PNNL SFA: Role of Microenvironments and Transition Zones in Subsurface Reactive Contaminant Transport

Multiscale Reactive Transport Modeling

Tim Scheibe

Pacific Northwest National Laboratory, Richland, WA

http://www.pnl.gov/biology/sfa/

SFA Project Meeting
February 25-26, 2009

Office of Science
U.S. DEPARTMENT OF ENERGY

Environmental Remediation Sciences

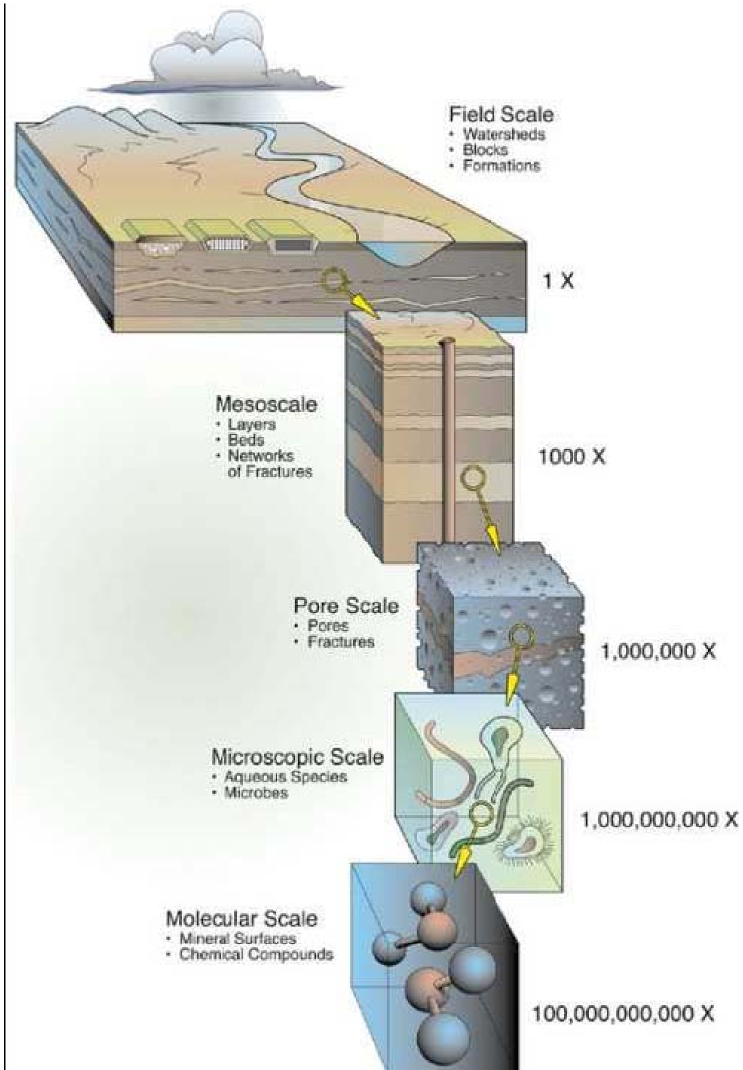
William R. Wiley EMSL

Pacific Northwest NATIONAL LABORATORY

PNNL-SA-65087

Objectives

- **Serve as the framework for quantitative integration among the experimental elements of the SFA**
  - Quantitative understanding of coupled flow, transport and reactions at fundamental scales (molecular / pore)
  - Develop and test upscaled models that rigorously incorporate fundamental scale process understanding
  - Predict laboratory- and field-scale experimental observations using pore-scale, upscaled, and hybrid models
- **Provide support for experimental design (with iterative updating based on new experimental results) and support post-experimental analysis and interpretation.**

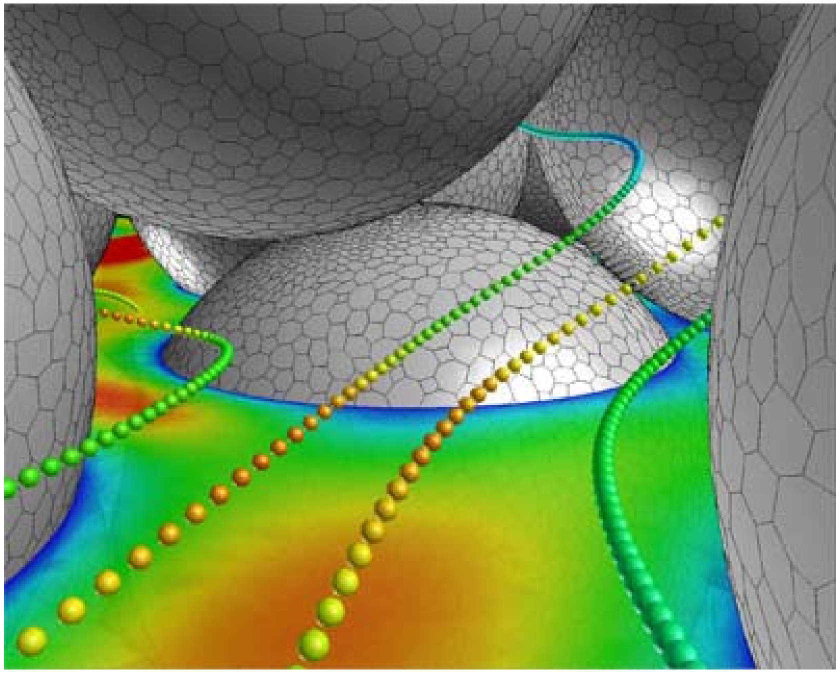


Fundamental Science Problems

- Scale issues are central to the SFA theme and hypotheses (microenvironments and transition zones are local-scale features that exert control on field-scale phenomena)
  - Quantitative understanding of coupled flow, transport and reaction at the pore scale (mass transfer of uranium)
  - Development and testing of rigorous continuum-scale models based on pore-scale simulations
  - Prediction of laboratory- and field-scale experimental observations using upscaled, pore-scale, and hybrid models (with minimal “calibration”)

Scope

- Initial focus:
  - Hanford IFC field site
  - Mass transfer controls on uranium transport
  - Diffusion/dispersion and dissolution/sorption.
- Future broadening:
  - Other field sites
  - Other contaminants (Tc, Pu)
  - Biogeochemical reactions
- Major elements:
  - Pore-scale model development and application
  - Rigorous upscaling
  - Column- and field-scale model application and testing



Pacific Northwest NATIONAL LABORATORY

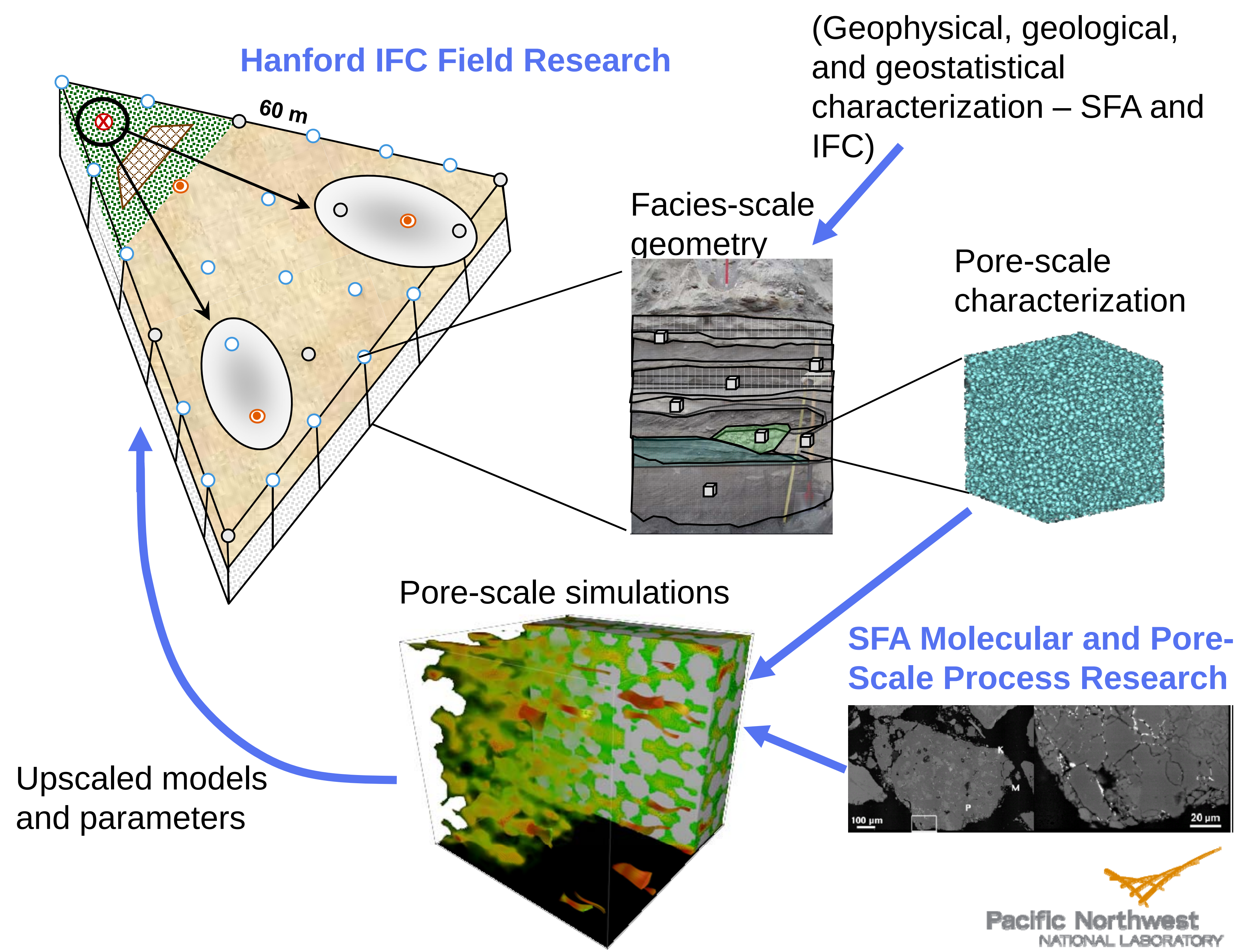
Primary Research Team

- SFA Co-PI and Project Lead: Tim Scheibe
- PNNL technical contributors:
  - Alexandre Tartakovsky (pore-scale modeling with SPH)
  - Marshall Richmond, Cindy Rakowski, Bill Perkins (pore-scale modeling with CFD and numerical upscaling)
  - John Serkowski (pore-scale visualization)
  - Yilin Fang (continuum-scale modeling)
  - Mark Rockhold (field-scale IFC model)
- External collaborator:
  - Brian Wood (Oregon State University): Theoretical and numerical upscaling (pore-to-continuum)

Hanford Motivation / Problem Linkage

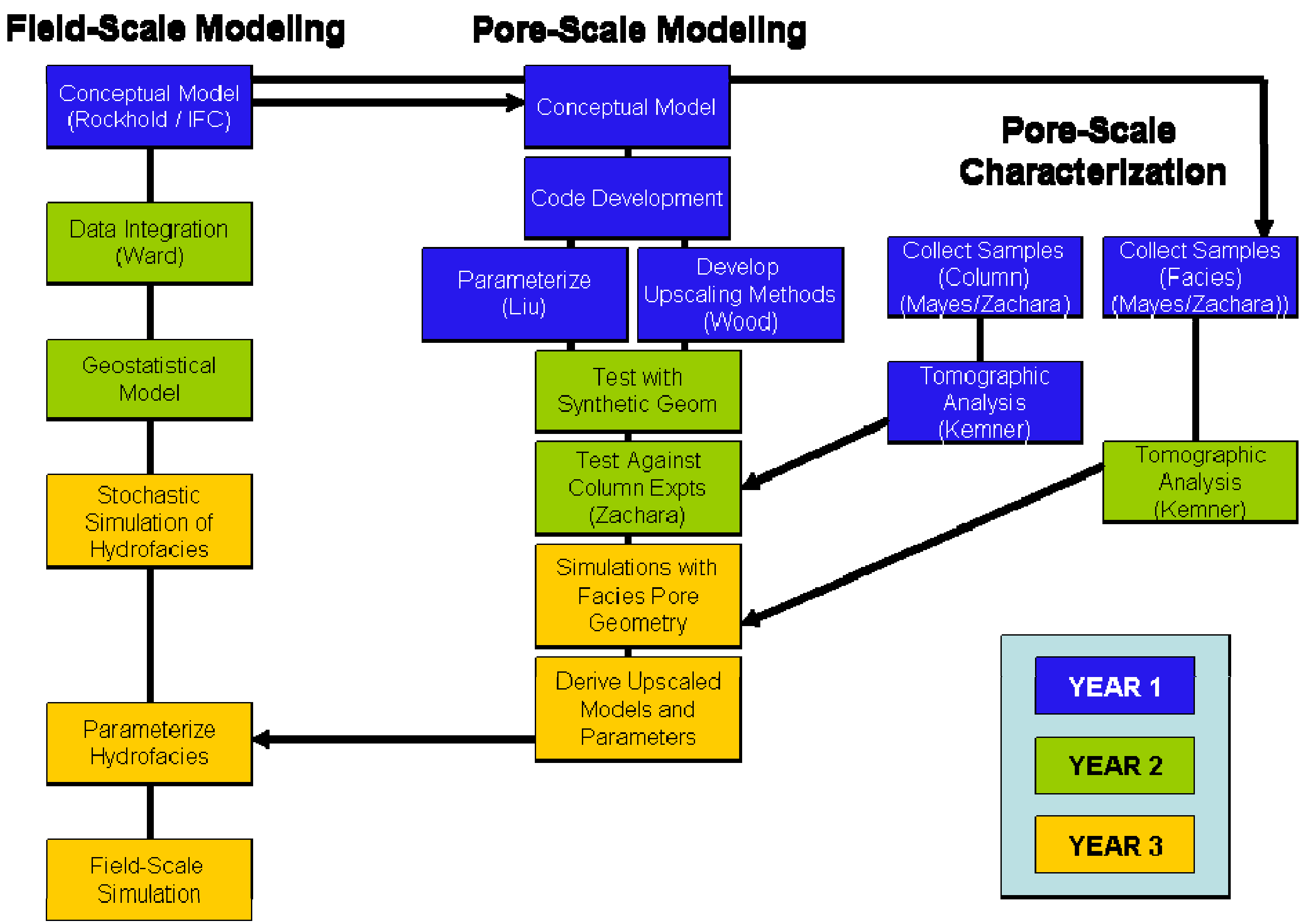
- Models will be initially applied to simulate uranium transport at the 300-area Integrated Field Challenge site.
- Developed models of Hanford Formation sediments will be applicable to other Hanford Formation problems (e.g., 100-H chromium site, 200-areas vadose zone)
- General approach/methodology of model development and upscaling will be broadly applicable to Hanford Site and beyond.

Pacific Northwest
NATIONAL LABORATORY



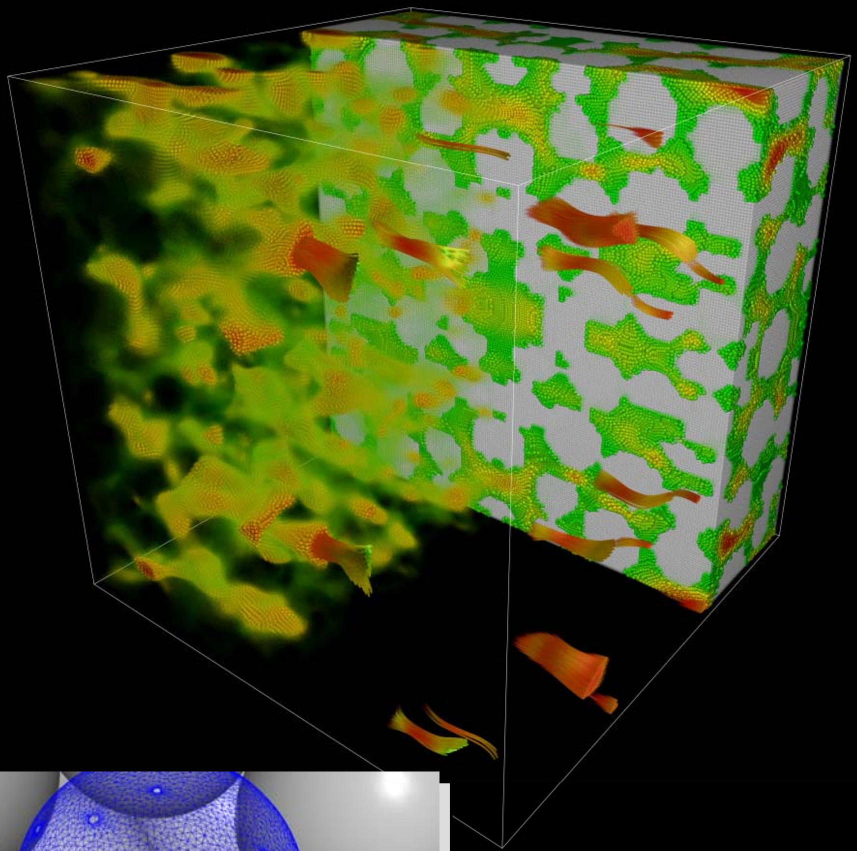
Pacific Northwest
NATIONAL LABORATORY

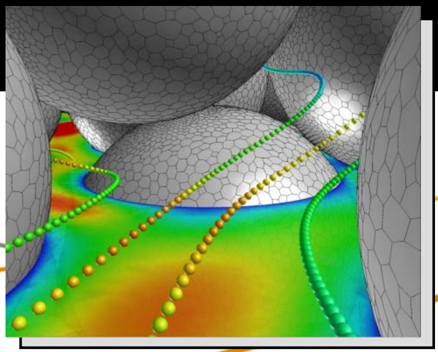
Research Design and Timeline

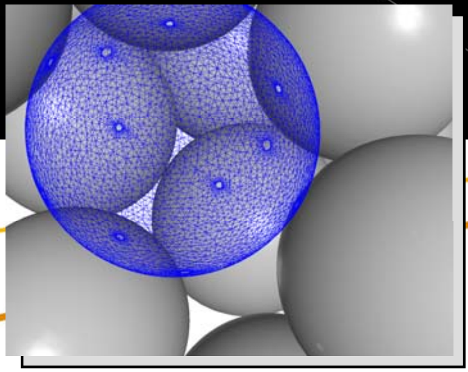


Pore-Scale Simulation

- Microbiological and geochemical processes are controlled by local (pore) environments
- Pore-scale simulation serves as the foundation for fundamentally-sound models at larger scales
- Grid- and particle-based methods implemented on parallel computers



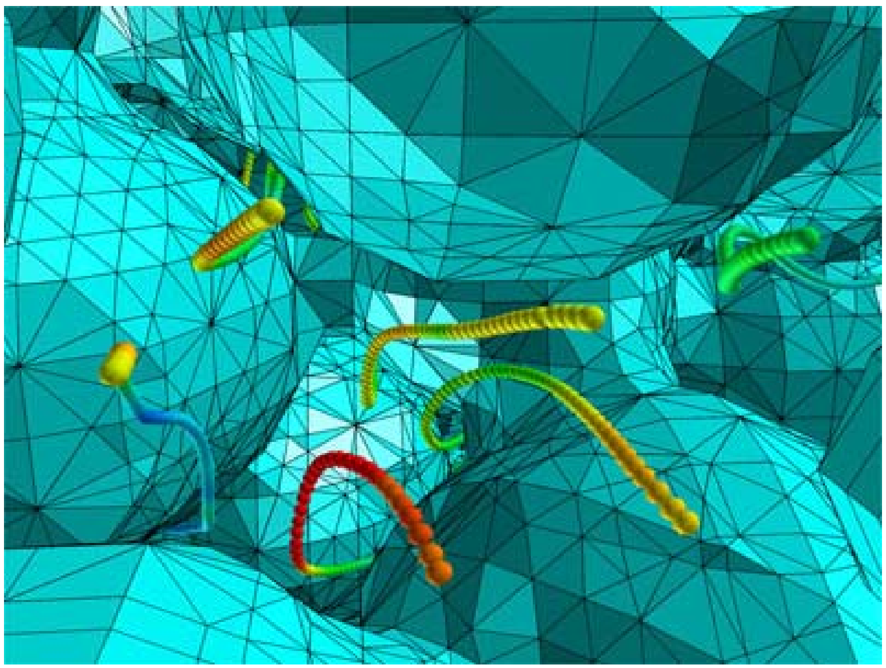


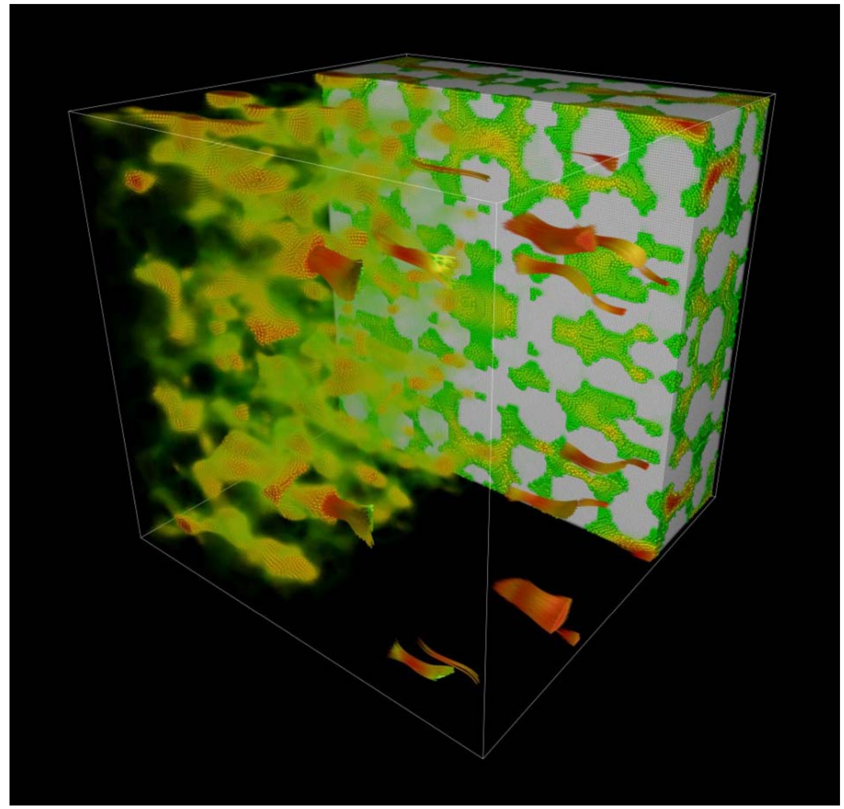


Pacific Northwest NATIONAL LABORATORY

Pore-Scale Modeling

- Two primary approaches:
  - Smoothed Particle Hydrodynamics (SPH)
  - Computational Fluid Dynamics (CFD)

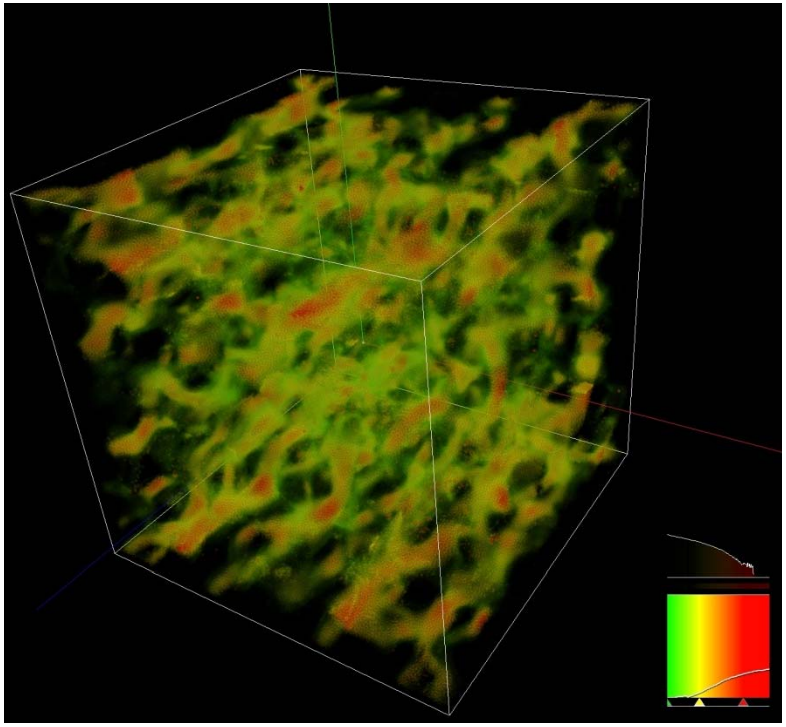




Pacific Northwest
NATIONAL LABORATORY

SPH Pore-Scale Model of Uranium Diffusive Mass Transfer

- 3D parallel SPH code runs on EMSL supercomputer (fluid flow and diffusion) using 500+ processors and 7 million particles (EMSL Science Theme allocation – SciDAC)
- Currently developing capability for intragranular diffusion and surface sorption of uranium (with Chongxuan Liu)
- Run series of simulations with varying amount and distribution of particles with intragranular sites
- Calculate effective dispersion and reaction rates (upscaling) using residence time distributions



Pacific Northwest
NATIONAL LABORATORY

CFD Pore-Scale Flow and Transport Model

- Goal: Numerically solve volume averaging closure equations for arbitrary pore geometry → define effective properties such as dispersion tensors
  - Implement numerical methods within CFD code
  - Test using standard problems (flow between plates, flow in a wavy tube)
  - Cross-validate computations against other methods (e.g., SPH, Lattice-Boltzmann) and data (MRI data from Joe Seymour, Montana State University)

Code Development and Testing

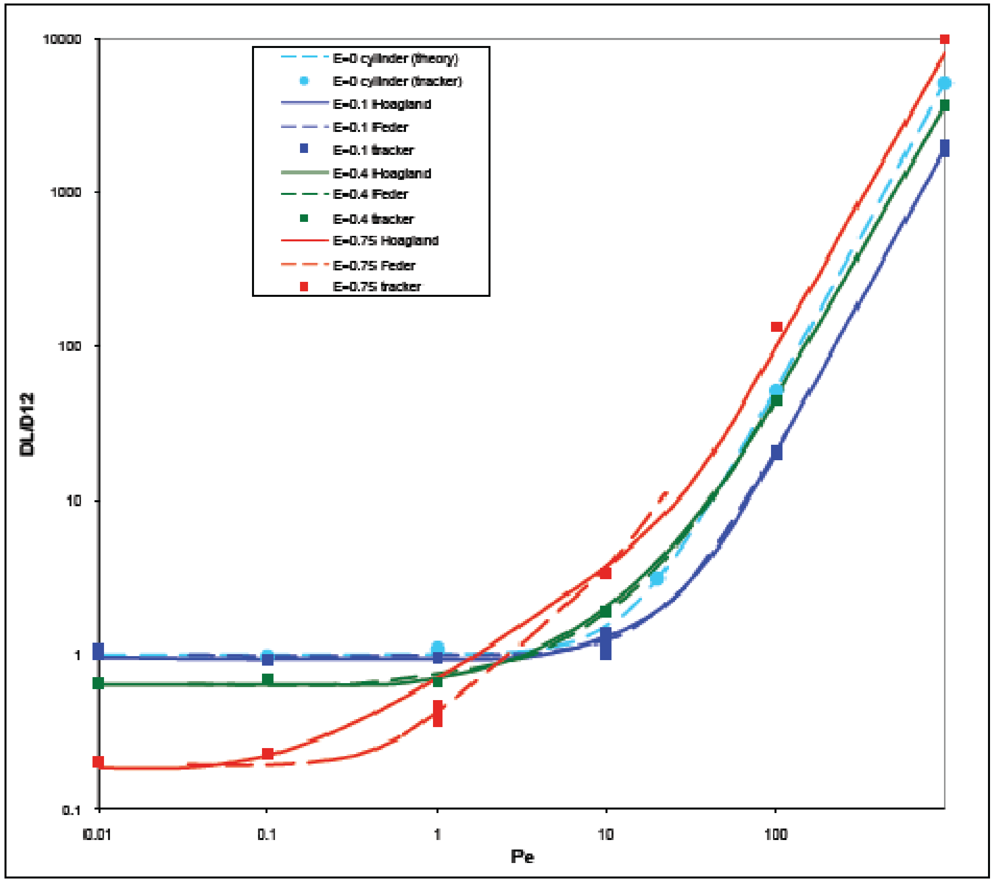
- SPH model enhancements: Received feedback on draft model design document from Liu and others. Scheibe (with Palmer / SciDAC) has initiated work on modifying the 3D parallel SPH code to incorporate intraparticle diffusion and reactions.
- Computational resources: In January we received a 2009 allocation from the NERSC supercomputing center. We are currently porting TETHYS (pore-scale CFD code) to Franklin and also are pushing for CCA software to get built there so we can also port our SPH code.

Upscaling Methods Development

- We have been working on developing and testing numerical upscaling (using volume averaging and particle tracking methods) using a wavy-tube model for which there are solutions in the literature for comparison. Some preliminary results:

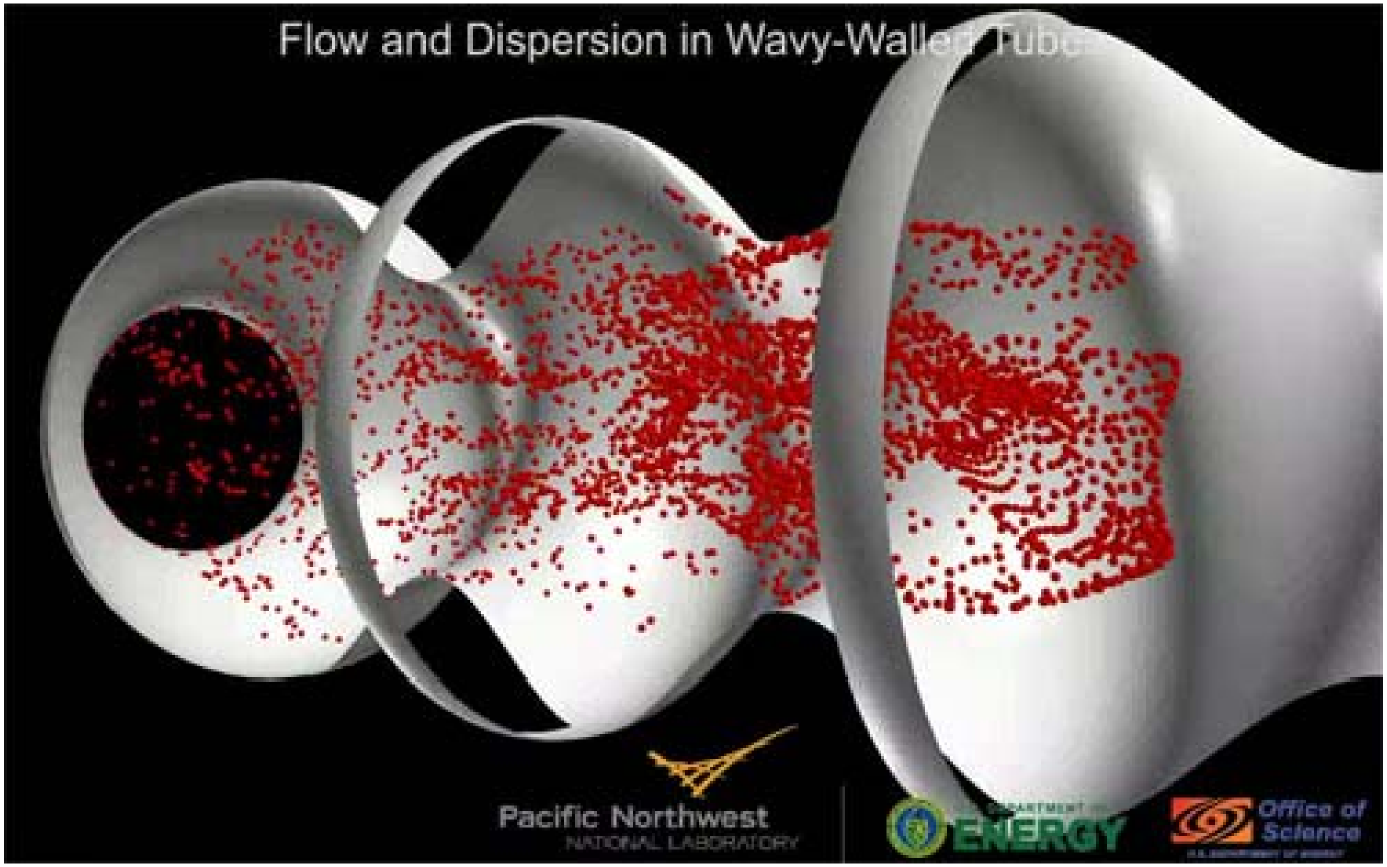
•These CFD simulations were run for a Reynolds number of 0.1 to correspond to the low Reynolds number, creeping flow used by Hoagland.
•Axial dispersion computed using our Lagrangian particle tracker code with 5000 particles.
•Also compared to results from Federspiel and Fredburg (1988) who also used Hoagland's results for validation of their calculations. We confirm their finding that for an amplitude of 0.75 (very wavy) Hoagland's results are incorrect.

•→ Conclusion: Particle tracking model is working correctly



Numerical Methods Testing

- Animation



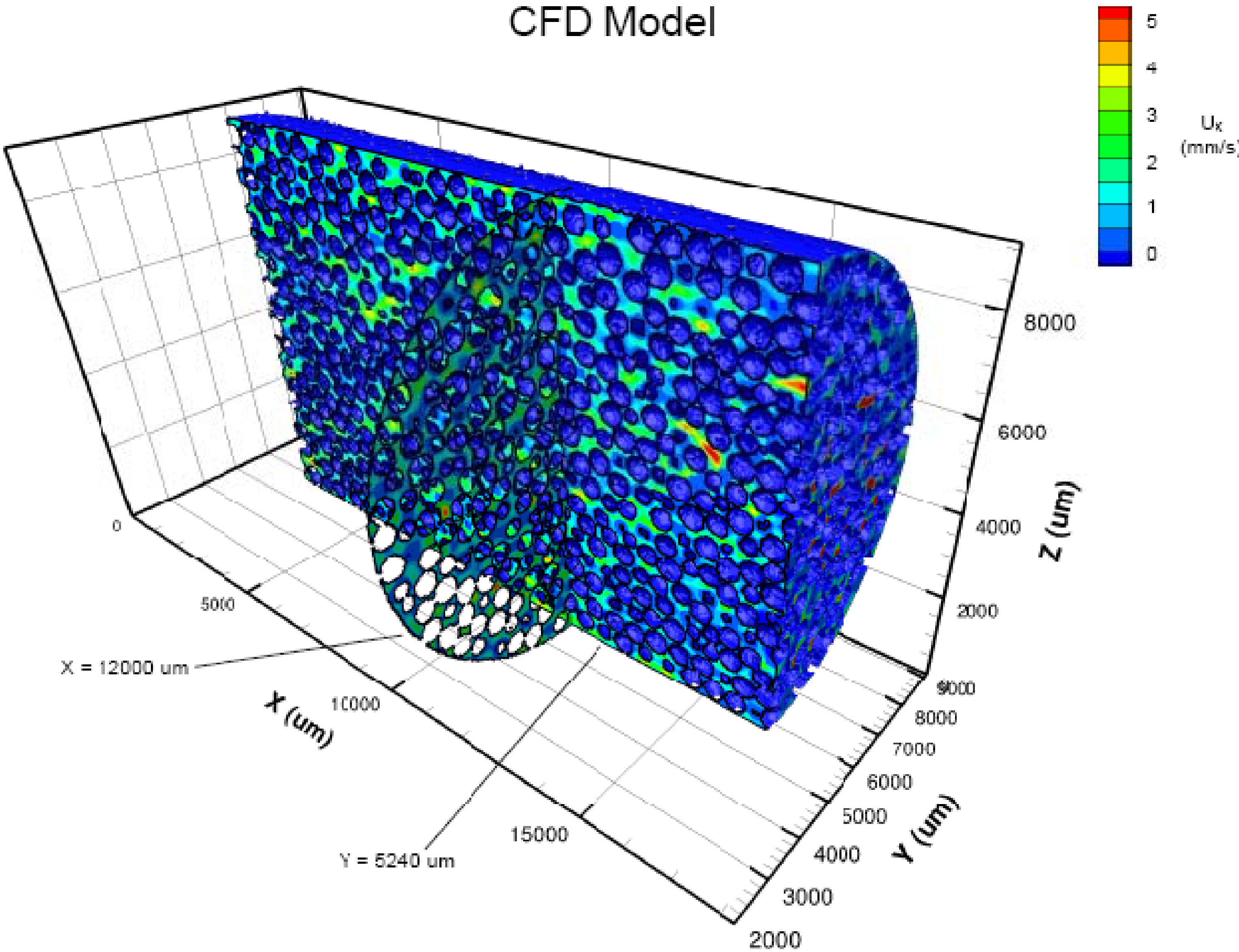
Model Cross-Validation

- Bruce Palmer has provided a 3D simulation of pore-scale flow using SPH in a randomly-generated synthetic pore geometry.
- Marshall Richmond is currently simulating the same problem using the CFD approach and will perform cross-validation once the results are available.
- We have contacted external researchers (Mike Sukop, FIU) that are interested in applying Lattice-Boltzmann methods to the same dataset for further cross-comparison of methods.
- We expect that this will lead to an interesting publication since the relative advantages/disadvantages of the various pore-scale simulation methods have not been quantitatively evaluated to date.

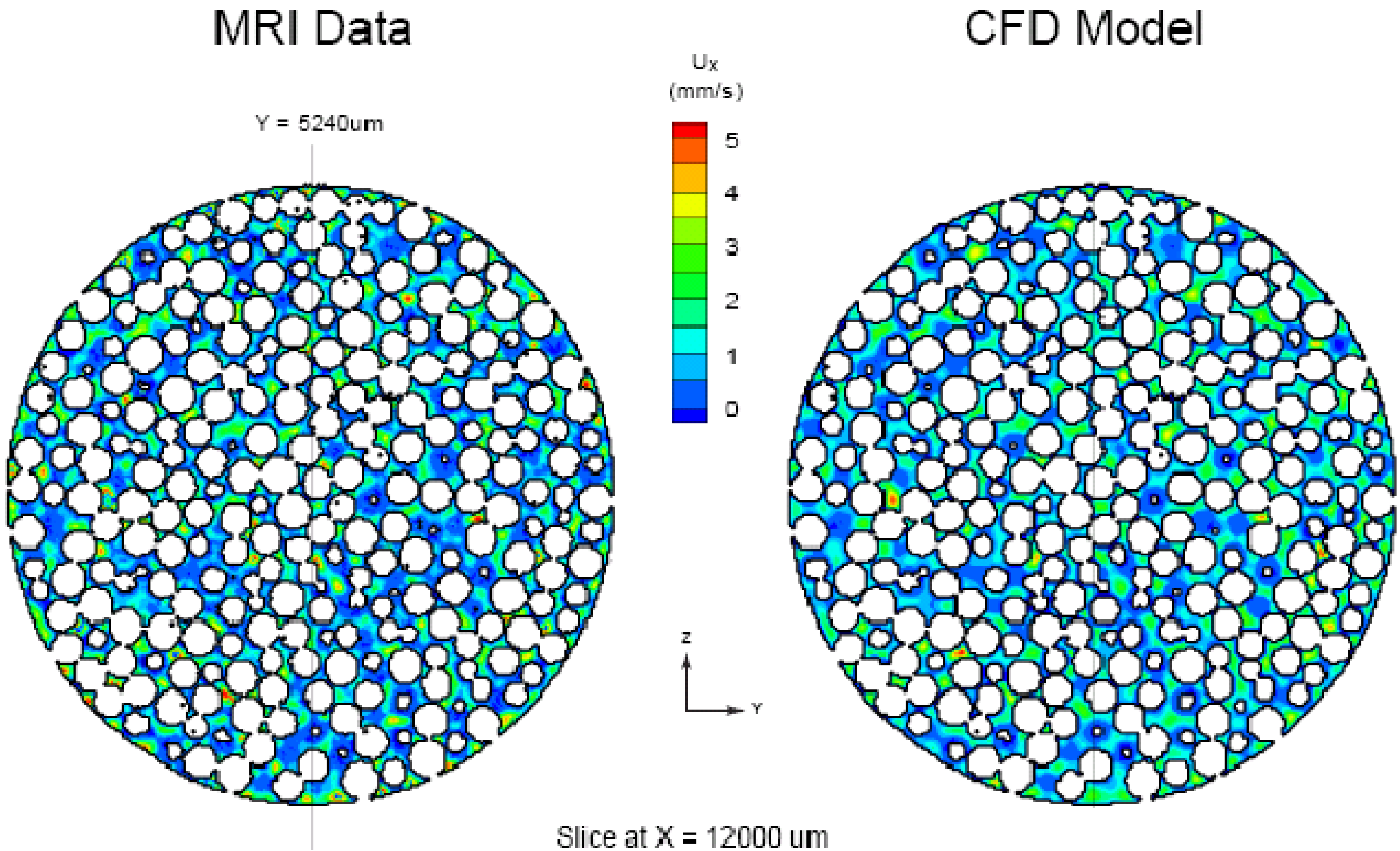
Pore-Scale Characterization

- Joe Seymour (Montana State University) provided a 512x256x256 dataset describing z-component of velocity in a 500 micron monodisperse beadpack, measured using MRI.
  - Resolution is 40 mm^3.
  - This will provide an excellent validation dataset for our SPH and CFD pore-scale flow models
  - Measurement of x- and y- components in the same beadpack are ongoing.

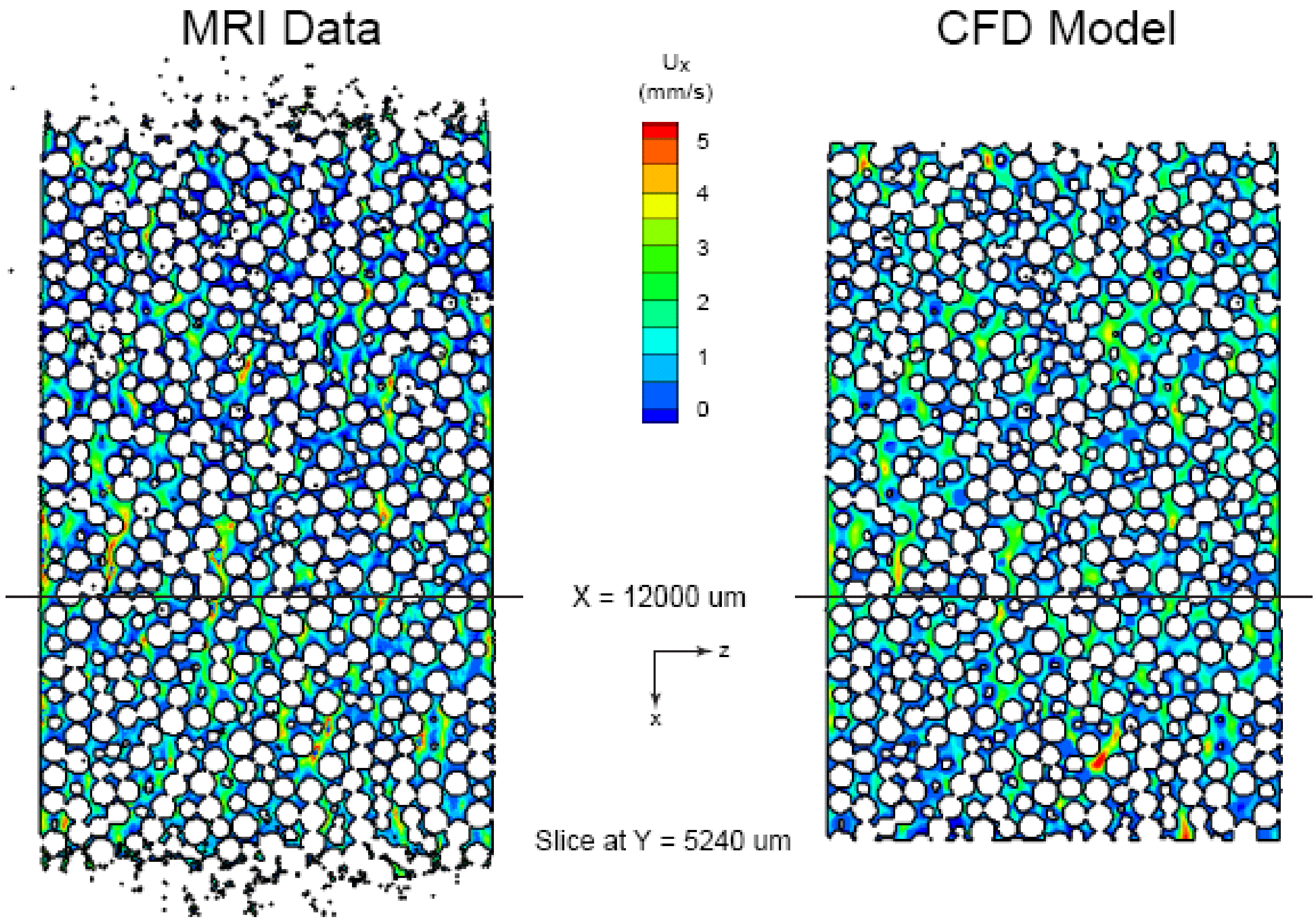
CFD Model



Pacific Northwest
NATIONAL LABORATORY

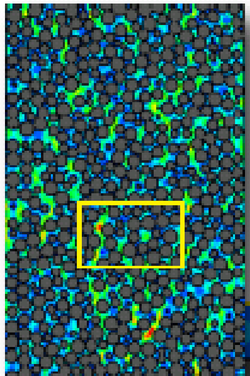


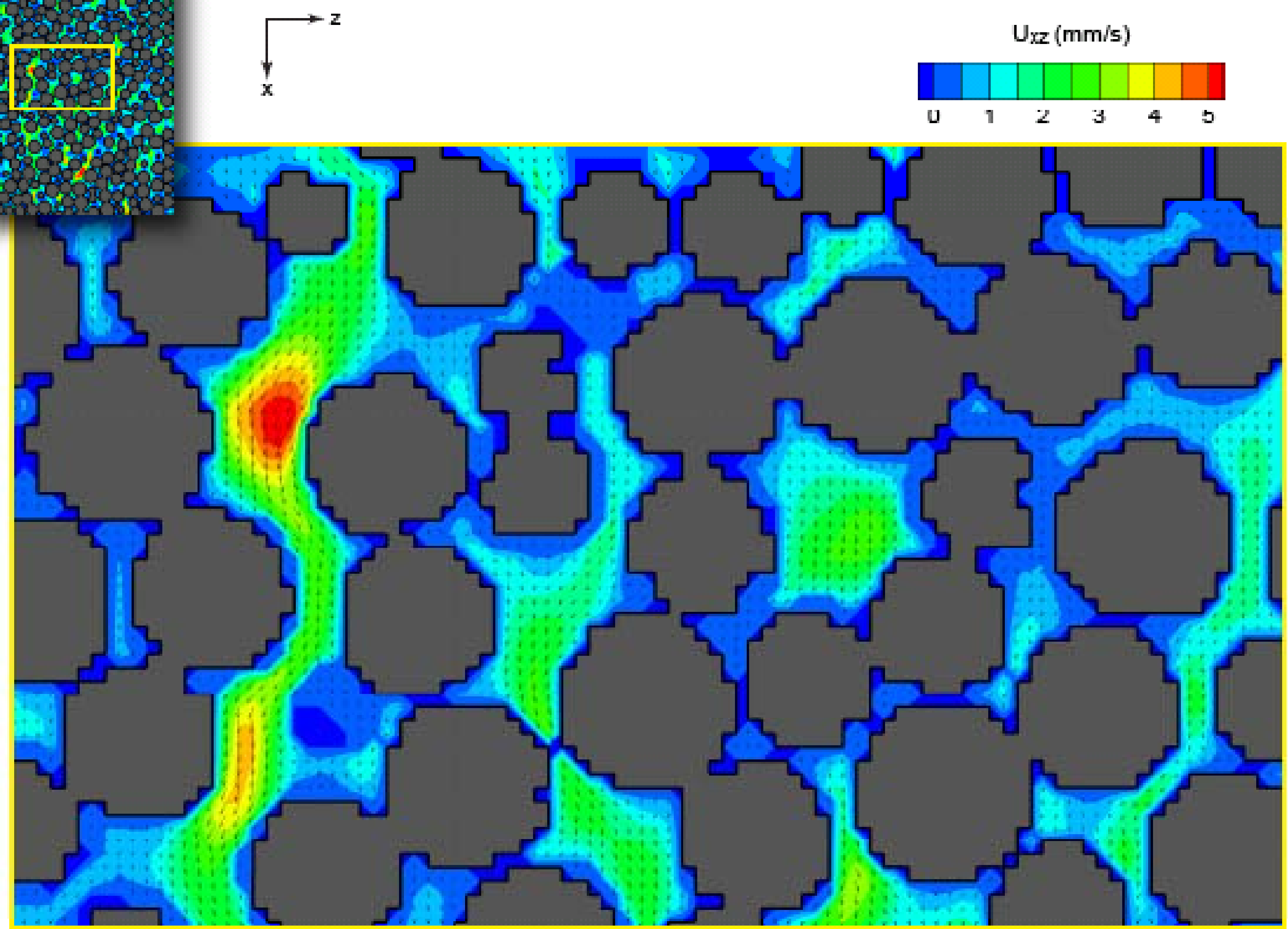
Pacific Northwest
NATIONAL LABORATORY



Pacific Northwest
NATIONAL LABORATORY

CFD Model



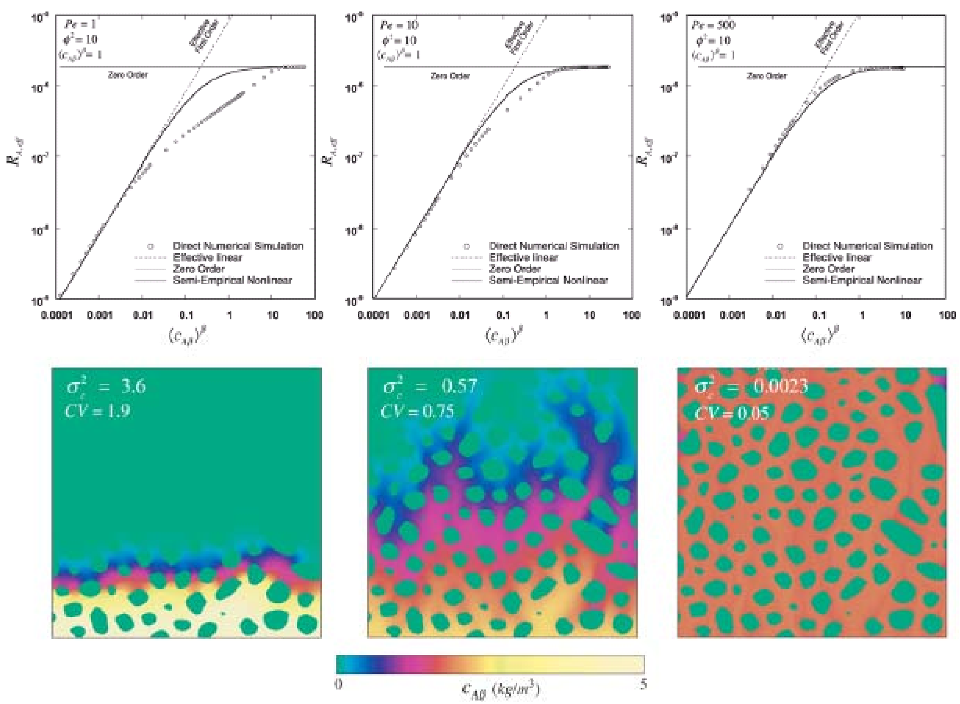


Slice at Y = 5240 um

Pacific Northwest
NATIONAL LABORATORY

Upscaling:

- Volume averaging method w/ direct numerical simulation[1]
  - Lagrangean methods[2,3]
  - Particle tracking methods[4,5,6]
  - Hybrid pore / continuum models[7]



1. Wood, B. D., Radakovich, K. & Golfier, F., Adv. Water Resour. 30: 1630-1647, 2007.
2. Yabusaki, S. B., Steefel, C. I. & Wood, B. D., J. Contam. Hydrol. 30: 299-331, 1998
3. Ginn, T. R. J. of Contam. Hydrol. 47:1-28, 2001
4. Scheibe, T. D. & Cole, C. R., Water Resour. Res. 30: 2027-2039, 1994
5. Scheibe, T. D., Fang, Y. L., Tartakovsky, A. M. and Redden, G. D., EOS Trans. AGU 88:H33H-1727, 2007
6. Scheibe, T. D. & Wood, B. D., Water Resour. Res. 39, 2003
7. Tartakovsky, A. M., D. M. Tartakovsky, T. D. Scheibe and P. Meakin, SIAM J. on Scientific Computing, 30(6):2799-2816, 2008.

Specific Science Milestones (2 Years)

- Implement SPH model of diffusive intragranular mass transfer and surface sorption of U(VI) with input from molecular-scale studies. (Liu/Tartakovsky)*
- Define field-scale hydrofacies framework for 300 Area IFC. Compile existing field data and develop preliminary geostatistical model of hydrofacies distribution. Begin initial numerical model development. (Rockhold/Fang)
- Collect intact sediment samples from each of the defined hydrofacies and submit for synchrotron analysis. (Zachara/Kemner)
- Develop and test combined numerical/theoretical upscaling approach for uranium mass transfer / sorption / dispersion. (Wood/Richmond)*
- Integrate geophysical observations into the geostatistical model of hydrofacies distributions for 300 Area IFC. (Ward)

***Peer-reviewed publications**

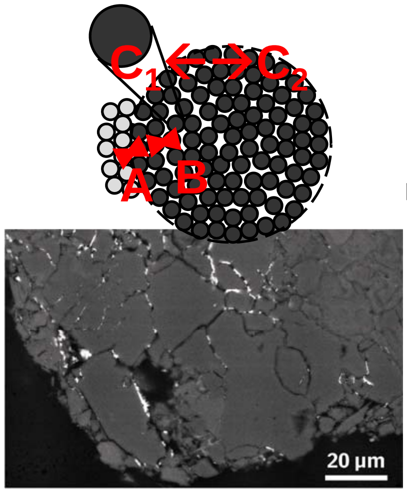
Pacific Northwest
NATIONAL LABORATORY

Expected Accomplishments and Impact

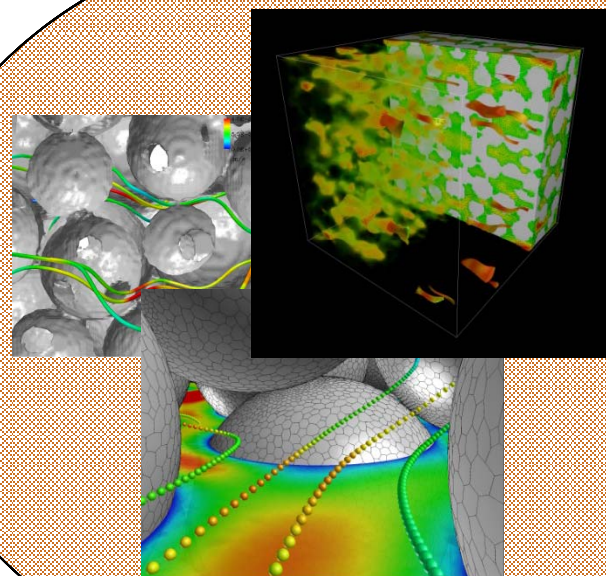
- We will undertake the first serious attempt to quantitatively utilize information from molecular and pore scales to drive predictions in a field-scale model. **<u>Impact: Reduce reliance on "calibration" (parameter fitting) of field-scale models and improve predictive capability.</u>** *(directly addresses ERSP long-term measure)*
- We will implement novel pore-scale models of diffusive mass transfer, dispersion, and sorption. **<u>Impact: New insights into the nature of coupled processes at fundamental scales.</u>**
- We will develop and test new upscaling methods based on combined numerical and theoretical approaches. **<u>Impact: Upscaling methods with fewer restrictive assumptions (linearity, periodicity, etc.).</u>**
- We will create a quantitative basis for integration across projects within the SFA, and between the SFA and the IFC. **<u>Impact: A much higher level of project synergy and multidisciplinary collaboration will increase the value and productivity of all research.</u>**

OBJECTIVE: Bridge the gap between fundamental process understanding and field-scale reactive transport prediction

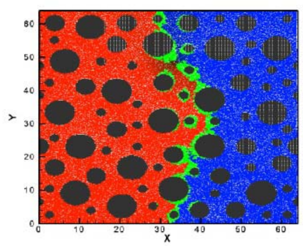
Diffusion-controlled dissolution and transport of U (PNNL SFA project – collaboration with molecular-scale modelers (Liu) and computational scientists (SPH – SciDAC)



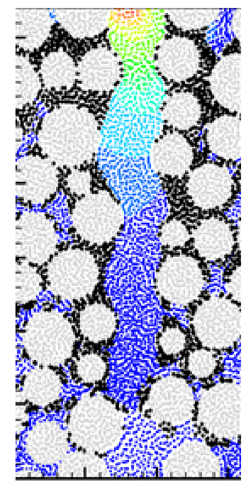
http://subsurface.pnl.gov



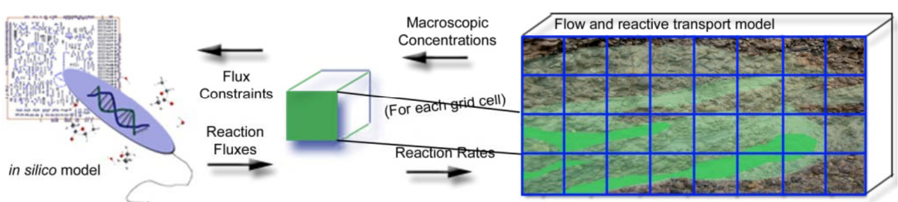
Pore-Scale Process Modeling



Hybrid Multiscale Modeling
(Tartakovsky et al., 2008a; 2008b; Battiato et al., submitted).



Biofilm Dynamics
(Tartakovsky et al., in press)



Genome-scale Metabolic Modeling (Scheibe et al., 2009) – collaboration with mircobiologists at U Mass and U Toronto

Pacific Northwest
NATIONAL LABORATORY