Hybrid Numerical Methods for Multiscale Simulations of Subsurface Biogeochemical Processes

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Abstract. Many subsurface flow and transport problems of importance today involve coupled non-linear flow, transport, and reaction in media exhibiting complex heterogeneity. In particular, problems involving biological mediation of reactions fall into this class of problems. Recent experimental research has revealed important details about the physical, chemical, and biological mechanisms involved in these processes at a variety of scales ranging from molecular to laboratory scales. However, it has not been practical or possible to translate detailed knowledge at small scales into reliable predictions of field-scale phenomena important for environmental management applications. A large assortment of numerical simulation tools have been developed, each with its own characteristic scale. Important examples include 1. molecular simulations (e.g., molecular dynamics); 2. simulation of microbial processes at the cell level (e.g., cellular automata or particle individual-based models); 3. pore-scale simulations (e.g., lattice-Boltzmann, pore network models, and discrete particle methods such as smoothed particle hydrodynamics); and 4. macroscopic continuum-scale simulations (e.g., traditional partial differential equations solved by finite difference or finite element methods). While many problems can be effectively addressed by one of these models at a single scale, some problems may require explicit integration of models across multiple scales. We are developing a hybrid multi-scale subsurface reactive transport modeling framework that integrates models with diverse representations of physics, chemistry and biology at different scales (sub-pore, pore and continuum). The modeling framework is being designed to take advantage of advanced computational technologies including parallel code components using the Common Component Architecture, parallel solvers, gridding, data and workflow management, and visualization. This paper describes the specific methods/codes being used at each scale, techniques used to directly and adaptively couple across model scales, and preliminary results of application to a multi-scale model of mineral precipitation at a solute mixing interface.

1. Introduction

Hybrid multiscale numerical modeling methods are those that combine multiple models defined at fundamentally different length and time scales within the same overall spatial and temporal domain.

In many cases, the models also have fundamentally different ways of representing the physical, chemical and biological processes. For example, several models in the materials science literature couple molecular dynamics (MD) simulations at the molecular scale to continuum mechanics (typically finite element) simulations at larger scales.

Such simulations are motivated by classes of problems in which large-scale phenomena of interest (e.g., overall material strength) are strongly influenced by processes occurring at much smaller scales (e.g., microfracture propagation) that are not well represented by effective or averaged processes or properties. Executing an exhaustive simulation of processes at the smallest scales for a domain of engineering significance is currently impractical, and likely to remain so for a very long time. However, the hybrid multiscale approach, in which a small-scale model with high resolution is utilized in a fraction of the overall domain and is linked to a large-scale model with coarse resolution over the remainder of the overall domain, can provide necessary efficiency of characterization and computation that will render solution of these problems practical. Here we use the term "hybrid multiscale modeling" as that seems to us to be the clearest descriptor of this concept. However, the terms "adaptive algorithms" (the use of different model algorithms at different scales in a manner analogous to adaptive mesh refinement, e.g., [1]) and "multi-physics modeling" (the simultaneous use of multiple fundamentally-different process representations in a single model, e.g. [10]) have also been used to describe the same concept.

Although hybrid multiscale techniques have been developed and applied in a number of other science and engineering disciplines, they have only been previously applied to subsurface water flow and reactive transport to a very limited extent. Balhoff *et al.* [2] describe a hybrid model that utilizes a network model to simulate pore-scale water flow in a sand-filled fracture linked with a continuum-scale finite element model of flow in a porous rock matrix. To our knowledge, this is the only published example of a hybrid multiscale model applied to subsurface flow. A new SciDAC Science Application with the same title as this paper was initiated this year to develop and apply hybrid numerical techniques to simulate complex subsurface flow and biogeochemical reactions of relevance to subsurface contaminants at Department of Energy sites. This paper provides a brief introduction to the problems of interest, gives an overview of hybrid multiscale modeling techniques as applied in other disciplines, and provides results from our first hybrid multiscale simulation.

Important subsurface biogeochemical processes (e.g., microbial respiration or complexation of solutes with mineral surfaces) are currently best understood and defined at very small scales, typically ranging from molecular to cellular to small batch and column experimental scales (with time scales of minutes to days). However, the scales at which we are interested in predicting phenomena for engineering applications (e.g., fate and transport of contaminants in aquifers) are very large, typically ranging from meters to kilometers (with time scales of months to years or even centuries). A large degree of variability of natural subsurface properties exists across this broad spectrum of spatial and temporal scales. From a computational standpoint, this problem is manifested in the fact that numerical grids cannot simultaneously cover large (e.g., field-scale) domains and achieve extremely high (e.g., pore-scale) resolution. In simple terms, we cannot computationally solve problems at the scale of tens of meters (let alone kilometers) while explicitly resolving pore and grain structures, even if we had characterization data to populate such a model. Accordingly, application of multicomponent, multi-phase, multi-porosity, multi-dimensional continuum reactive transport codes at relatively high spatial resolution (e.g., grids with dimensions on the order of meters, with adaptive grids or multi-continua approaches sometimes achieving even higher resolution) represents the current state-of-the-art in high performance subsurface transport modeling. For many important subsurface reactive transport problems, the current approach is completely appropriate and adequate. However, some types of problems are not amenable to this approach and motivate a hybrid modeling approach. In this paper, we focus specifically on porous media systems that exhibit strong coupling between flow, transport, and reaction processes, such as reactions involving biofilm development and/or mineral precipitation. In these systems, the biogeochemical reactions (controlled by flow and transport processes) lead to changes in pore structure, which in turn modifies local flow and transport behavior.

This coupling/feedback leads to strong non-linearity in apparent continuum-scale behavior, and this behavior is not well represented by averaged properties and state variables.

The experiment shown in Figure 1 provides a relevant example of such a system. In this experiment, two solutes mix and react to precipitate calcium carbonate minerals (e.g., calcite) within a very narrow zone in the center of the experimental cell. We have performed pore-scale simulations of the mixing and reaction processes in this type of system [8] as shown in Figure 2. The simulation results indicate that 1) strong mixing of the two solutes is limited to a very local region (only a few grains wide), and 2) the mixing is inhibited by mineral precipitation leading to a strong negative feedback or coupling between the reaction and transport across the narrow mixing zone in which precipitation occurs. In this case, the precipitation/dissolution reaction described in detail by the pore scale model is not easily represented at the continuum scale, but it could be efficiently modeled by simulating the narrow mixing zone with the SPH model at the pore scale and simulating the remainder of the model domain with a computationally efficient continuum-scale model.

Figure 1. Mesoscale experimental flow cell (60 cm by 60 cm). The flow cell is filled with 0.5 mm quartz sand and is relatively thin in the third dimension. Two solutes are injected along two halves of the lower boundary as indicated by the red and blue arrows. The reaction causes precipitation of calcium carbonate minerals (the white zone approximately 0.5 cm wide in the center of the flow cell).

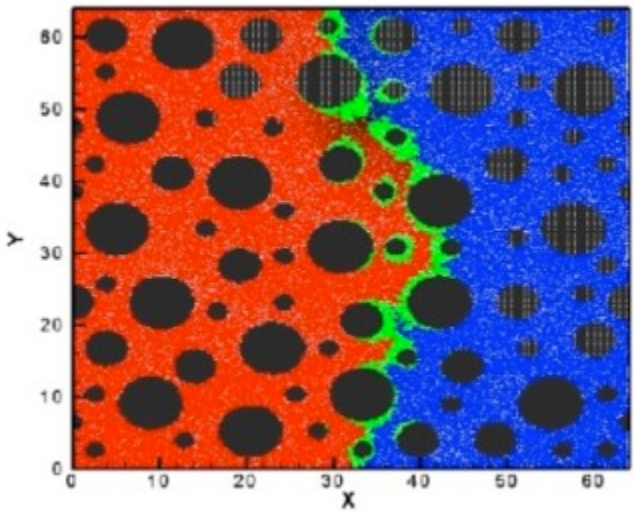

Figure 2. Pore-scale simulation of mixing of two solutes (blue and red) and reaction to form precipitated solid mineral (green). Details of the simulation method are provided in [8].

2. Hybrid Multiscale Modeling Methods

Published reviews of hybrid multiscale modeling concepts are provided by [5, 7]. Hybrid multiscale modeling methods have been most widely applied in the fields of materials science and chemical engineering, in which atomic-scale models of molecular dynamics (MD) have been linked to continuum-scale models of material deposition, strength, deformation, and failure. A recent review of

multiscale methods applied to materials science is given by [3]. Hybrid multiscale methods have also been applied in chemical engineering, catalysis and reactor processes (e.g., [12]), life sciences (e.g., [11]), and fluid mechanics (e.g., [4]).

Although terminology varies by discipline, two general approaches have been developed for integrating different models at disparate spatial and temporal scales. The first, hierarchical modeling, uses fine-scale models to inform and update coarse-scale models in overlapping domains. In other words, the coarse-scale (e.g., continuum) model is used over the entire computational domain but a higher-resolution (e.g., discrete particle pore-scale) model is applied on selected subdomains and used to estimate and update parameters within corresponding grids of the coarse model. In essence, the finer-scale models are used to train or inform the coarser scales, and the overall computation is done on the coarsest grid. An alternative to the hierarchical approach, often called concurrent modeling, uses different models simultaneously over different sub-domains. The various models run simultaneously and perform a "handshake" at boundaries between the model subdomains to define boundary fluxes for each model scale. Obviously a critical issue is when and where to apply more detailed models in a simulation domain in time and space. Again, two general approaches have been widely applied. The first involves estimation of the spatial distribution of model errors across the overall model domain, and application of detailed models only where the error in the coarse model is unacceptable, e.g., [6]. The second approach involves application of heuristic rules to adaptively select and modify regions for model refinement. For example, regions where the rate of porosity change is high or where a high degree of chemical disequilibrium exists might be selected for refinement.

3. A Hybrid Multiscale Model of Diffusion and Reaction in Porous Media

In this section we present results from our first multiscale hybrid model application. The model is based loosely on the system shown in Figures 1 and 2, except that the vertical flow in the system is turned off. Therefore, transport of the two solutes (and resulting mixing and reaction) is by diffusion only. We simulate mixing and precipitation in a thin strip of porous medium as shown in Figure 3. Initially, the concentration of the two solutes ("A" and "B") is set to unity in each half of the simulation domain (with no mixing); the boundaries at each end of the system are subject to constant concentration conditions ($C_A = C_B = 1.0$). The multiresolution hybrid model is constructed using the mesh-free Smoothed Particle Hydrodynamics (SPH) method [8] at two distinct scales. In the middle portion of the domain where mixing and precipitation is active, pores and grains are explicitly represented using high numerical resolution. In the outer portions of the domain, where little mixing or precipitation occurs, the system is treated as a continuous porous medium with coarse numerical resolution. Figure 3 shows a snapshot of the system state at a selected time. Favorable comparisons were drawn with analytical solutions and with a single-resolution model using high resolution throughout the model domain. Details of the methods and additional results are presented in [9].

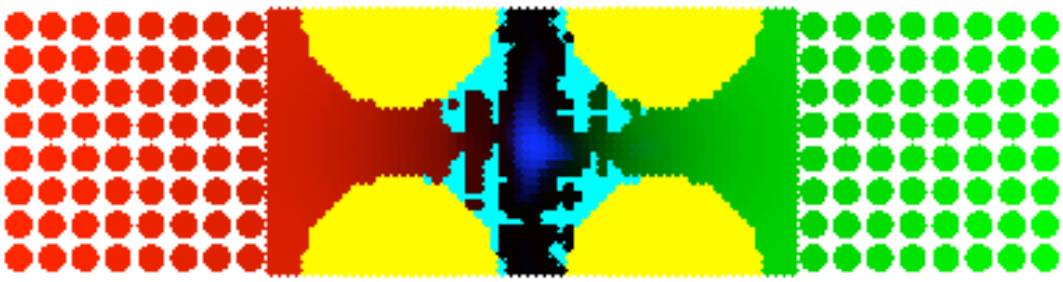

Figure 3. Visualization of hybrid simulation results at a single snapshot in time. The two diffusing and mixing solutes are represented by red and green (mixing into dark blues). Yellow indicates solid grains. Light blue represents precipitated mineral phases. The central portion is directly simulated at the pore scale whereas the outer zones are simulated using a continuum porous media approximation.

4. Concluding Remarks

Our research addresses the development of multiscale hybrid numerical methods for simulation of subsurface flow and biogeochemical reactions. We have developed and presented here an initial hybrid two-scale model of diffusion and reaction in a model porous medium. Current efforts are aimed at 1) developing and testing a similar two-scale system that combines SPH at the pore scale with grid-based (finite volume) methods at the continuum scale, and 2) extending the hybrid model system to include advective fluid flow to better simulate the system shown in Figure 1.

The hybrid models being developed will be implemented using Common Component Architecture (CCA) technologies and integrated into a general data management and visualization workflow framework. Further information on the CCA and workflow/data management efforts supporting this science application are provided by Palmer et al. (this issue) and Schuchardt et al. (this issue).

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