Hybrid Numerical Methods for Multiscale Simulations of Subsurface Biogeochemical Processes

Tim Scheibe, Alexandre Tartakovsky, Bruce Palmer, Karen Schuchardt - Pacific Northwest National Laboratory
Daniel Tartakovsky - University of California San Diego
Paul Meakin, George Redden - Idaho National Laboratory

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Hybrid Multiscale Modeling

The images below schematically show the concept and a possible implementation of the hybrid multiscale modeling approach. ***Figure 1*** is a photograph of an intermediate-scale quasi-2D experimental flow cell (courtesy of George Redden, Idaho National Laboratory). In this experiment, two solutes are injected into the system along the bottom boundary and flow upward, mixing along the centerline. A reaction between the two solutes forms the mineral CaCO3 (calcite), shown in the photo as a narrow whitish band. The mixing zone, within which concentration gradients are very strong, is very narrow, and the precipitated mineral inhibits solute mixing leading to strong coupling between the reaction and transport processes. While a grid-based porous media continuum approach is appropriate for most of the domain (***Figure 2***), the processes in the mixing zone are better described by a grid-free particle method (Smoothed Particle Hydrodynamics or SPH as shown in ***Figure 3***) which is able to explicitly model the geometry of grains and pore spaces. Red and green colors represent the two solutes; green particles indicate locations of precipitated minerals, and black circles denote soil grains. Model hybridization requires definition of an algorithm for matching conditions at the sub-model domain boundaries that enforces conservation of mass (both fluid and solutes).

Figure 1

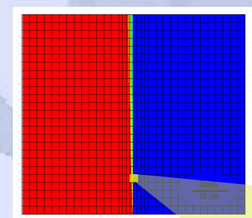


Figure 2

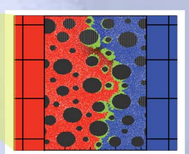


Figure 3

This project is developing and applying a computational framework for hybrid modeling of challenging subsurface reactive transport problems. In the hybrid modeling approach (also called adaptive algorithms or adaptive physics), two or more models at different scales, and with fundamentally different representations of physics, chemistry, and biology are coupled and executed together. The more computationally expensive model (in this case, a pore-scale model) is used only in that portion of the model domain where it is needed and linked to a less demanding model over the remainder of the domain.

Figure 4

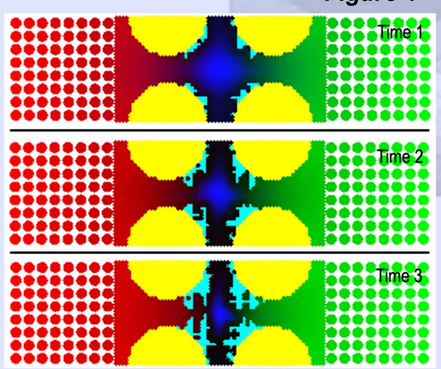


Figure 4 shows results of our first hybrid simulation. This model represents the mixing and reaction of two solutes (with diffusion only, no advection) using the SPH method for both the discrete pore-scale and continuum-scale models. Simulation results are shown for three times. Green and red particles represent the two solutes; blue tones represent the mixed fluid, yellow represents individual grains in the pore-scale model, and light blue represents the precipitated solid phase mineral that results from the reaction of the two solutes.

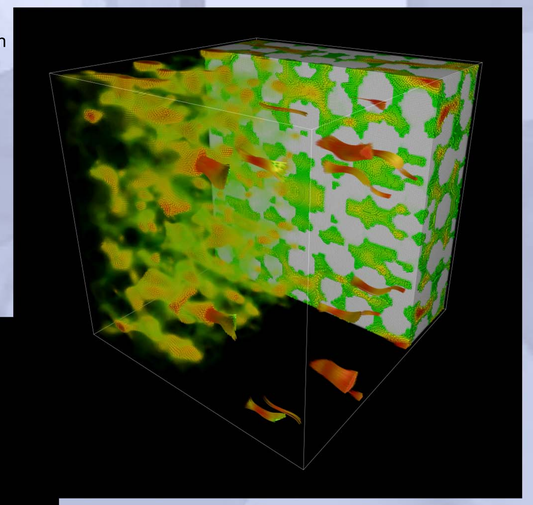
Pore-Scale Modeling Using Particle and Grid Methods

Figures 5 and 6 are based on simulated fluid flow through a complex 3D pore geometry. The simulation method is "Smoothed Particle Hydrodynamics" (SPH) as described in Tartakovsky et al. (2007a; 2007b). Visualizations were created by Chad Jones and Kwan-Lui Ma of the SciDAC Institute for Ultrascale Visualization at UC Davis.

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

Tartakovsky, A. M., P. Meakin, T. Scheibe, and B. D. Wood, 2007b. "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.

Figure 6



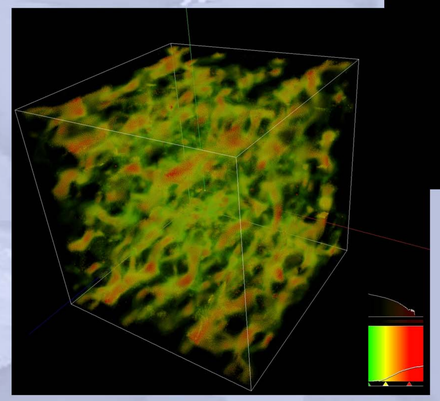


Figure 5

Figure 7

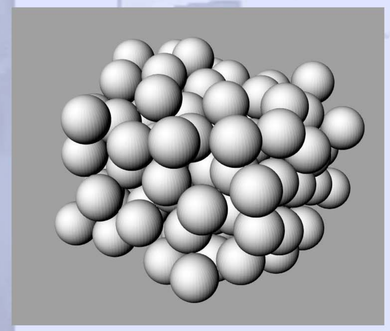
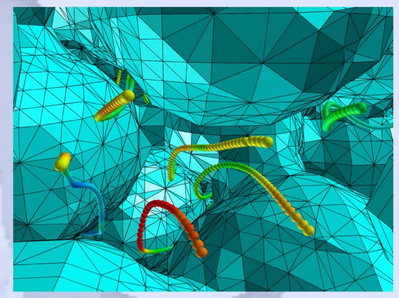
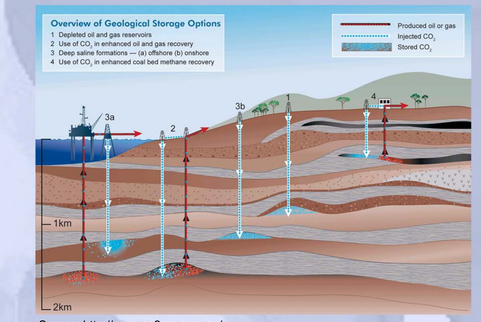


Figure 8



Pore-scale models are also being developed using grid-based methods implemented in computational fluid dynamics (CFD) codes. ***Figure 7*** shows a representation of 100 monodisperse spheres created by a synthetic sphere packing model. ***Figure 8*** shows a three-dimensional rendering of porous media grains (blue mesh planes) with colored particles indicating 3D pathlines in the computed flow field (visualization created by John Serkowski, PNNL).

Relevance to Geological Carbon Sequestration



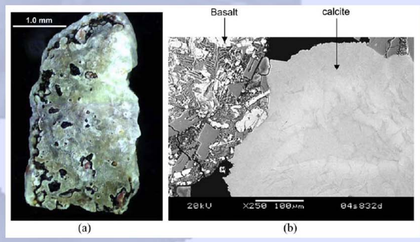
Source: http://www.co2crc.com.au/

Figure 9

Hybrid multiscale simulation methods are most needed for problems in which there exist strongly localized processes that are not well represented by average or bulk (upscaled) models. Some situations relevant to geological carbon dioxide sequestration (***Figure 9***) include:

- Gas or fluid flow through preferential pathways (e.g., fractures in low-permeability cap layers)
- Unstable fingering of dense fluids in CO2-rich brines
- Dissolution of carbonate rocks by low-pH fluids at a mixing interface
- Precipitation of calcite minerals in basalt reservoirs (***Figure 10***) including coupled effects on flow, transport, and release of Ca and other reactive ions from basalt grains.

Figure 10



(a) Optical photo of grain of Rocky Coulee basalt flow top after 32 weeks of exposure to deionized water and CO2 at 10.3 MPa and 90?C. Nearly the entire grain surface is coated with calcite. (b) SEM micrograph of basalt grains removed from the same test. Light areas of the basalt grains are pyroxene and the darker regions are plagioclase feldspar and glassy mesostasis. The precipitate on the right was identified by XRD as calcite. Figure from McGrail et al., *Journal of Geophysical Research*, 111: B12201, doi:10.1029/2005JB004169, 2006

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