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Linking Pore- and Darcy-scale Models of Reactive and Non-Reactive Transport

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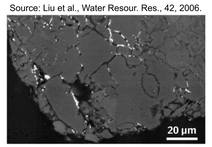
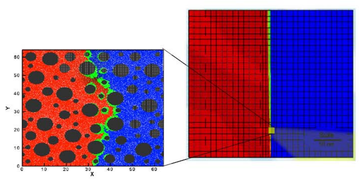
Project Objectives:

1) Develop and test a multiscale hybrid modeling framework for subsurface flow and reactive transport simulation, for problems with high levels of localization and process coupling.
2) Develop and test an upscaling approach for quantatively incorporating molecular and laboratory scale information into field-scale models through application of pore-scale models.

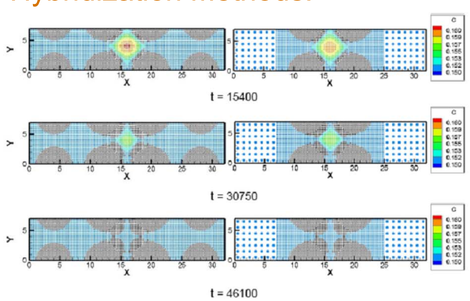
Source: Liu et al., Water Resour. Res., 42, 2006.



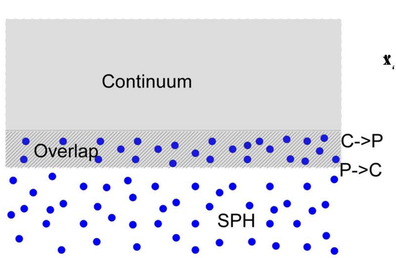
Source: George Redden, Idaho National Laboratory



Hybridization Methods:



Hybrid two-scale SPH model of diffusion and reaction with mineral precipitation. Left images: pore-scale-only model results at three simulation times. Right images: hybrid pore-Darcy scale model results. From Tartakovsky et al., SIAM J. Sci. Comp., 2008.

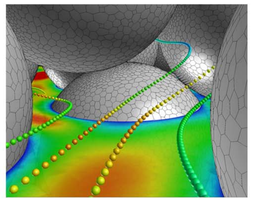


$$\dot{\mathbf{v}}_i = \frac{\mathbf{F}_i}{m} - \frac{1}{N_J m}\sum_{i=1}^{N_J}\mathbf{F}_i + \frac{D\mathbf{u}_J(t)}{Dt}$$

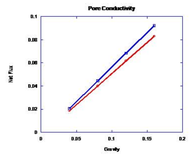
Left: Schematic diagram of coupling between SPH pore-scale and grid-based continuum-scale models. Above: Modified force equation for particles in the matching zone (after Nie et al., *J. Fluid Mech.*, 2004).

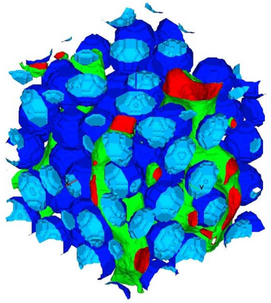
Pore-Scale Modeling:

We are developing and applying both grid-based methods (top image below) and grid-free methods (bottom image below and images to the right) to simulation of pore-scale fluid flow and reactive transport.

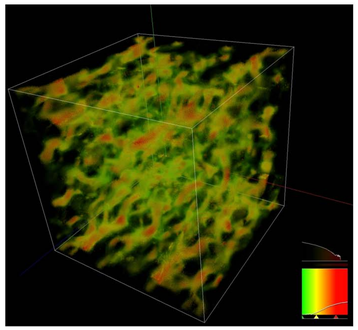


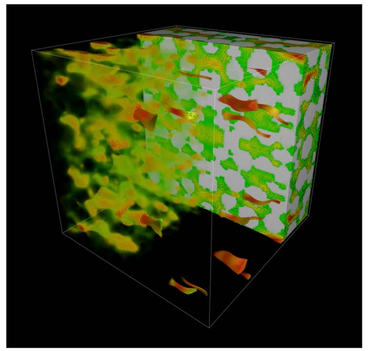
Simulation performed by Cindy Rakowski (PNNL); Visualization created by John Serkowski (PNNL)



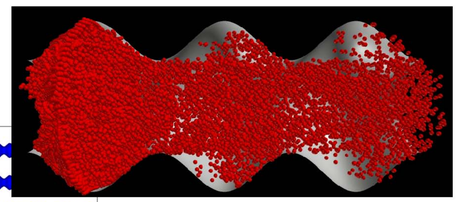


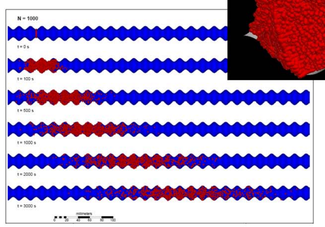
Simulations were performed by Bruce Palmer on the Hewlett-Packard Linux-based supercomputer MPP2 at the Environmental Molecular Sciences Laboratory, a national scientific user facility sponsored by the Department of Energy's Office of Biological and Environmental Research and located at Pacific Northwest National Laboratory.





Figures above are based on simulated fluid flow through a complex 3D pore geometry. The simulation method is Smoothed Particle Hydrodynamics (SPH). Visualizations were created by Chad Jones and Kwan-Lui Ma of the SciDAC Institute for Ultrascale Visualization at UC Davis.





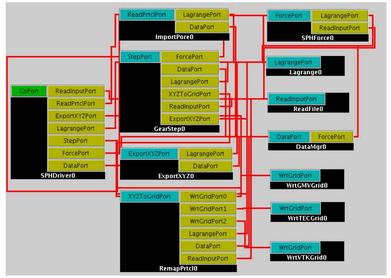
Left and above: Cross-sections of simulated Lagrangian particles moving through a 3D wavy tube, computed using grid-based CFD methods. Visualization above created by John Serkowski (PNNL). See also the animation on laptop accompanying this poster.

Science Application Partnerships:

Component Software Infrastructure for Achieving High Level Scalability in Groundwater Reactive Transport Modeling and Simulation (Bruce Palmer, PNNL, PI)

Major Components:

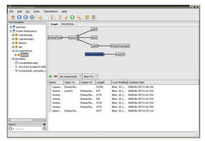
- Component-based SPH (pore-scale) and STOMP (continuum-scale) codes - in testing/validation
- Application of parallel SPH code to 3D simulation of uranium dissolution and diffusion-limited transport in intra- and inter-granular pore spaces - under development
- Implementation of a two-scale hybrid model in the component framework - planned

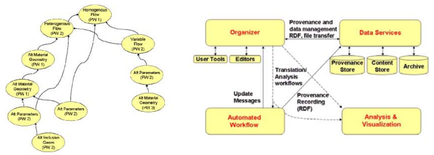


ISSUES:
> Definition: What functionality and data belong together?
> Granularity: Componentization vs. performance
> Abstraction of Interfaces: Support multiple model implementations?

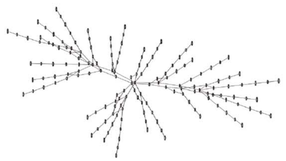
Process Integration, Data Management, and Visualization for Subsurface Simulation (Karen Schuchardt, PNNL, PI)

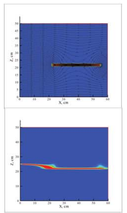
- **Major Components**
  - **Organizer Tool**
  - **Scientific workflow automation**
  - **Data and metadata management**
  - **Large-scale data visualization**





Top right: A screen shot of the Organizer tool.
Middle right: Relationship diagram
Above and Below: Network plots for a series of calcite precipitation experiments (lower right).





Publications:

Tartakovsky, A. M., G. Redden, P. C. Lichtner, T. D. Scheibe, and P. Meakin, "Mixing-induced precipitation: Experimental study and multi-scale numerical analysis," Water Resources Research, 44, W06S04, doi:10.1029/2006WR005725, 2008.

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Tartakovsky, A. M., D. M. Tartakovsky, T. D. Scheibe and P. Meakin, "Hybrid simulations of reaction-diffusion systems in porous media," SIAM Journal on Scientific Computing, 30(6):2799-2816, 2008.

Tartakovsky, A. M. and S. P. Neuman, "Effects of Peclet number on pore-scale mixing and channeling of a tracer and on directional advective porosity," Geophysical Research Letters, 35, L21401, doi:10.1029/2008GL035895, 2008

Schuchardt, K., G. Chin, Jr., J. Chase, J. Daily, and T. Scheibe, "Experiences in the design of scientific workflows for subsurface sciences," submitted March 2008 to IEEE Transactions on Automation Science and Engineering , special issue on Scientific Workflow Management and Applications, in review

Meakin, P. and A. Tartakovsky, "Modeling and simulation of pore scale multiphase fluid flow and reactive transport in fractured and porous media," submitted February 2008 to Reviews in Geophysics, in review

Tartakovsky A. M., P. Meakin, T. D. Scheibe, and R. M. Eichler West, "Simulations of reactive transport and precipitation with smoothed particle hydrodynamics." Journal of Computational Physics, 222(2):654-672, 2007. doi:10.1016/j.jcp.2006.08.013

Tartakovsky, A. M., P. Meakin, T. Scheibe, and B. D. Wood, "A smoothed particle hydrodynamics model for reactive transport and mineral precipitation in porous and fractured porous media," Water Resources Research, 43(5):Art. No. W05437, doi:10.1029/2005WR004770, 2007.

Tartakovsky, A. M., T. D. Scheibe, and P. Meakin, "Pore-scale model for reactive transport and biomass growth," accepted March 2008 for publication in Journal of Porous Media, in press.

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The Pacific Northwest National Laboratory, located in southeastern Washington State, is a U.S. Department of Energy Office of Science laboratory that solves complex problems in energy, national security and the environment, and advances scientific frontiers in the chemical, biological, materials, environmental and computational sciences. The Laboratory employs 4,000 staff members, has a $760 million annual budget, and has been managed by Ohio-based Battelle since 1965.

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