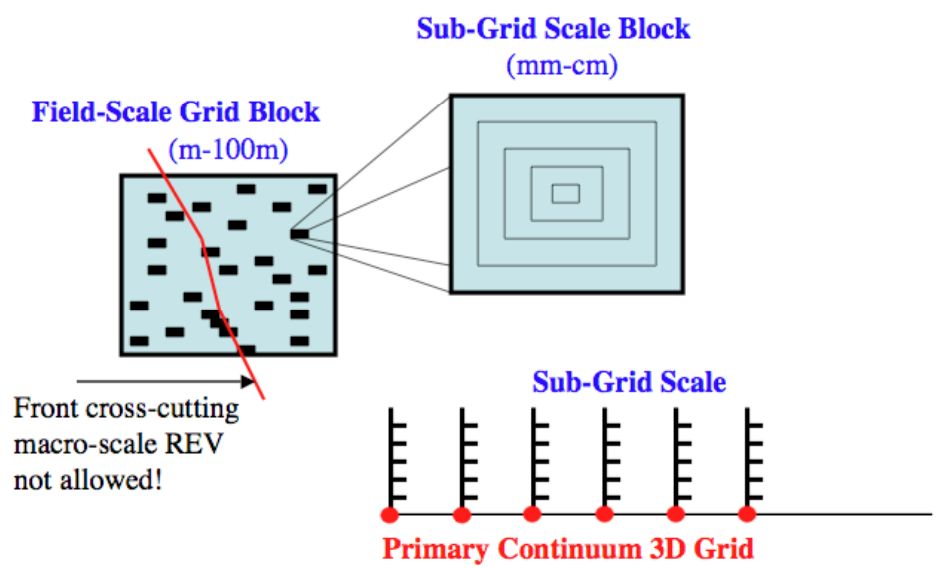
  - Modeling multiscale processes
    - New challenges is system characterization and computational algorithms



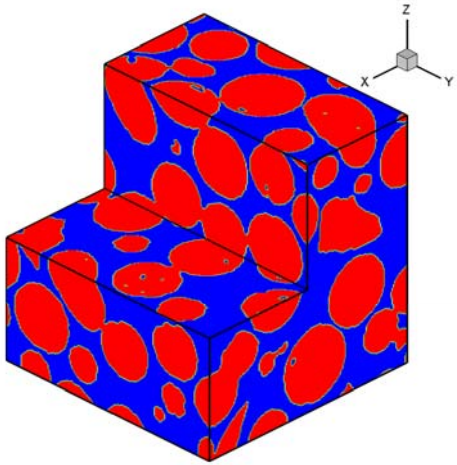
Multiscale Processes

- 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
  - 1D computational domain
  - Multiple sub-grid model attached to primary continuum nodes
  - Degrees of freedom: $N \times N_K \times N_{DCM} \times N_c$

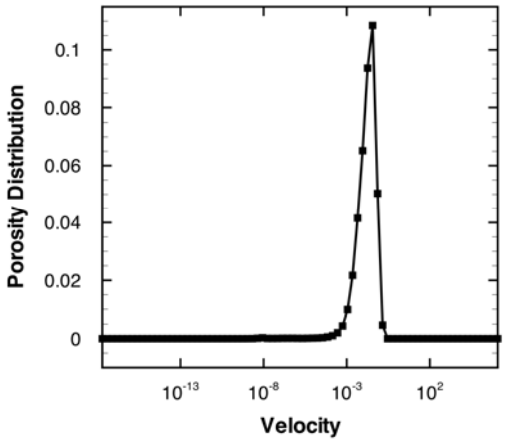


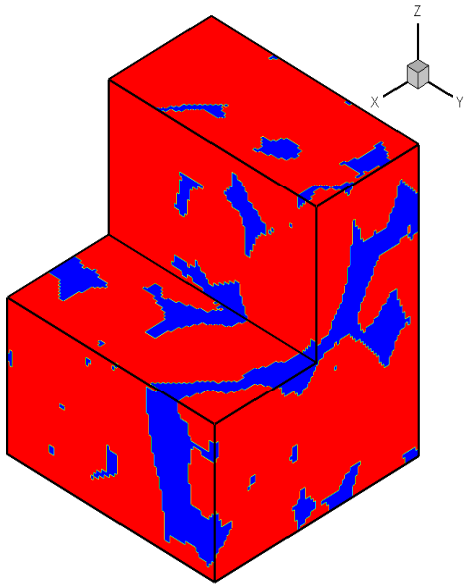


LBM Applied to 3D Porous Media

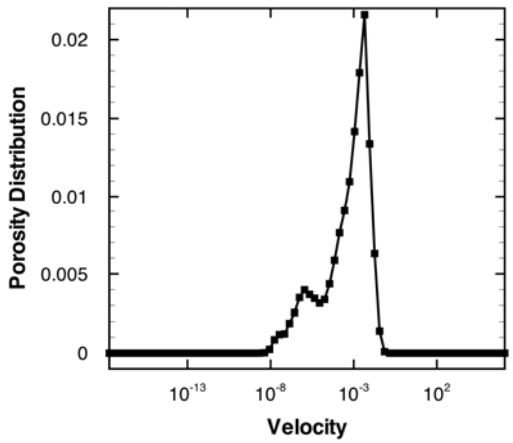


Glass Beads



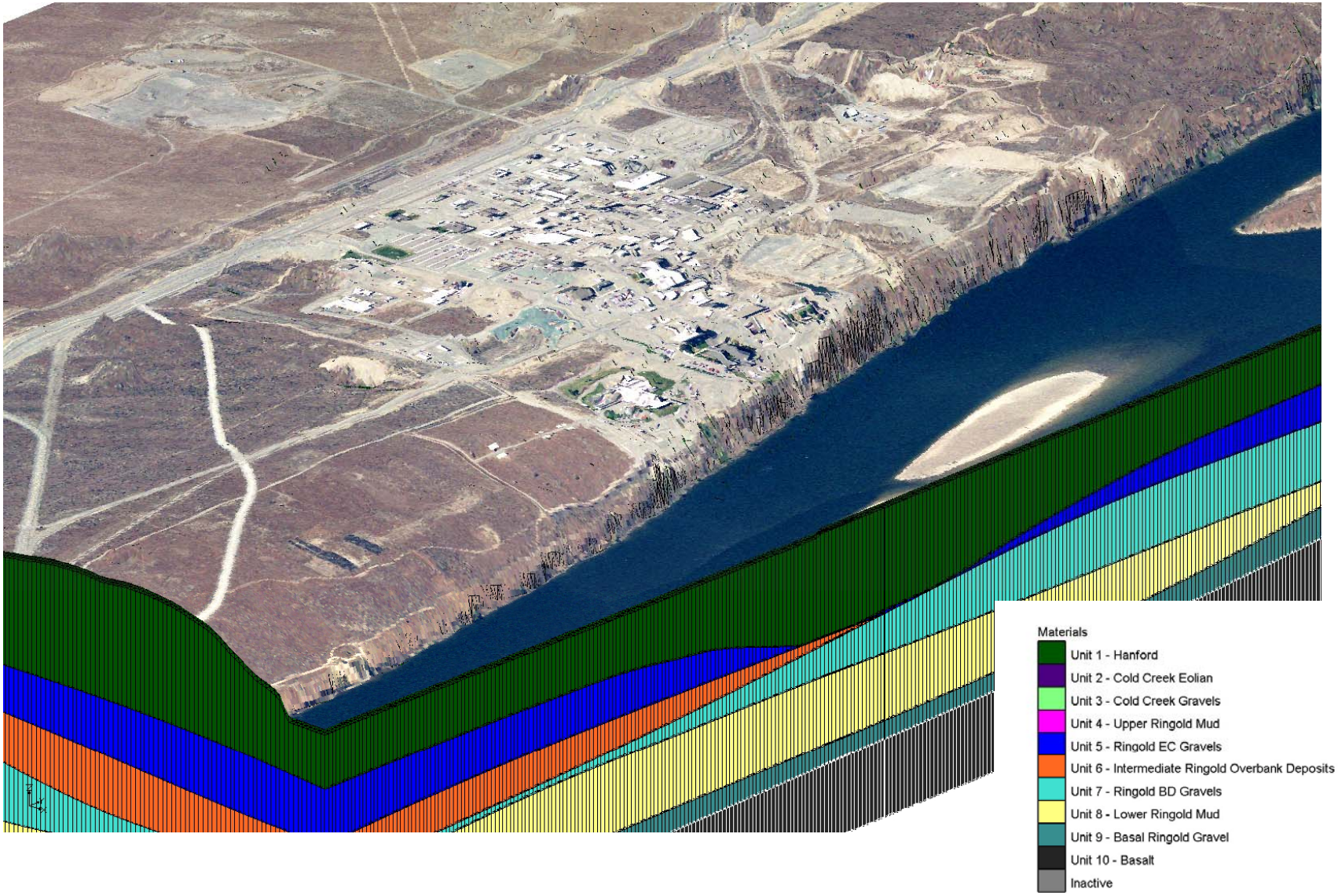


Fontainebleau Sandstone

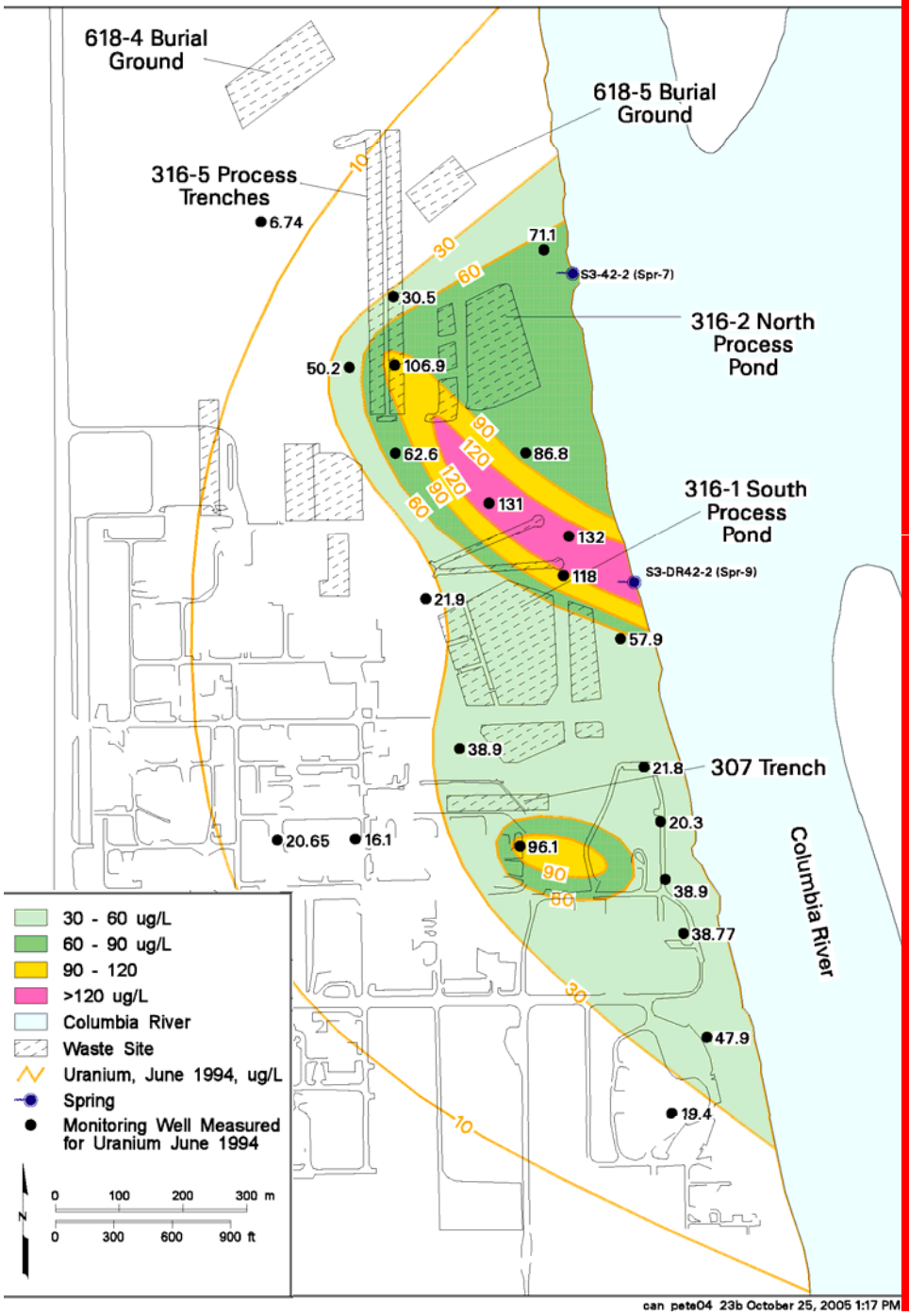


Hanford 300 Area

Hanford 300 Area: Layered Hydrostratigraphy



Shaded 300 Area Uranium, June 1994



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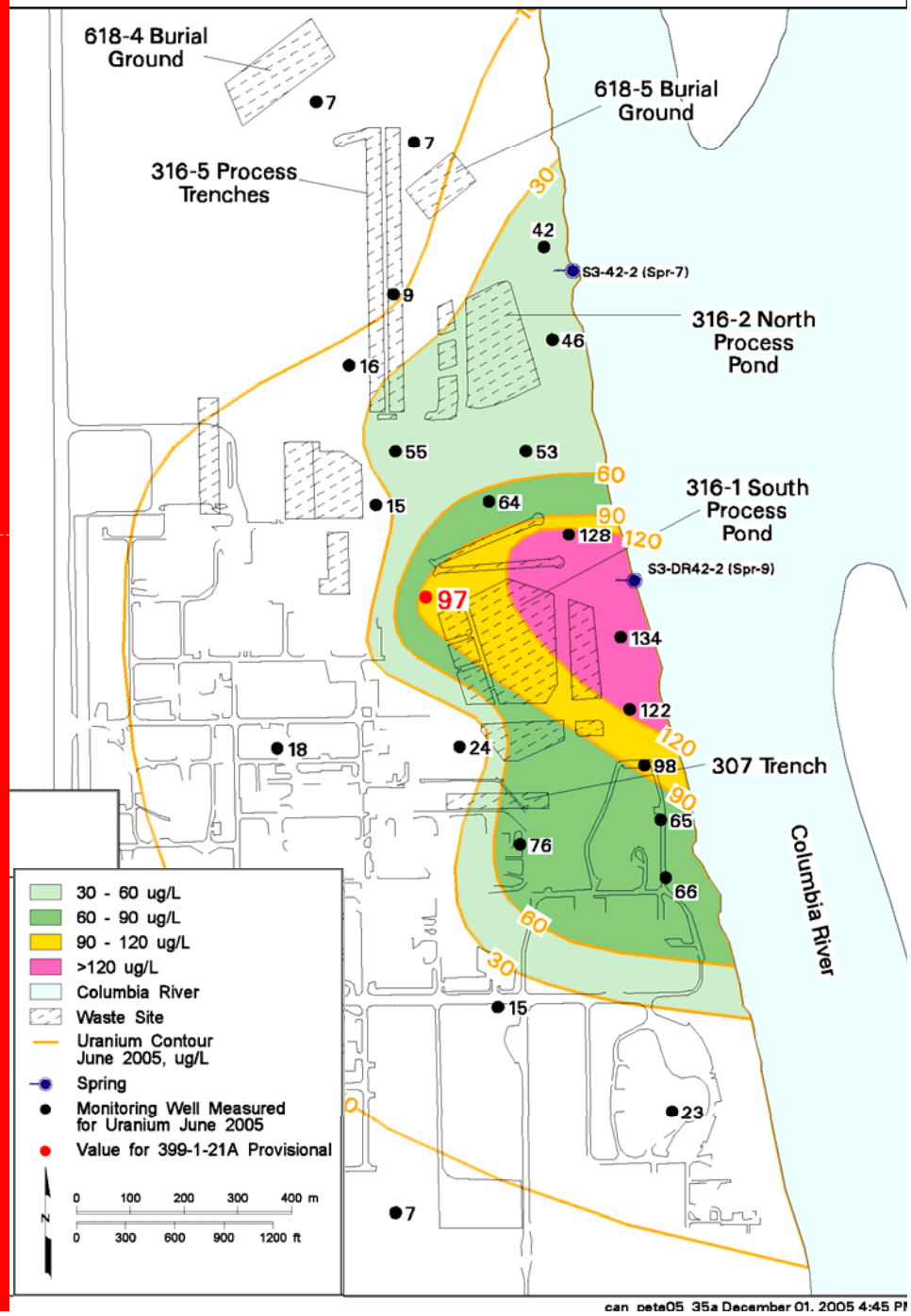
Shaded 300 Area Uranium, June 2005



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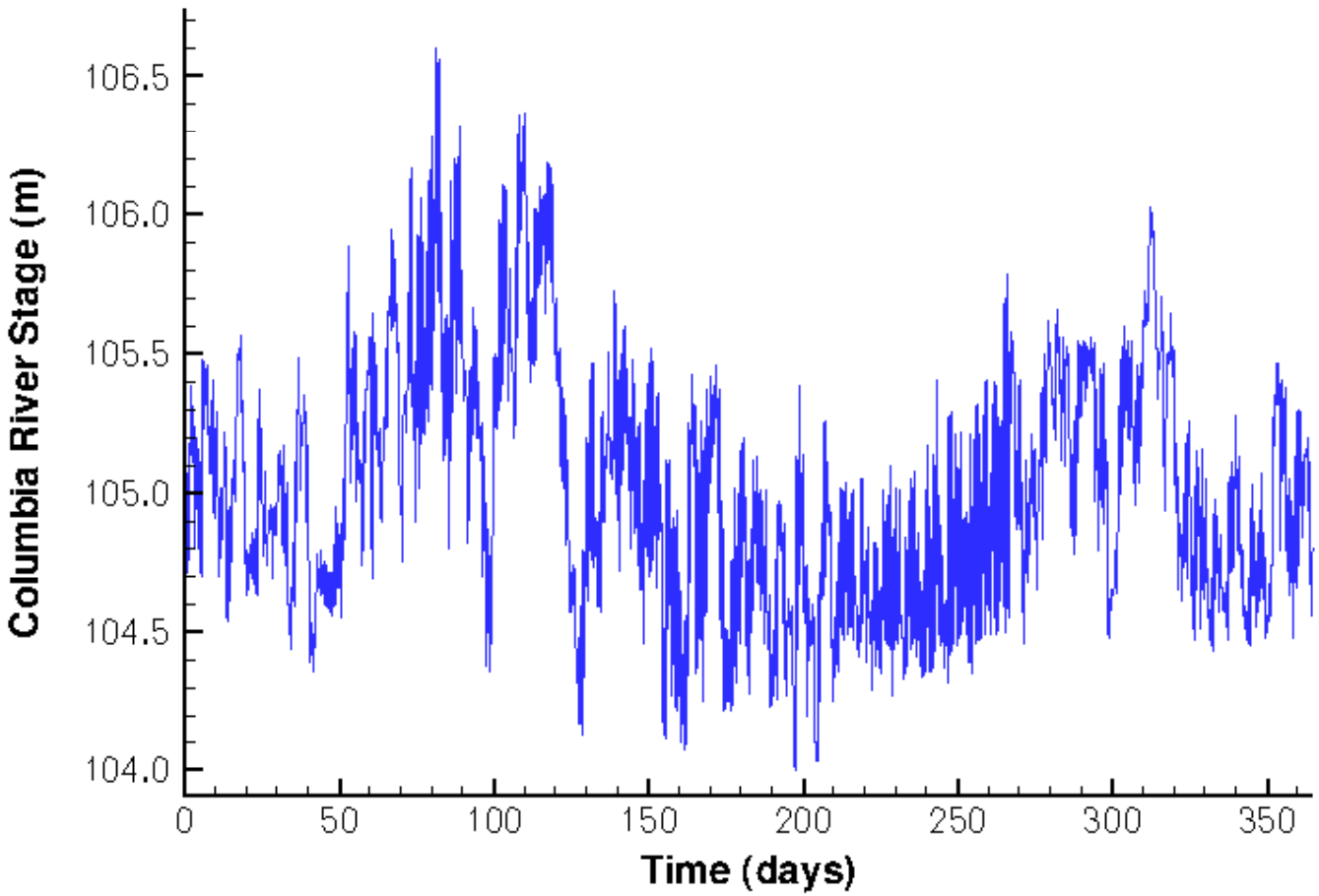
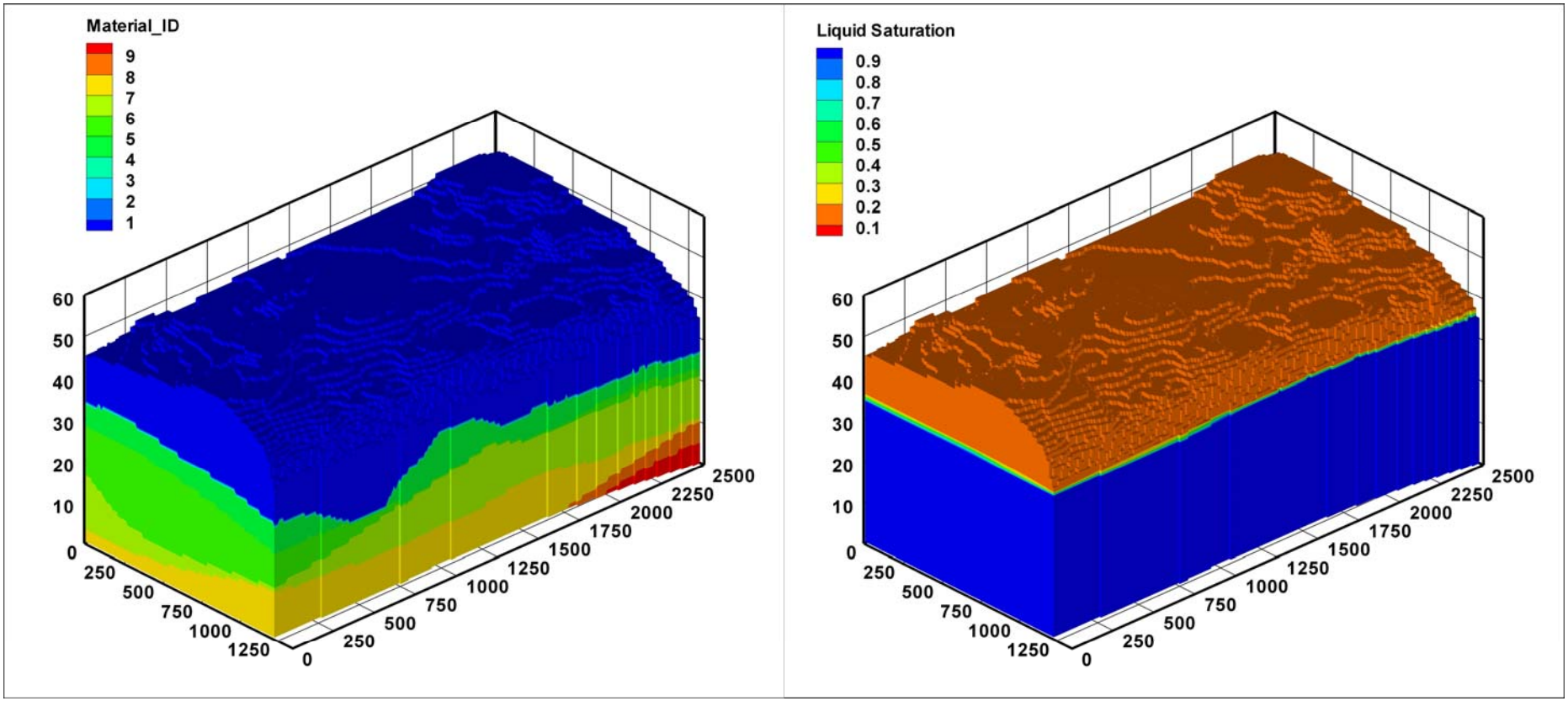
Hanford Modeling Challenges

- 3D Domain: length and time scales
  - field scale domain (~km)
  - hourly river fluctuations, ~ 1000 year predictions
  - fast flow rates (~5 km/y)
- Complex chemistry: Na-K-Ca-Fe-Mg-Br-N-CO_2-P-S-Cl-Si-U-Cu-H_2O (~15 primary species)
- Multiscale processes (μm-m)
- Highly heterogeneous sediments
  - fine sand, silt; coarse gravels; cobbles
- Variably saturated environment

River Stage Fluctuations



Preliminary Scoping Results



20 day simulation with 1024 processor cores took 4 hours on Jaguar
135 x 250 x 60 grid (10m x 10m x 1m resolution)

Multiple Interacting Continuum Model

- **Primary continuum (α = primary fluid):**

$$\frac{\partial}{\partial t}\epsilon_\alpha \varphi_\alpha R_j^\alpha \Psi_j^\alpha + \nabla \cdot \epsilon_\alpha \Omega_j^\alpha = -\epsilon_\alpha \sum_m \nu_{jm} I_m^\alpha - \sum_\beta a_{\alpha\beta} \Omega_j^{\alpha\beta}$$

- **Secondary continua (β^{th} continuum):**

$$\frac{\partial}{\partial t}\epsilon_\beta \varphi_\beta R_j^\beta \Psi_j^\beta + \nabla \cdot \epsilon_\beta \Omega_j^\beta = -\epsilon_\beta \sum_m \nu_{jm} I_m^\beta$$

- **Boundary conditions:**

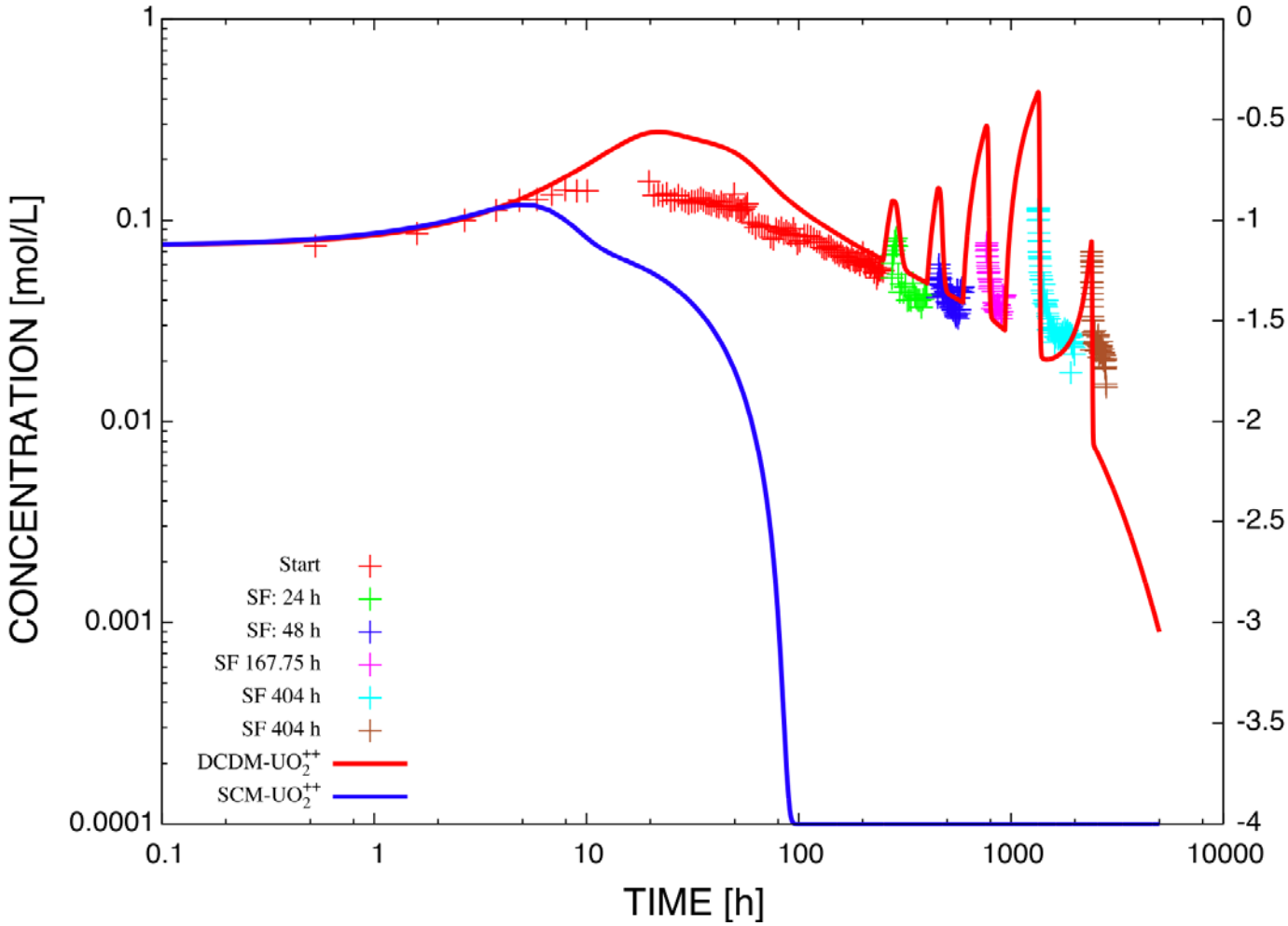
$$\Psi_j^\beta(0, t\,|\,r) = \Psi_j^\alpha(r, t), \qquad \Omega_j^{\alpha\beta} = -\varphi_\beta D_\beta \left(\frac{\Psi_j^\alpha - \Psi_j^\beta}{d_{\alpha\beta}} \right)$$

- **Mineral mass transfer:**

$$\frac{\partial \varphi_s^\alpha}{\partial t} = \overline{V}_s I_s^\alpha, \qquad \frac{\partial \varphi_s^\beta}{\partial t} = \overline{V}_s I_s^\beta$$

PNNL Hanford Large Column Exp. NPP1-14

Multiscale Model of Hanford Large Column Exp.



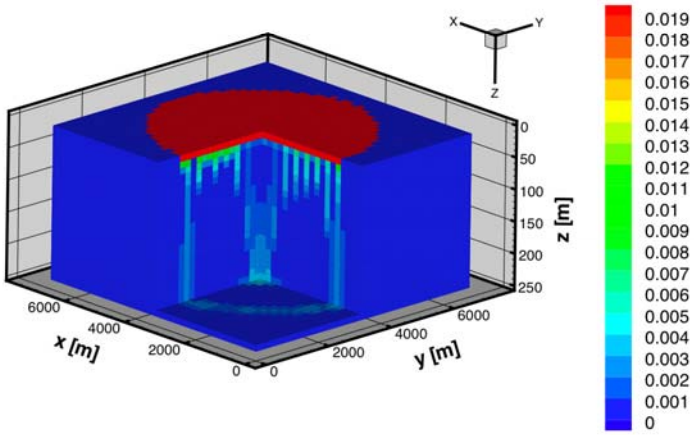
Hanford 300 Area: Projected Ultrascale Modeling Requirements

- **Uniform grid:**
  - Problem domain: 1500 × 2500 × 60 meters
  - Structured grid spacing: 1.0 × 1.0 × 0.25 meters
  - 900M grid nodes (spatial degrees of freedom)
  - 2+ continua (spatial degrees of freedom)
  - 10-20 chemical components (chemical degrees of freedom)
  - 10-20B+ unknowns (~100K processors)
- Local grid refinement through the use of unstructured grids (or AMR) should reduce the number of unknowns by many orders of magnitude and improve resolution

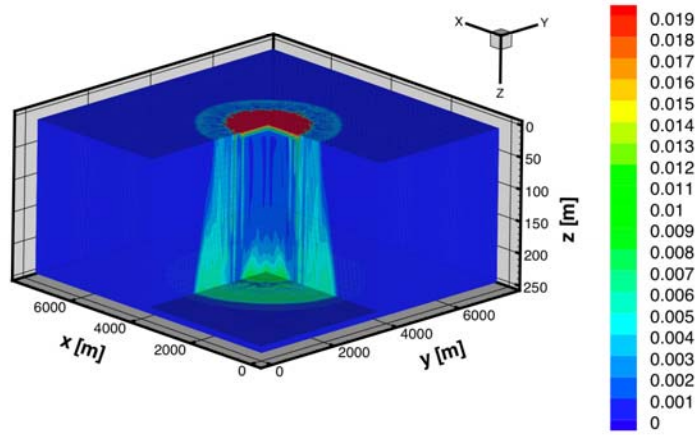
CO_2 Injection in a Sandstone Aquifer

QuickTime™ and a
BMP decompressor
are needed to see this picture.

3D Simulation of Geologic CO_2 Sequestration



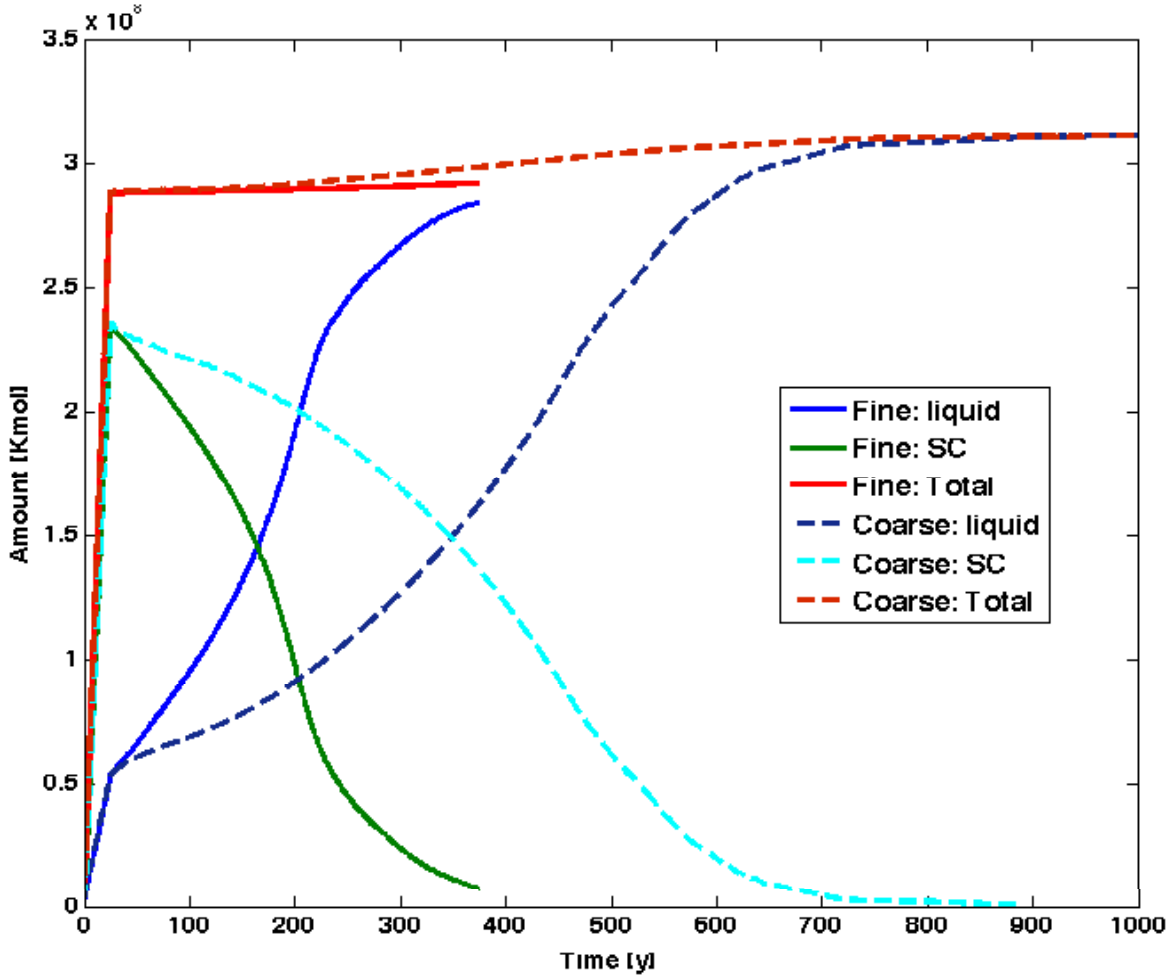
Coarse Grid (175 x 175 x 10 m)



Fine Grid (45 x 45 x 10 m)

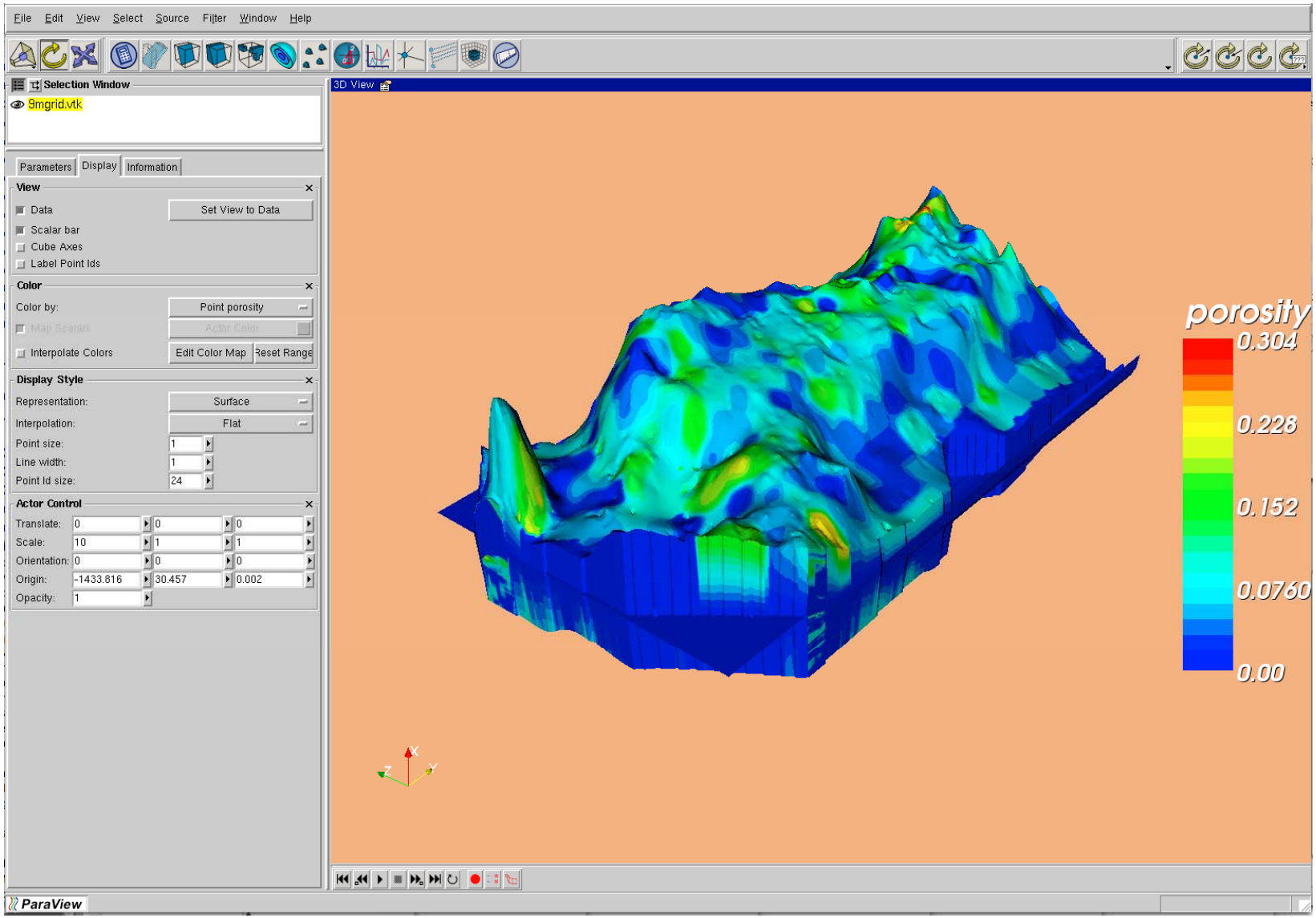
- Fingering phenomena results as supercritical CO_2 is injected into a reservoir and dissolves into the aquifer formation brine
- Critical finger wavelength is inversely proportional to permeability and predicted to be on the order of decimeters or smaller for a sandstone host rock
- Spatial resolution of fingers is crucial for prediction of the rate of dissipation of the supercritical CO_2 which may involve several thousand years depending on the brine composition
- Ultrascale computing will be required to adequately resolve spatial scales
- Develop upscaling techniques to represent fingering

CO_2 Plume Lifetime



SACROC 9M Node Grid (1200 m depth)

Scurry Area Canyon Reef Operators Committee

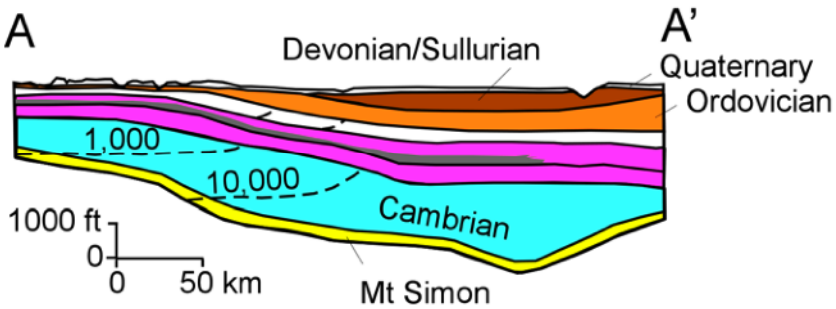


SACROC [Cont.]

Scurry Area Canyon Reef Operators Committee

- Oldest continuously operated CO_2 EOR site in U.S. beginning in 1972
  - West Texas oil field
  - 93 million tons CO_2 injected/38 million tons produced
- Carbonate reef complex (limestone & shale)
- Domain size: 4 km x 10 km x 200 m
- Over 200 injection and extraction wells

CO_2 Injection into Illinois Basin



Potential petascale computational problem

225 x 10^6 metric tons CO_2/year

Mark Person (unpublished, Univ. Indiana, Bloomington)

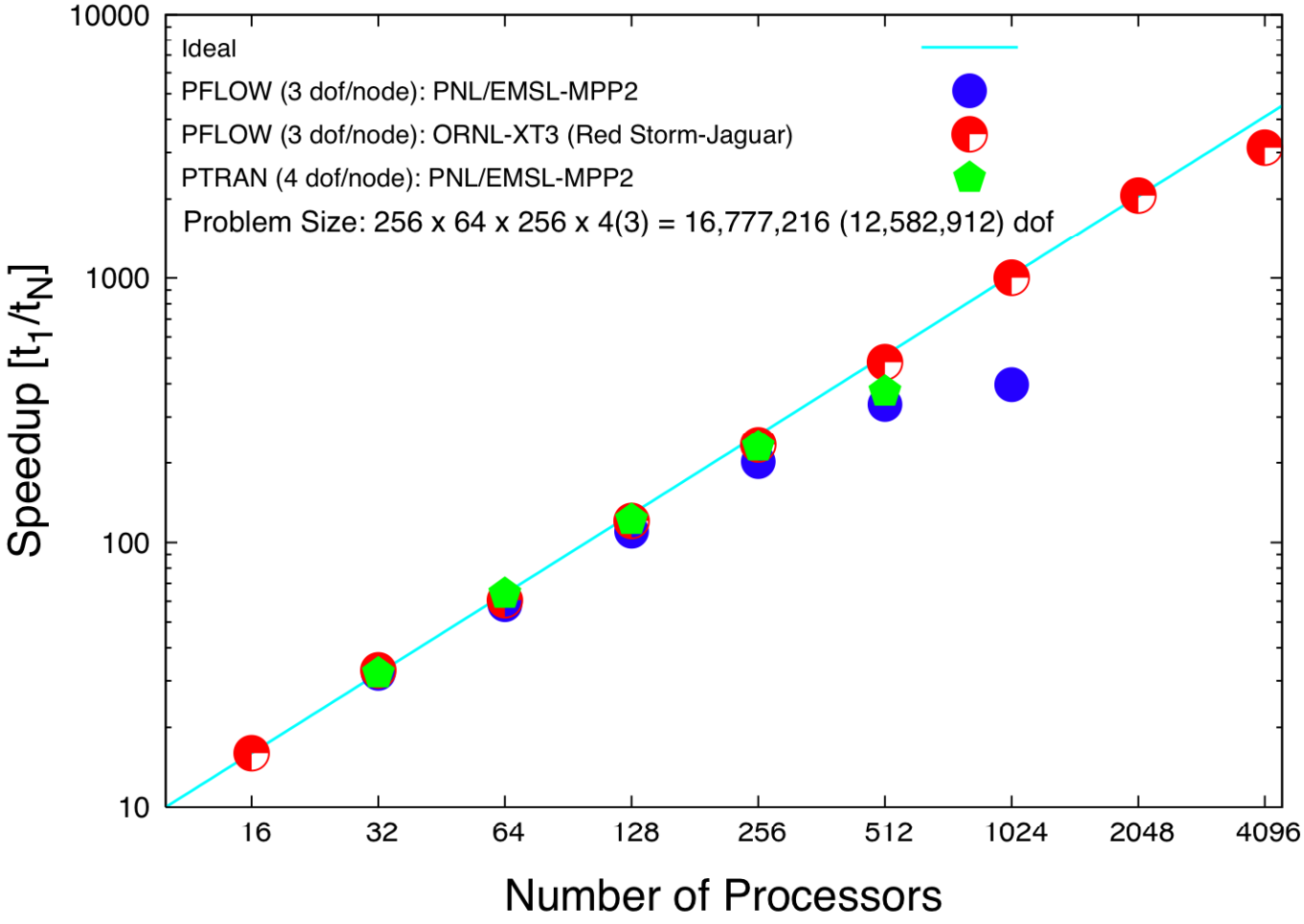
Summary: HPC Challenges

- Large (~km) spatial scales
- Long simulation times (thousands of years)
- Multicomponent/multiphase systems
- Multiple length and time scales: multiple interacting continua for representing multi-scale processes
- Need advances in solver and preconditioner algroithms (multilevel solvers) for solving heterogeneous multiphase systems to achieve weak scaling
- Load balancing with sub-grid model
- Need higher order finite volume methods to obtain positive def. solutions with tensors and eliminate spurious grid effects

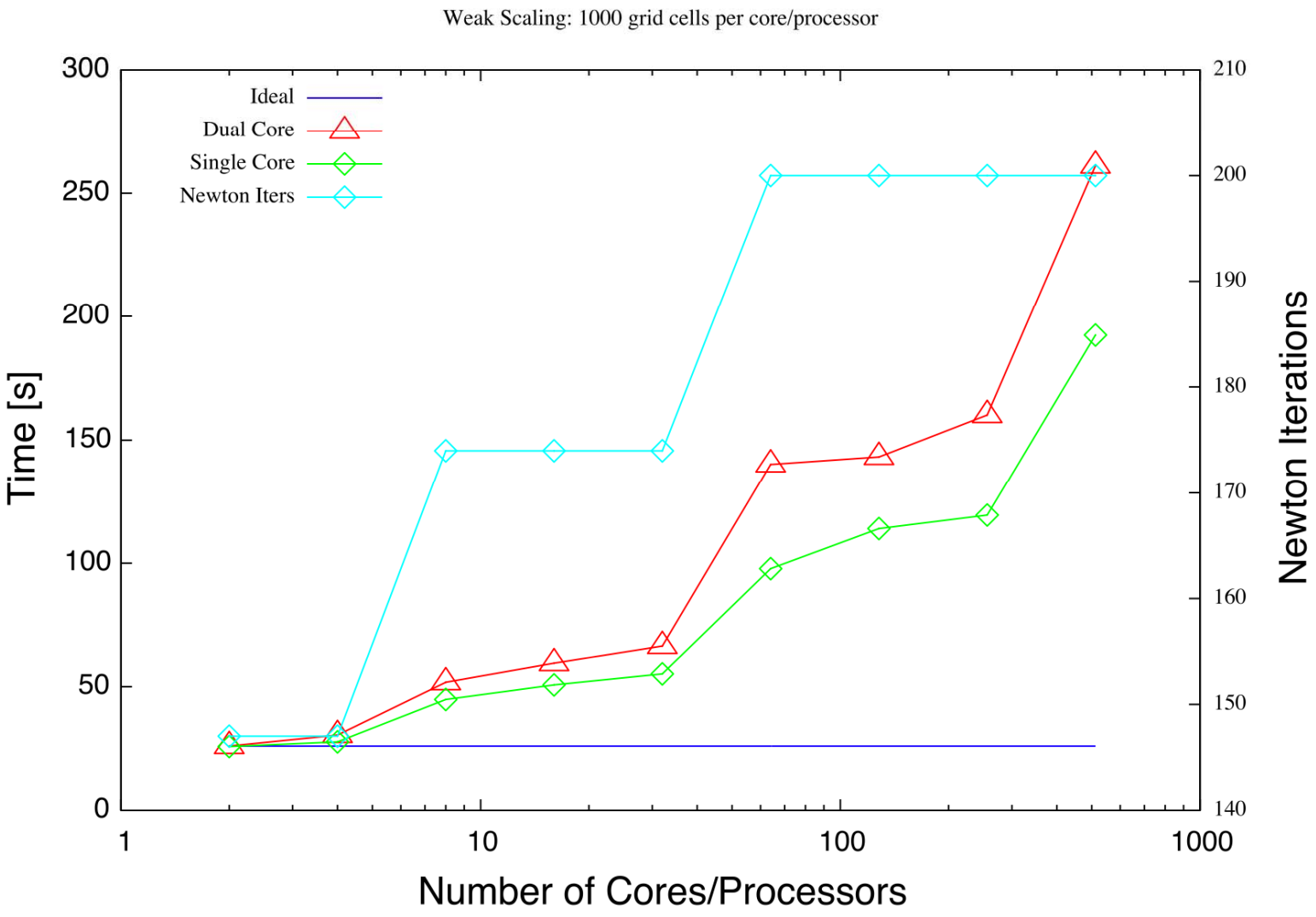
PFLOTRAN: PFLOW + PTRAN

- Solve mass & energy conservation equations
  - PFLOW: multiphase (CO_2, H_2O, Oil, gas)
  - PTRAN: multicomponent reactive transport
  - PFLOW and PTRAN sequentially coupled
- Finite Volume discretization
  - Positive definite solution (solve for log C_j)
  - Logically structured grid
- Mercurial (Hg) code repository
- Open Source
- Parallel I/O using HDF5

PFLOTRAN: Strong Scalability

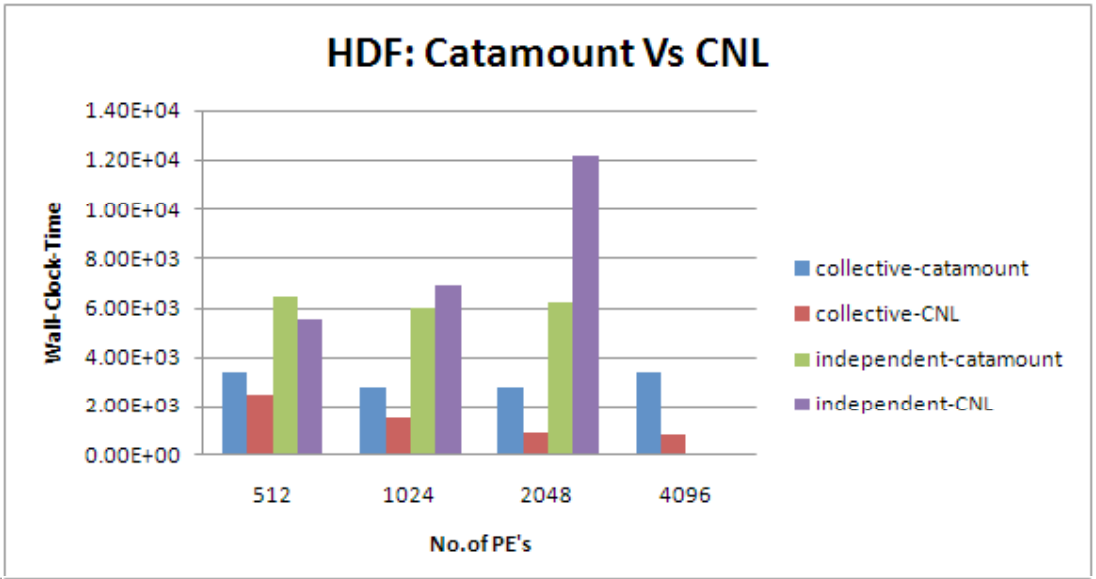


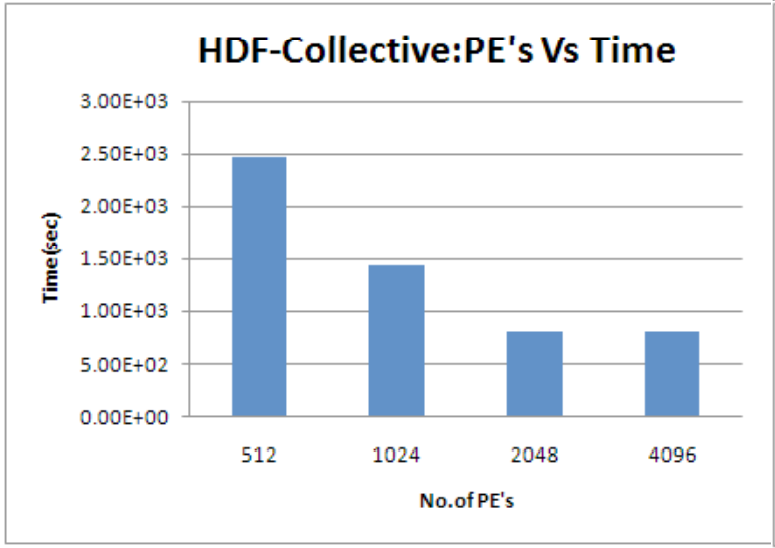
PFLOTRAN: Weak Scalability

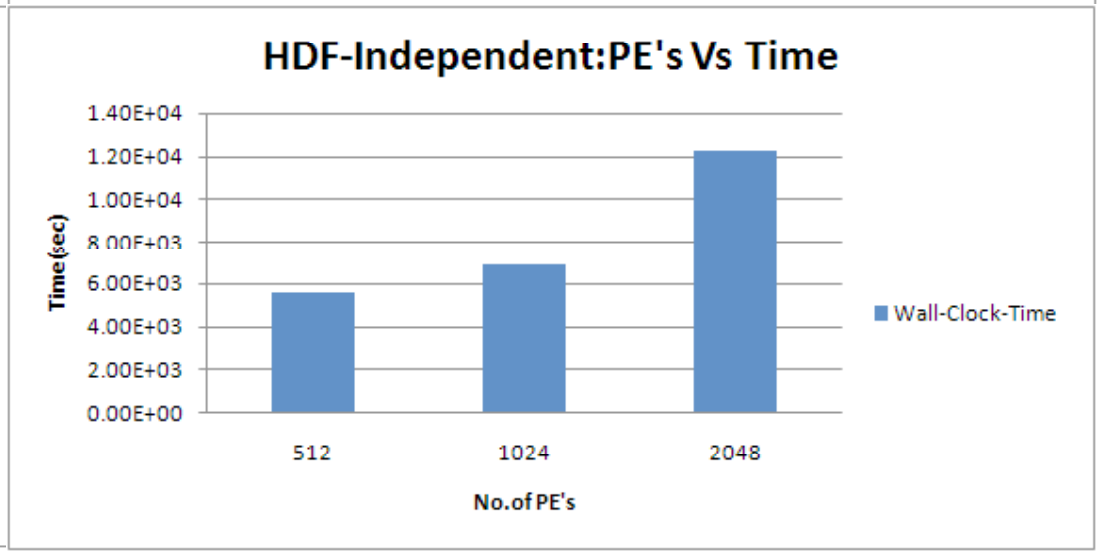


HDF5 I/O Performance

PFLOTRAN Results
(Kumar Mahinthakumar,
NC State–SciDAC PERI)





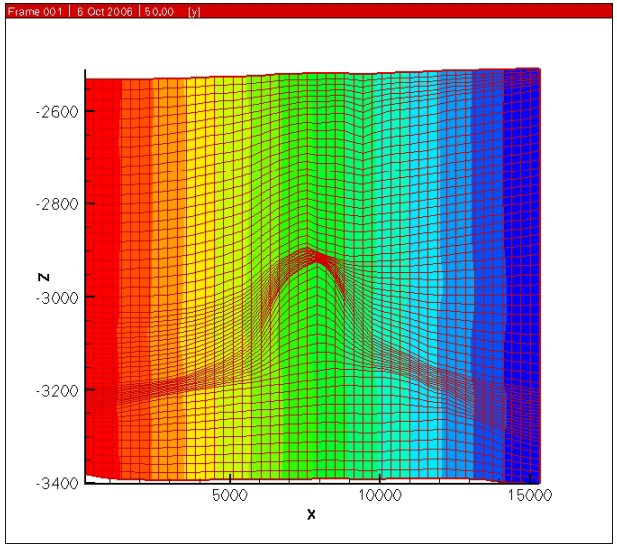


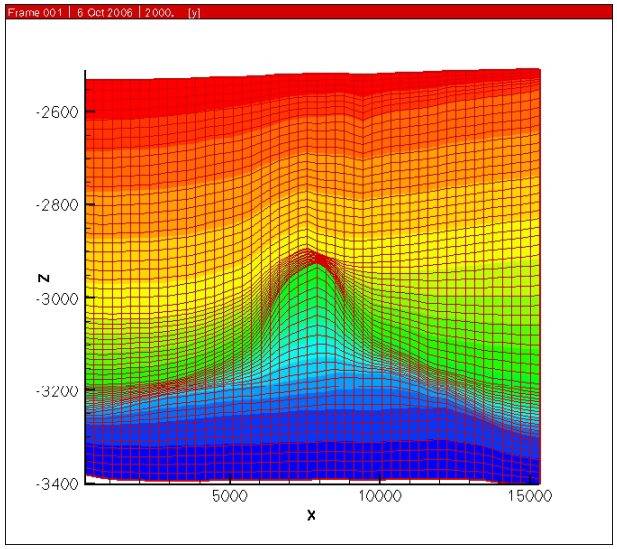
Multilevel Solvers and Preconditioners

- Need solvers and preconditioners that provide weak scaling
  - Multilevel solvers
  - physics based preconditioning
- Need to restructure PFLOTRAN to handle multiple grids
- Need to generalize conventional multilevel solvers:
  - multiphase systems with variable switching to account for phase changes—or revise phase change approach to persistent variables
  - heterogeneous systems with scale-dependent coefficients (e.g. permeability)

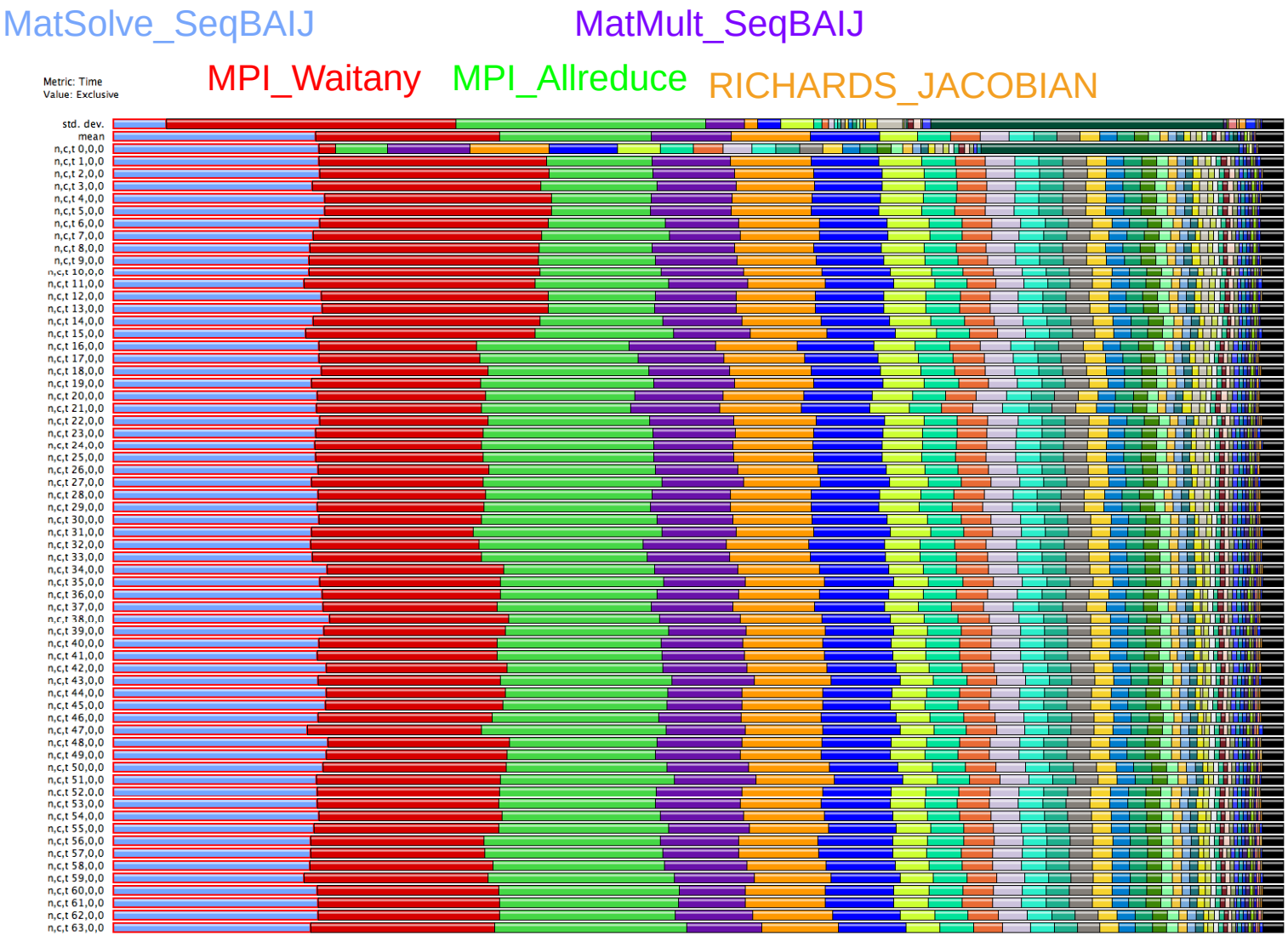
Grid Effects

- SACROC logically structured grid with equal Δx, Δy and variable Δz
- Need higher order methods
- No known method that includes full dispersion tensor and preserves positive definiteness of solution



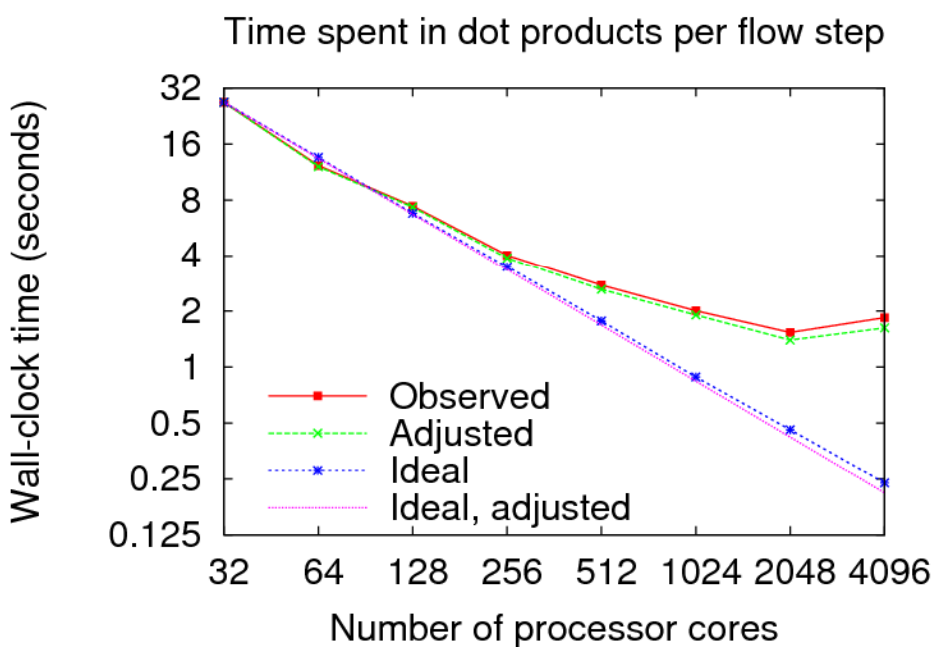


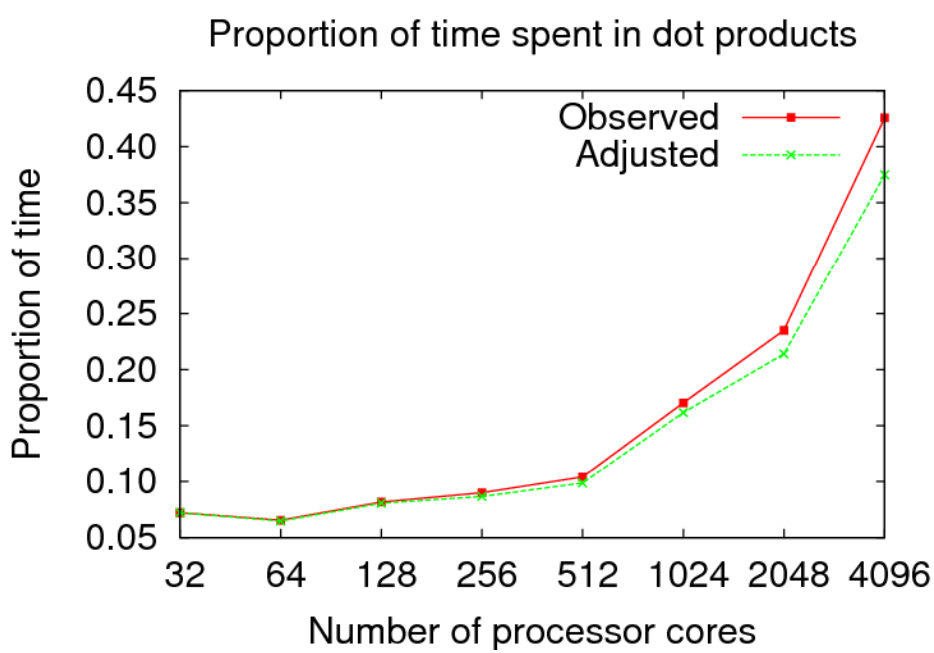
PFLOTRAN: Profiling using TAU



Factors limiting strong scaling

- Parallel dot-products (AllReduce operations) limit strong scaling.
- Keep in mind: Only 6144 unknowns per processor core at 4096 cores.
- Block-Jacobi preconditioner loses effectiveness with more processors (due to smaller subdomains)...
- ...but the effect on scalability is minor (slow growth in BiCGSTAB iterations)





Impact of Ultrascale High Performance Computation on Hanford 300 Area Modeling

- High-resolution grids:
  - Reduce discretization error for flow and transport (improved accuracy)
  - Capture the effects of small scale-heterogeneities (e.g. sand lenses)
- Increased biogeochemical complexity:
  - Increased # of chemical components
  - Increased # and sophistication of chemical reactions (computing power to include more chemistry)
  - Sub-grid scale geochemical model (multi-continuum formulation)
- Unstructured grids:
  - Alignment of grid cells with irregular stratigraphy (i.e. high-permeable Hanford and low-permeable Ringold units
  - Grid refinement in regions of interest (e.g. uranium source zone, fluctuating water table)
- Uncertainty analysis:
  - Ability to simulate large numbers of realizations of stochastic parameters on high-resolution grids
- SciDAC & others Collaborations:
  - PETSc, SAMRAI, Hypre, TAO, PERI, Zoltan, ParaView, VisIt

Publications

- Hammond, G., Lichtner, P.C., Lu, C. (2007) Subsurface Multiphase Flow and Multicomponent Reactive Transport Modeling using High-Performance Computing, Journal of Physics Conference Series, 78, 012025 doi:10.1088/1742-6596/78/1/012025.

- Mills, R., Lu, C., Lichtner, P.C., Hammond, G. (2007) Simulating Subsurface Flow and Transport on Ultrascale Computers using PFLOTRAN, Journal of Physics Conference Series, 78, 012051 doi:10.1088/1742-6596/78/1/012051.

- Lu, C. and Lichtner, P.C. (2007) High resolution numerical investigation on the effect of convective instability on long term CO_2 storage in saline aquifers, Journal of Physics Conference Series, 78, 012042 doi:10.1088/1742-6596/78/1/012042.

- Lichtner, P.C. and Q. Kang (2007) Upscaling Pore-Scale Reactive Transport Equations using a Multi-Scale Continuum Formulation, WRR, in press.

- Tartakovsky, A. M., G. Redden, P. Lichtner, T. Scheibe, P. Meakin (2007) Pore-Scale Smoothed Particle Hydrodynamics Model of Mixing Induced Precipitation, Wat. Res. Res, in press.

- Zachmann, D., Schiebe, T., Lichtner, P.C, and Meakin, P., SciDAC Review, in preparation.