Hybrid Numerical Methods for Multiscale Simulations of Subsurface Biogeochemical Processes: An Overview of Visualization Needs

Vicky Freedman

Pacific Northwest National Laboratory

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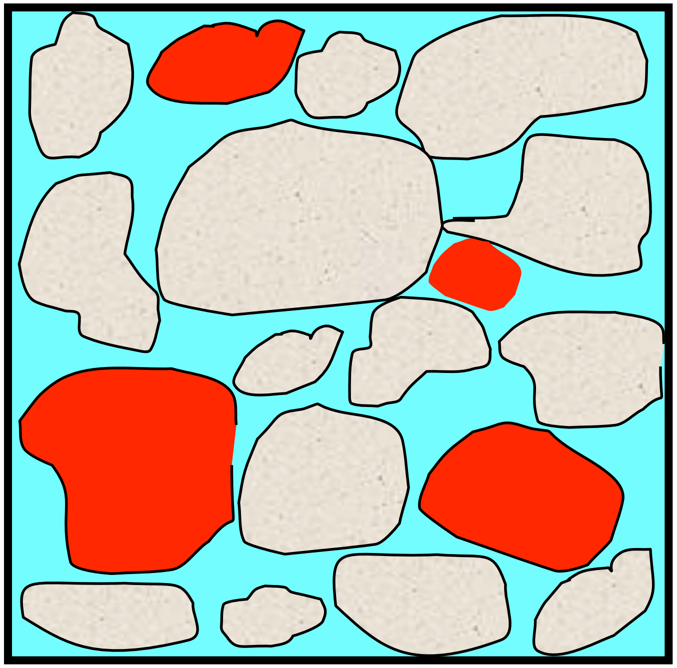
Project Overview

- Project Title: *Hybrid Numerical Methods for Multiscale Simulations of Subsurface Biogeochemical Processes* (http://subsurface.pnl.gov/)
- Sponsor: SciDAC-2 Science Application (Groundwater) jointly funded by BER and ASCR
- Science goals: Develop an integrated multiscale modeling framework with the capability of directly linking different process models at continuum, pore, and sub-pore scales (groundwater flow and biogeochemically reactive transport)
- Principal Investigator: Tim Scheibe (PNNL)
- Participating institutions: Pacific Northwest National Laboratory, UC San Diego, Idaho National Laboratory, Oak Ridge National Laboratory
- Project History: Started FY07 – This is second of four years
- Science Application Partnerships:
  - Process integration, data management, and visualization framework for subsurface sciences (Karen Schuchardt, PNNL)
  - Component-based framework for subsurface simulations (Bruce Palmer, PNNL)

Motivation

- Chemical heterogeneities of porous media exist in a range of length scales
- Traditional modeling approaches
  - Pore-scale
    - Represents microscopic properties of individual pores and pore-size distributions
  - Continuum scale
    - Represents bulk flow characteristics at a larger (field) scale
    - No detailed quantification of local-scale variations in physical and/or chemical properties



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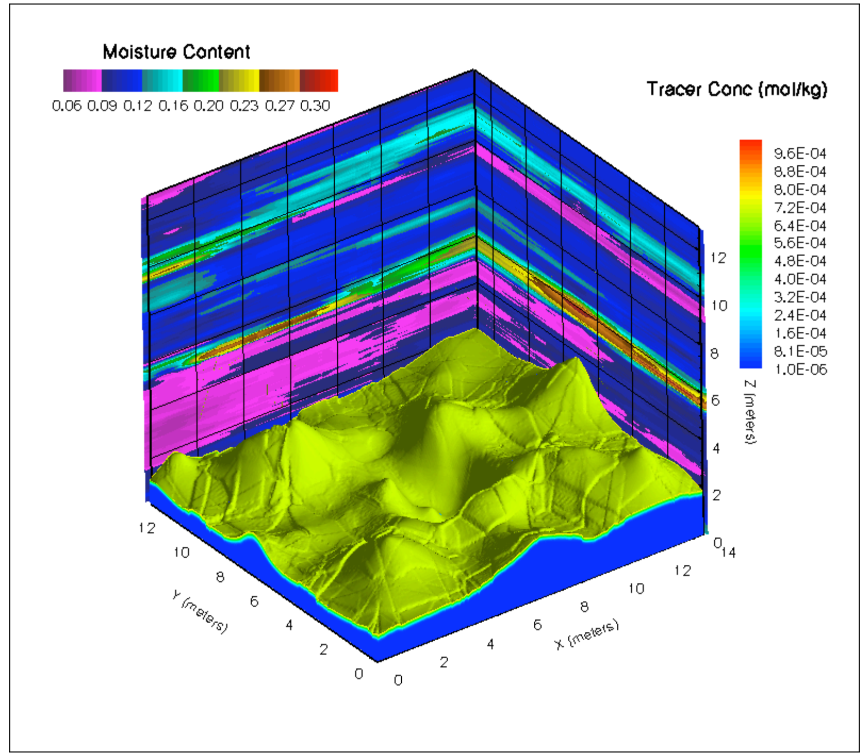
Continuum Scale Modeling

- Macroscopic continuum-scale simulations
  - traditional partial differential equations solved by finite difference or finite element methods)
  - application of multicomponent,multi-phase, multi-porosity, multi -dimensional continuum reactive transport codes at relatively high spatial resolution represents current state of the art



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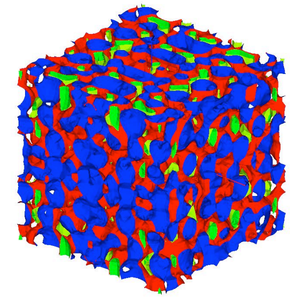
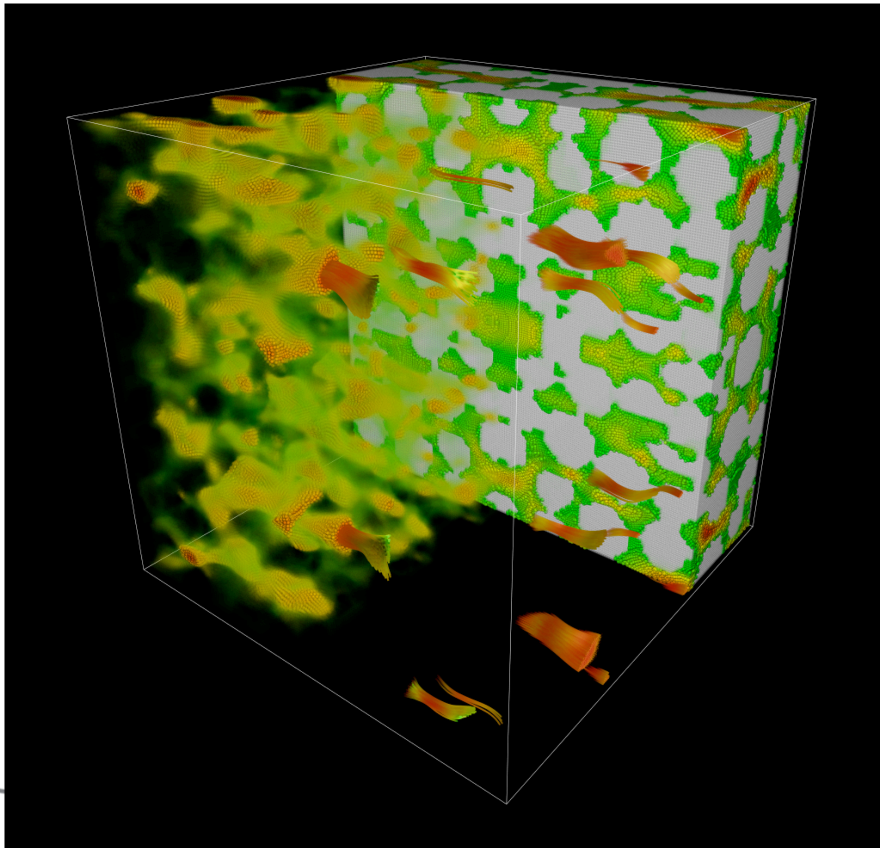
Pore-Scale Modeling Approaches



- Smoothed Particle Hydrodynamics (SPH)

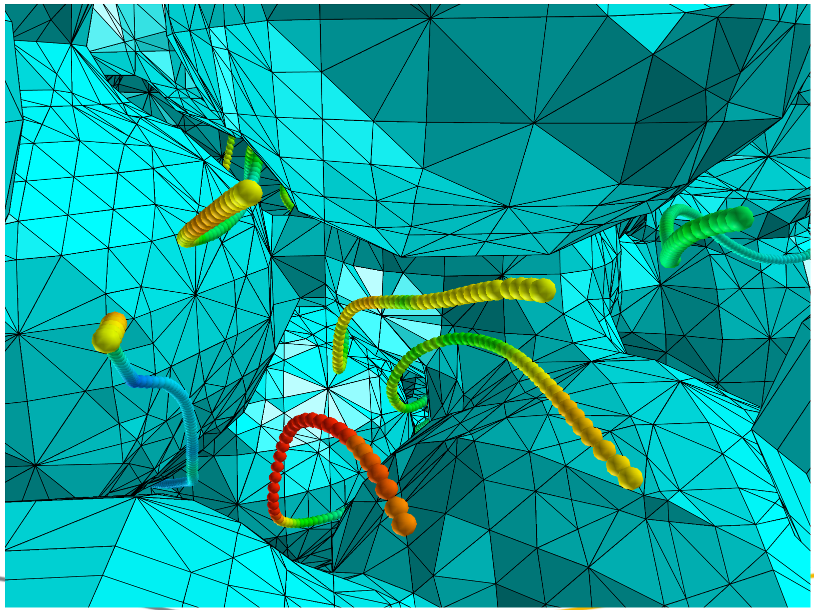


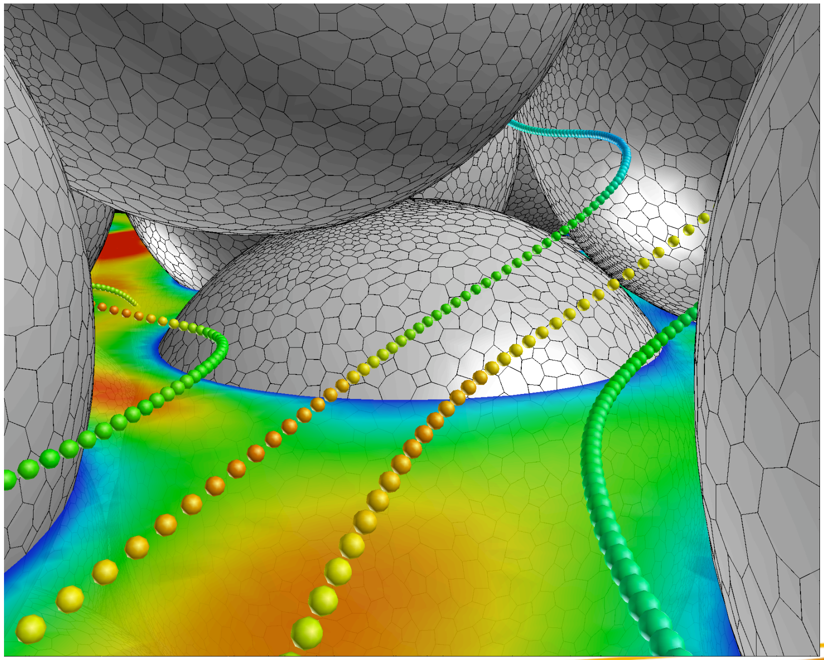
  - 3D parallel SPH code runs on Environmental Molecular Sciences Laboratory supercomputer (fluid flow and solute advection/diffusion) using 500+ processors and 7 million particles

SPH simulation by Bruce Palmer (PNNL); particle visualization by Kwan-Liu Ma,(UC Davis)

Pore-Scale Modeling Approaches

- Computational Fluid Dynamics (CFD)
  - Development of efficient computational mesh is significant effort
  - Parallel code for efficiency
  - 3D visualization

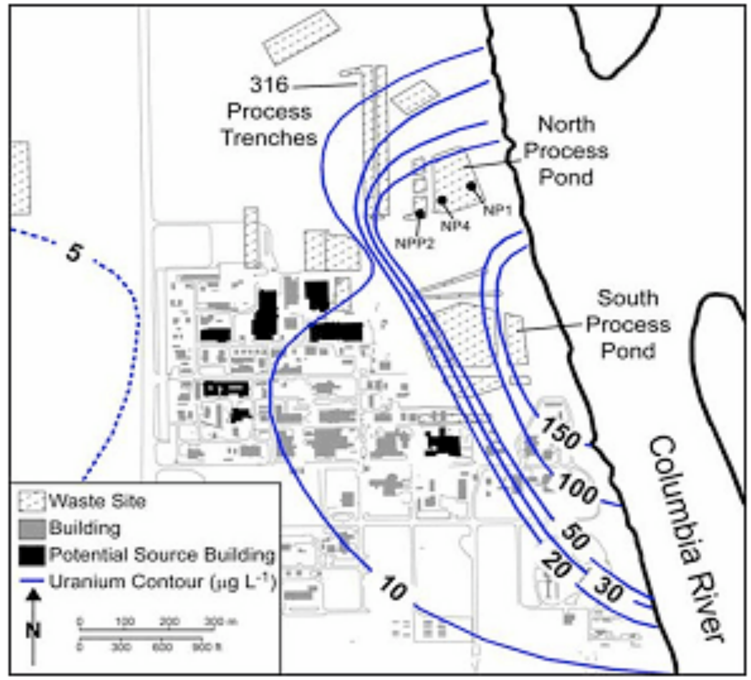




Field Example: Mass Transfer Controls on Transport of Uranium

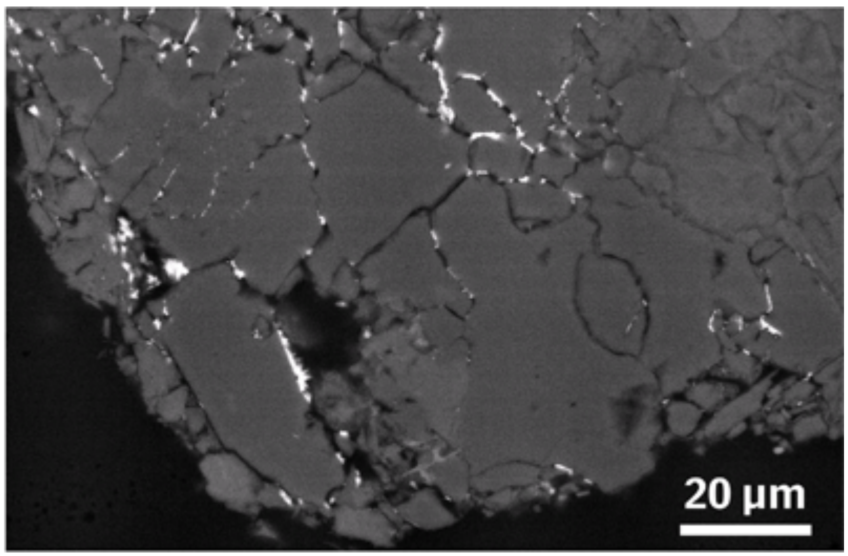
- Uranium historically disposed to trenches and ponds at the Hanford Site 300 Area (1943-1994)

- After initial sharp decline, the plume has persisted at near-constant concentrations and extent



Mass Transfer Controls on Transport of Uranium

- Subsequent studies have shown that uranium is in the form of mineral precipitates in intragranular fractures in a small fraction (4%) of grains and its transport is controlled by kinetics of dissolution and diffusion-limited mass transfer.

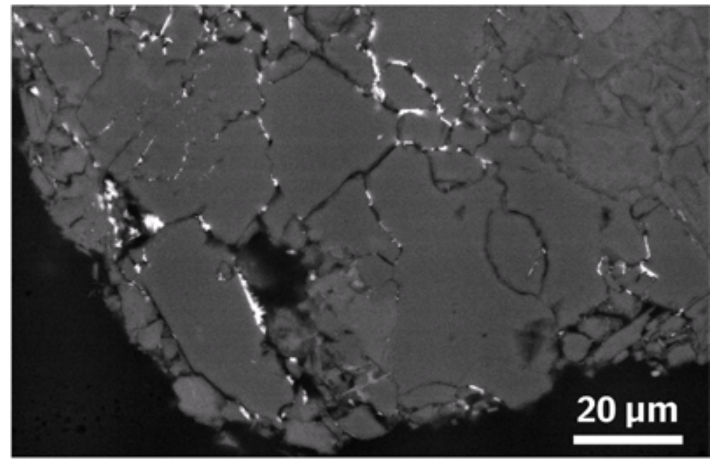


Back-scattered electron SEM images showing intragrain distribution of U(VI) precipitates (white) within a feldspar grain.

Liu, C. X., Zachara, J. M., Yantasee, W., Majors, P. D. & McKinley, J. P. Microscopic reactive diffusion of uranium in the contaminated sediments at Hanford, United States. Water Resources Research 42 (2006).

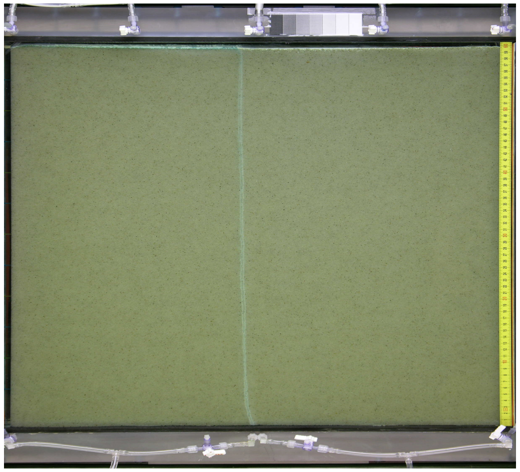
Pore-Scale vs. Continuum Scale

- Area too large to model at pore-scale, though pore-scale processes control uranium reactions and transport
- Upscaling
  - Spatial distribution of grains with uranium precipitates (relative to dominant flow paths)
  - Effective mass transfer rates related to dissolution and diffusion rates within microfractures (with non-linear dissolution reaction kinetics)
  - Dispersion in complex pore geometry
  - Local (reacting) concentrations do not equal bulk (average) concentrations



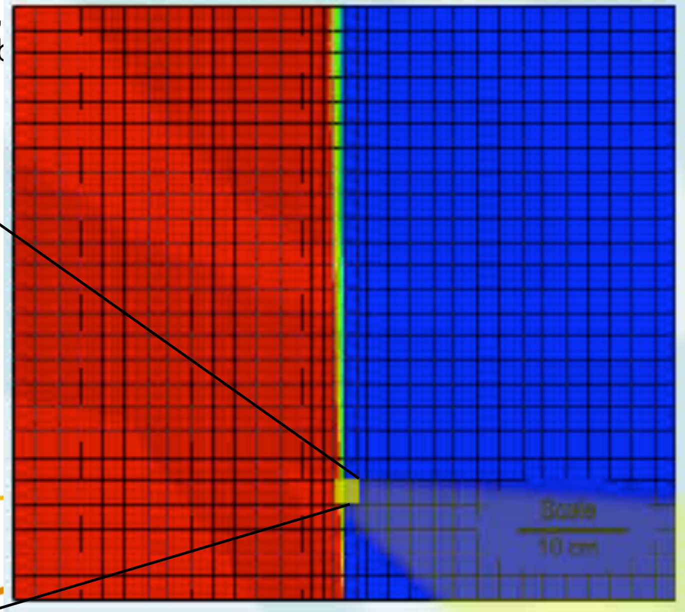
Laboratory Example: Mixing Controls on Mineral Reactions

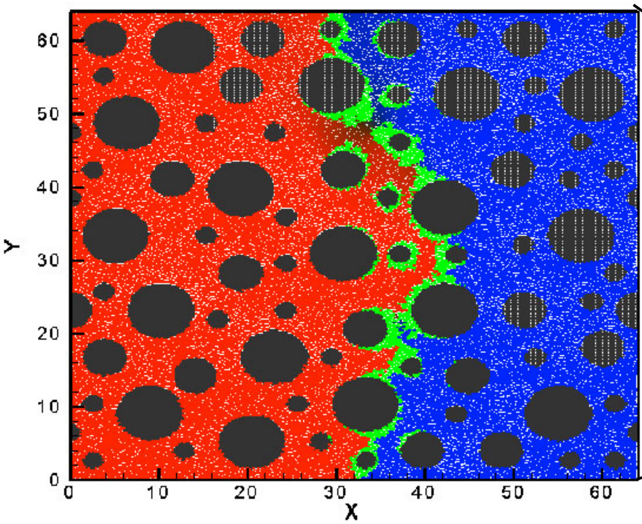
- Interest in controlling calcium carbonate precipitation for in-situ sequestration of strontium (Fujita et al. 2004)
  - Mixing of two solutes is limited to local region
  - Precipitation/dissolution reaction described in detail by the pore scale model is not easily represented at the continuum scale



Na_2CO_3 $CaCl_2$

Fujita, Y., G. D. Redden, J. C. Ingram, M. M. Cortez, F. G. Ferris, and R. W. Smith, Strontium incorporation into calcite generated b bacterial ureolysis, Geochim. et Cosmochim. Acta, 68(15): 3261-3270, 2004.





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Hybrid Multiscale Modeling

- **Conclusion:** In some situations, pore-scale modeling provides a more fundamental description of mixing-controlled reactions that are not straightforward to upscale to the continuum scale.
- **Problem:** Pore-scale modeling is extremely computationally intensive. Simulation at application-relevant scales is impractical.
- **Potential Solution:** Hybrid multiscale modeling – directly couple simulations at two scales (pore and continuum).

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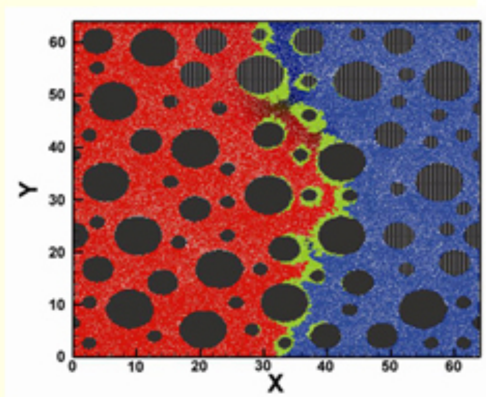
Visualization and Analysis

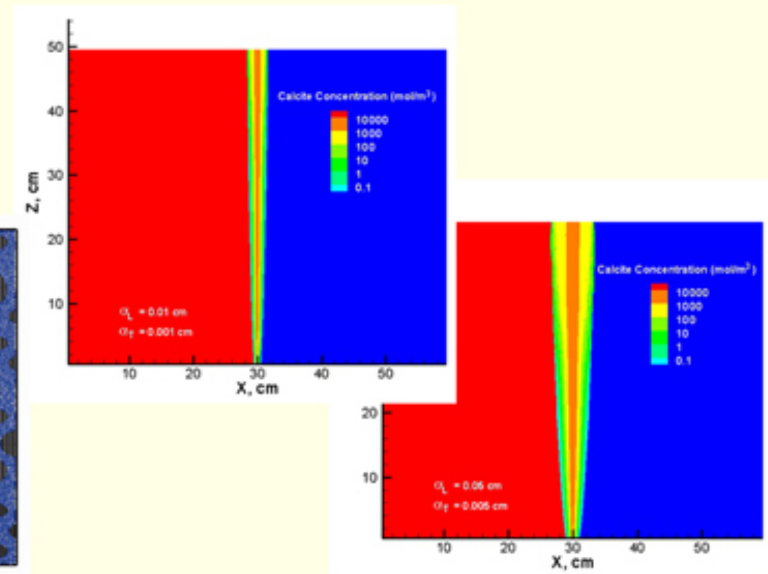
- Data to be explored within Kepler workflow environment

Visualization

- Support for a variety of visualization tools including VisIt and Tecplot for grid based data
- Organizer integration to automate multi-step data translations and visualizations
- Plan to support new hybrid visualization techniques



Pore-scale Visualization of Benchmark Problem



Continuum Model Visualizations of Benchmark Problem

Visualization Needs

- Pore scale: Smoothed Particle Hydrodynamics (SPH).
  - Solves Navier-Stokes equations using discrete particle method
  - Grid free with particles
- Porous medium scale: STOMP Finite Volume model.
  - Finite-difference PDE approximation solved using PETSc (linear and non -linear iteration)
  - Structured grid, cell-centered properties
- Coupled pore- and continuum-scale models
  - Pore-scale only where mixing and reaction are occurring
  - Need to simultaneously represent both scales graphic

Visualization Challenges

- Large 3D data sets
  - Time to read data
    - Manipulating data in software with large data sets can be slow (parallel visualization?)
    - Determining resolution needed
    - Transient data
  - Best methods for manipulating data in software to extract useful information (feature identification)
  - Ability to extract 3D subgrids
  - Parallel processing
- Integration of particle and continuum data sets
  - Flagging of active sub-regions; ability to drill down into different types of data
- Plotting gridless particle data sets
  - Feature identification and selection of subsets of data

Current Methods

- Particle visualization
  - TecPlot
  - Institute for Ultrascale Visualization
- Gridded data visualization
  - TecPlot
  - FieldView