

Pore-Scale Simulation and Upscaling of Uranium Transport in Groundwater

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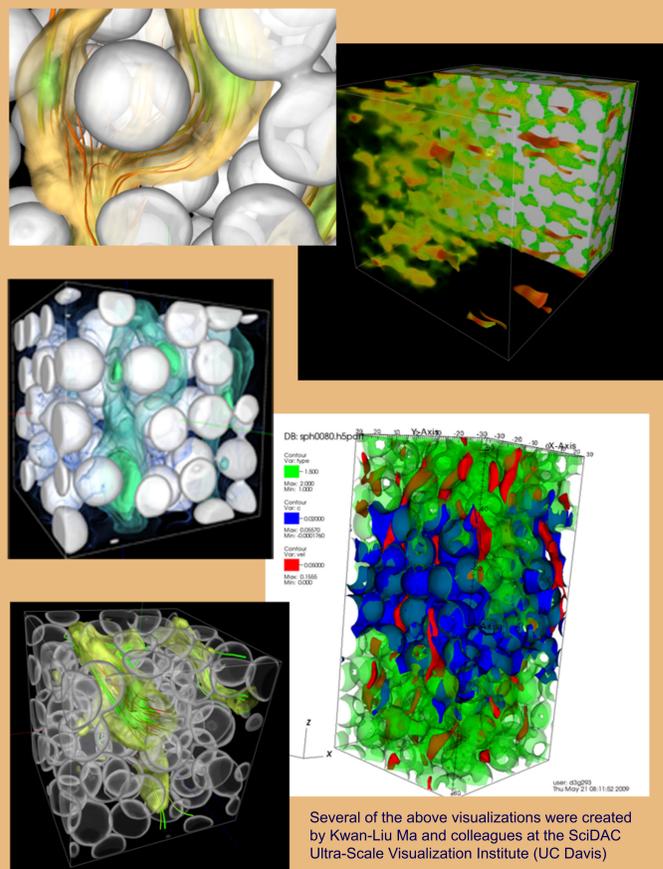
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PORE-SCALE SIMULATION

The transport and fate of uranium in the subsurface is strongly influenced by processes and properties that act predominantly at the scale of individual solid grains and fluid-filled (air or water) pore spaces. Pore-scale simulation (numerical modeling) provides a means of studying the emergent (larger-scale) character of multiple coupled processes acting at local scales. Critical challenges include 1) computationally intensity; 2) measurement of 3D pore geometry and mineral distribution in natural media; 3) experimental validation of complex pore-scale simulations; and 4) defining quantitative models of larger-scale (upscaled) behavior. This poster describes our recent advances in these four areas, ongoing research, and application to key uranium transport processes.

Smoothed Particle Hydrodynamics:

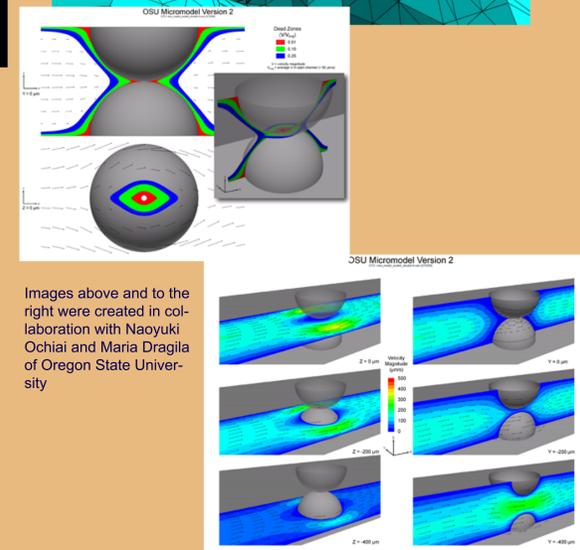
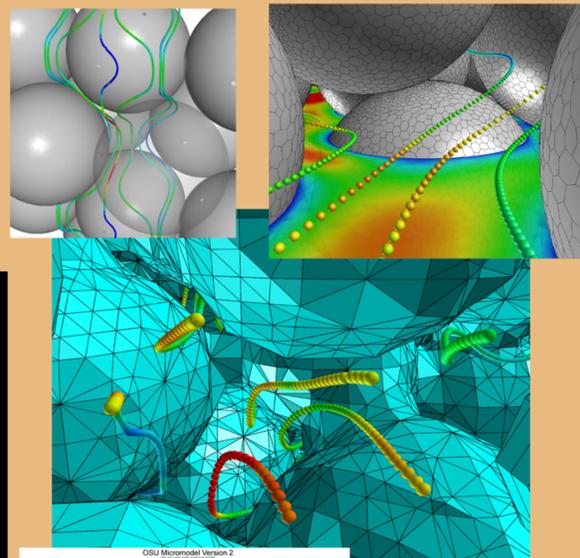
Smoothed Particle Hydrodynamics (SPH) is a particle-based (mesh-free) simulation method that is well-suited to pore-scale simulation. Our research group has applied this technique to simulation of multiphase flow and solute transport in porous media (Tartakovsky and Meakin, *Vadose Zone Journal*, 2005; Tartakovsky and Meakin, *Phys. Rev. E*, 2005; Tartakovsky et al., *Physics of Fluids*, 2007), pore-scale mineral precipitation (Tartakovsky et al., *Journal of Computational Physics*, 2007; Tartakovsky et al., *Water Resources Research*, 2007 and 2008), and biofilm development in porous media at the pore scale (Tartakovsky et al., *Journal of Porous Media*, 2009). We have developed a three-dimensional parallel SPH code for performing high-resolution pore-scale modeling in arbitrary 3D pore geometries. The images below visualize simulated fluid velocities and solute concentrations in synthetic and measured pore geometries.



Several of the above visualizations were created by Kwan-Liu Ma and colleagues at the SciDAC Ultra-Scale Visualization Institute (UC Davis)

Finite Volume CFD Methods

We are also applying grid-based finite volume methods drawn from the field of Computational Fluid Dynamics (CFD) to pore-scale simulation of flow and reactive transport. Grid generation issues for arbitrary and highly complex pore geometry are significant, particularly in the vicinity of grain-to-grain contacts. We have developed a method for automatically generating numerically accurate grids, and we have conducted 3D pore-scale flow simulations using both STAR-CD and a PNNL-developed code (TE2THYS) running on computational systems ranging from local workstations to the Franklin supercomputer at NERSC.

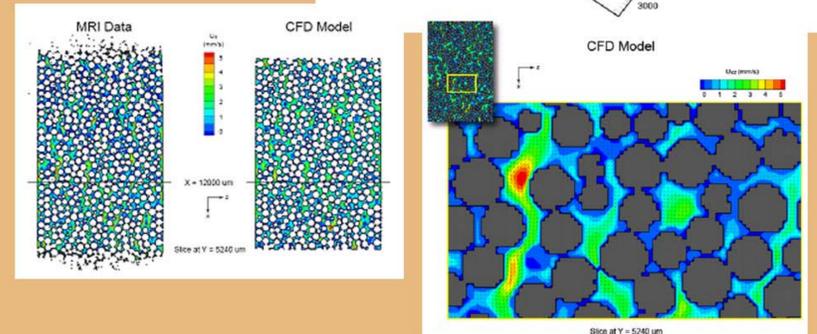
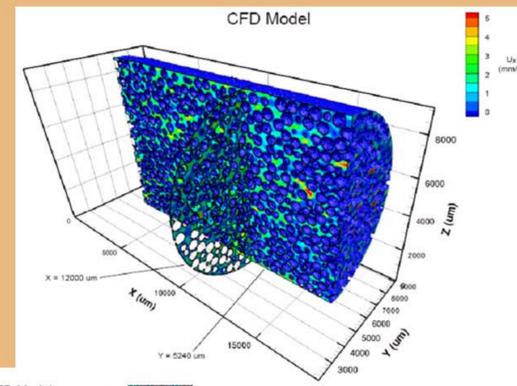


Images above and to the right were created in collaboration with Naoyuki Ochiai and Maria Dragola of Oregon State University

CHARACTERIZATION AND VALIDATION

Example: Magnetic Resonance Imaging

3D MRI dataset describing pore geometry and z-component of velocity in an experimental glass beadpack (courtesy Dr. Joseph Seymour, Montana State University). The dataset is resolved in 40-micron voxels. We are using this dataset to test our 3D CFD and SPH models of pore-scale flow. Right: A 3D CFD simulation of flow in the experimental beadpack. Below: Comparison of MRI-measured velocities and simulated velocities in a 2D slice through the 3D model/data. Also shown is a close-up of a portion of the simulated velocity field, showing local high-velocity flow zones (preferential flow paths).



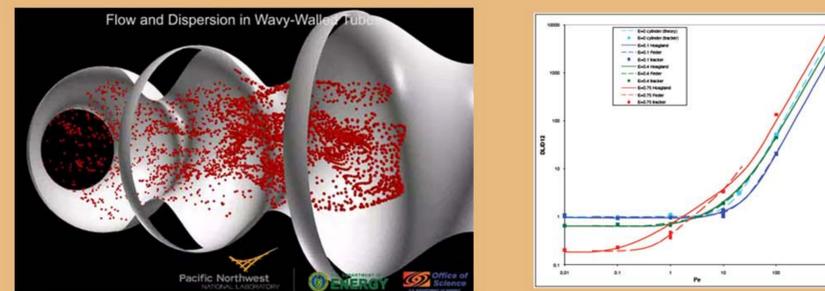
UPSCALING

Example: Volume Averaging - Numerical Solution

Volume averaging is one approach to rigorous upscaling; i.e., definition of macroscopic process models (equations) and parameters based on detailed knowledge of microscopic processes. Most reported applications rely on analytical solutions that require restrictive assumptions (e.g., periodic monodisperse media with perfect cubic packing). However, volume averaging methods can be implemented for more general cases (e.g., arbitrary pore geometries) by solving the closure equations numerically. Such solutions take very similar form to the numerical solutions of the underlying flow equation, and therefore are amenable to application of CFD codes (see above). In collaboration with Brian Wood of Oregon State University, we have performed initial numerical studies using a 3D wavy tube model that approximates pore throats and pore bodies, to develop and test our numerical methods. Once fully validated, the codes will be applied to generalized pore geometries.

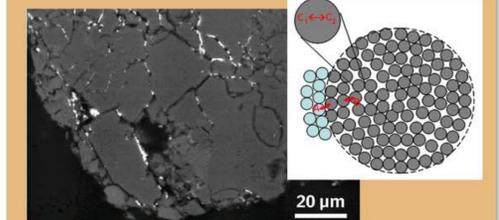
Below left: 3D visualization of simulated Lagrangian particles moving through a 3D wavy tube, computed using grid-based CFD methods.

Below right: Axial dispersion in the wavy tube, calculated using our CFD model and compared with literature reports.



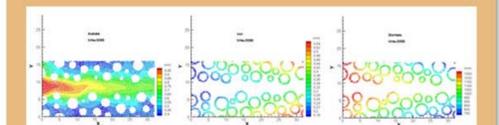
INTRAGRANULAR DIFFUSION

The image below shows a back-scattered electron SEM image indicating the intragrain distribution of U(VI) precipitates (white) within a feldspar grain (From Liu et al., *Water Resources Research*, 2006). The diagram on the right shows the implementation of a two-domain diffusive mass-transfer model in SPH. Grey particles represent solid phase; blue represent fluid phase. Diffusive transfer between fluid and solid phase particles in primary porosity (i.e. A) and between two solid particles (i.e. B) is implemented using the standard SPH diffusion model. Diffusive transfer between the primary and secondary porosity domains (C1 and C2) occurs only within each SPH particle as denoted by the enlarged gray particle. This approach is being implemented in the 3D parallel SPH code to allow simulation of pore-scale transport of uranium including diffusion-limited mass transfer.



SURFACE REACTIONS

Many reactions important to uranium transport and fate are associated with mineral surfaces (e.g., microbial reduction, surface complexation). We have developed an SPH model using a diffuse surface layer (Xu et al., *Phys. Rev. E*, 2009) that can be used to simulate these processes. Below is a sequence of images showing results of a pore-scale simulation of microbial iron reduction at grain surfaces under stimulation by a soluble electron donor (acetate, left image). Center image: Simulated distribution of surface-associated Fe(III) at a selected time step. Right image: Simulated distribution of surface-associated biomass.



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