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An Analysis Platform for Multiscale Hydrogeologic Modeling with Emphasis on Hybrid Multiscale Methods

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Abstract

One of the most significant challenges faced by hydrogeologic modelers is the disparity between the spatial and temporal scales at which fundamental flow, transport, and reaction processes can best be understood and quantified (e.g., microscopic to pore scales and seconds to days) and at which practical model predictions are needed (e.g., plume to aquifer scales and years to centuries). While the multiscale nature of hydrogeologic problems is widely recognized, technological limitations in computation and characterization restrict most practical modeling efforts to fairly coarse representations of heterogeneous properties and processes. For some modern problems, the necessary level of simplification is such that model parameters may lose physical meaning and model predictive ability is questionable for any conditions other than those to which the model was calibrated. Recently, there has been broad interest across a wide range of scientific and engineering disciplines in simulation approaches that more rigorously account for the multiscale nature of systems of interest. In this article, we review a number of such approaches and propose a classification scheme for defining different types of multiscale simulation methods and those classes of problems to which they are most applicable. Our classification scheme is presented in terms of a flowchart (Multiscale Analysis Platform), and defines several different motifs of multiscale simulation. Within each motif, the member methods are reviewed and example applications are discussed. We focus attention on hybrid multiscale methods, in which two or more models with different physics described at fundamentally different scales are directly coupled within a single simulation. Very recently these methods have begun to be applied to groundwater flow and transport simulations, and we discuss these applications in the context of our classification scheme. As computational and characterization capabilities continue to improve, we envision that hybrid multiscale modeling will become more common and also a viable alternative to conventional single-scale models in the near future.

Introduction

It is not an exaggeration to say that almost all problems have multiple scales. (E et al. 2003)

One of the most significant challenges faced by hydrogeologic modelers is the disparity between the spatial and temporal scales at which fundamental flow, transport, and reaction processes can best be understood and quantified (e.g., microscopic to pore scales and seconds to days) and at which practical model predictions are needed (e.g., plume to aquifer scales and years to centuries). While the multiscale nature of hydrogeologic problems is widely recognized, even the most sophisticated field-scale simulators utilize upscaled model representations of fundamental processes that invoke

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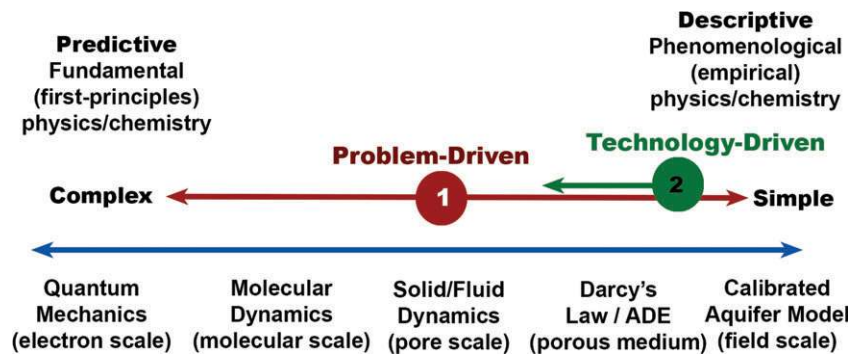


Figure 1. Complexity vs. simplicity in hydrogeologic modeling, represented in terms of physical length scales. The needed level of complexity, denoted by (1), depends on the problem to be answered by a modeling effort, whereas our ability to achieve a given level of complexity, denoted by (2), depends on technological advances (scientific understanding, system characterization, and computation).

potentially restrictive assumptions and approximations, often without a clear understanding of their implications. As subsurface problems of practical concern have become increasingly more complex, the shortcomings of conventional model formulations have been brought to light. For example, the fundamental processes of molecular diffusion, solute spreading due to pore-scale velocity fluctuations (microdispersion), and solute spreading due to larger-scale velocity variations associated with geologic heterogeneity (macrodispersion) are all typically lumped into a single apparent dispersion process and tensorial parameter in advection-dispersion equations (ADEs) describing solute transport. When used for simulating chemical reactions on a coarse grid, such models commonly give rise to artificially large degrees of mixing and accordingly overestimate the rate of reaction (e.g., Cirpka et al. 1999; Rajee and Kapoor 2000; Knutson et al. 2007; Tartakovsky et al. 2008a). As a result, laboratory-scale measurements of reaction rates in fully-mixed reactors cannot be directly used for field-scale predictions; instead, field-scale model parameters must be calibrated which raises questions about their applicability for prediction under conditions other than those for which the calibration was performed.

A 2006 National Science Foundation report on simulation-based engineering science (NSF 2006) refers to this problem as “the tyranny of scales”:

The tyranny of scales dominates simulation efforts not just at the atomistic or molecular levels, but wherever large disparities in spatial and temporal scales are encountered. Such disparities appear in virtually all areas of modern science and engineering.

This disparity in scales is in part responsible for the tension that exists between the need to develop parsimonious models that can be used for practical applications and the need for such models to be soundly based in first principles. The appropriate level of hydrogeologic model complexity has been actively debated in the recent literature (Gomez-Hernandez 2006; Hill 2006). As indicated in Figure 1, the degree of complexity needed depends on the nature of the problem to be solved, whereas

our ability to meet that need depends on technological advances.

In recent years, there have been significant efforts in a number of disciplines to address the tyranny of scales through the development of multiscale modeling approaches. A rapidly growing body of literature in material sciences, life sciences, chemistry, and other fields is focused on means of combining simulation models at multiple scales, allowing for the direct accounting of both small-scale process effects on larger-scale phenomena, and of large-scale forcings on small-scale processes. In hydrogeology, attempts to address multiscale problems have mostly taken the form of upscaling, in which a particular model representation of small-scale (microscopic) processes is used as the basis for deriving a larger-scale (macroscopic) process description that depends only on macroscopic variables. However, upscaling is only one of several multiscale simulation approaches and is not appropriate for all hydrogeologic problems. There is a need for a broader understanding of multiscale modeling issues and methodologies within the hydrogeologic modeling community, and for the development of a new set of multiscale simulation tools that can be brought to bear on today’s challenging problems.

In light of these issues, the objectives of this article are to (1) present a general multiscale simulation classification framework (our Multiscale Analysis Platform or MAP) within which the nature and applicability of various multiscale simulation approaches can be more clearly understood, and to (2) introduce the hydrogeologic community to recent advances in hybrid multiscale modeling methods and tools that may be brought to bear on hydrogeologic problems (with some example applications).

Length and Time Scales in Multiscale Systems

The structure of multiscale hierarchical systems has been discussed in some detail in the works of Baveye and Sposito (1984) and Cushman (1984, 1986). An understanding of such systems is essential for understanding hybrid models; so we briefly review some basic information regarding multiscale systems in this section. Although systems can be hierarchical in both

space and time, it is generally more intuitive to think about the spatial organization rather than the temporal one. In the discussion below, we will offer examples that are primarily spatial; however, the reader should keep in mind that the same kinds of arguments can be made for the temporal evolution of systems.

In the simplest, and classical (cf. Bear 1972), multiscale system we can think of two discrete scales (i.e., subpore and Darcy scales in Figure 2). We consider fixing a point within the fluid phase, and then measuring some medium property, γ , with a small volume. The quantity γ can be considered to be any statistical field quantity of interest; for example, γ could represent the average amount of pore space in the volume, in which case it would represent the macroscopic parameter porosity. Initially, the volume will sample only the fluid phase, and the measurement of γ will be constant (subpore scale). As we increase the size of the volume beyond the characteristic length of the microscale (l , typically the scale of a single pore), variations in the measurements of γ will be observed. Under suitable conditions, these variations will diminish as r increases, and the measurement of γ will again reach a constant value (Darcy scale). The smallest averaging volume where γ is essentially a constant (characteristic size r_0) is called a representative elementary volume (REV; Bear 1972). The second fundamental scale of interest for this system is that at which our assumptions about the constant value of the measurement of γ begin to fail. This length often represents the scale at which geologic heterogeneities become measured by our averaging volume so that fluctuations in γ are once again noted, defined by characteristic length L . Any volumes with characteristic size between r_0 and L are referred to as representative volume elements (RVE; Hashin 1983). Because the smallest representative volume rarely has any special role in upscaling, we will refer to any such volumes where the measurement of γ yields a constant value as an REV. Materials that are considered to be statistically homogenous only over bounded intervals of averaging volumes are referred to as quasi-stationary (Christakos 1992).

The existence of such a hierarchy of scales requires that (1) the underlying distribution functions for the structures of interest have finite means and variances and (2) there exists separation between the scales identified above such that $l \ll r_0 \ll L$. As pointed out by Wood and Valdes-Parada (2013), under these circumstances the quantities l and L can be given explicit interpretation in terms of the integral scales associated with the underlying fields of interest. Note, that although it is common to think about l and L as being related to the structure of the porous medium itself, these length scales actually represent features of the microscale and macroscale fields of interest. For example, in the case of solute transport, these length scales are generally related to the concentration field. However, in many cases, the characteristic lengths of the medium and the concentration fields are related, so that it may be useful

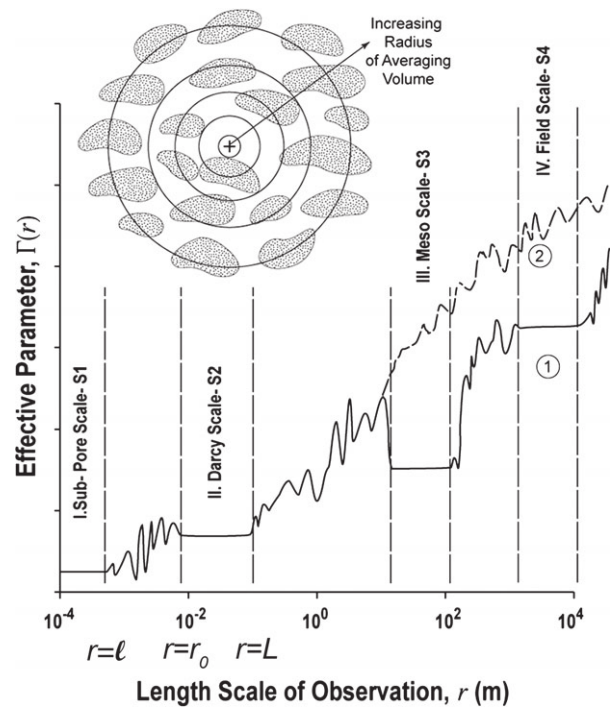


Figure 2. Two examples of how an effective parameter, g , might change with increase in observation scale. The curve indicated by (1) is a classical, discretely hierarchical system. The curve indicated by (2) indicates a system that shows mixed modes of behavior. At small enough length scales, it is discretely hierarchical; at larger length scales of observation, it becomes continuously evolving.

to approximate the characteristic lengths as being medium properties.

More generally, a system may have an evolving sequence of characteristic length scales, as illustrated in Figure 2. Such systems (with more than two characteristic scales) are conventionally thought of as *multiscale*. In Figure 2, two distinctly different kinds of hierarchical behavior are indicated. On the curve indicated by the numeral 1, the effective parameter γ behaves as a classical discretely hierarchical quantity. In other words, as the observation window increases in size, there is a sequence of scales at which the parameter γ can be considered to be quasi-stationary in space. In other words, we can explicitly identify a sequence of discrete scales S_1, S_2, S_3, \dots . Such systems have been studied in the context of averaging theory for some time, (e.g., Baveye and Sposito 1984; Cushman 1984; Whitaker 1999). The second curve, indicated by the numeral 2, represents a system that exhibits both discretely hierarchical stages (at sufficiently small scales of resolution), and continuously evolving scales. This kind of system has been recognized comparatively more recently, corresponding roughly with the discovery of fractal or power law structures in nature ushered by Mandelbrot (1967, 1977, 1982) and others. For multiscale discretely hierarchical systems, the terms microscale and macroscale are often used relatively rather than in an absolute sense. Thus, in Figure 2, if one were upscaling from S_1 to S_2 , then S_1 would represent

the microscale and S_2 would represent the macroscale; similarly, if upscaling from S_2 to S_3 , then S_2 would act as the microscale.

In such systems, there may be structures that prevent the system from exhibiting spatial (or temporal) quasi-stationary behavior. The practical effect of this kind of structure is that conventional upscaling (requiring that the sequence of scales be hierarchical and exhibit clear separation between the characteristic length scales) is no longer possible. For such systems there may be arbitrarily-long space and time correlation structures in the subsurface materials; thus, the behavior at any point in the system may, in principle, be a function of the time-space behavior at all other points in the domain. Because of this complex structure, fundamentally new approaches are required to handle such systems.

Under certain conditions, *nonlocal* models can be developed to represent the macroscale. A summary of the history of nonlocal models is well beyond the scope of this work, but nonlocal models have been reviewed by Edelen (1976) and Eringen (2002). For applications to porous media, there have been any number of nonlocal theories proposed, with the primary differences being the representation of the nonlocal behavior as (1) explicitly as a convolution integral or (2) through the use of fractional derivatives. Although the literature in this area is enormous, the applications to porous media are well represented by a number of excellent examples in the literature from both perspectives (Beran 1968; Koch and Brady 1987; Cushman and Ginn 1993a, 1993b; Neuman 1993; Benson et al. 2000; Neuman and Di Federico 2003; Berkowitz et al. 2006; Zhang et al. 2007; Neuman and Tartakovsky 2009). Nonlocal models are capable of predicting the behavior of systems that are not necessarily discretely hierarchical, such as the systems indicated in Figure 2, curve 2. Nonlocal models represent the increase in complexity of the system through space-time convolutions of the dependent variables. In essence, one can think of nonlocal models as arising from the fundamental integral solutions to the microscale equations which, for linear systems, are always expressible as convolutions over kernel functions (often simply referred to as Green's functions). Nonlocal models have more capacity to represent complex system behavior, and thus they require more information than do local ones. In principle, nonlocal models can be developed for essentially any kind of structure, regardless of the presence of statistical regularity. However, such nonlocal models would contain unique kernel functions at each point. In essence, this indicates that, without some kind of simplification, nonlocal models require the same amount of information as would the microscale model (Wood 2009; Wood and Valdes-Parada 2013).

With this in mind, then, under some conditions where the length (and time) scale constraints are not met, it may be as efficient and effective to simply solve the microscale problem directly. Of course, solution of a microscale problem over the full spatial and temporal extent of a practical problem is nearly always

computationally prohibitive. This situation motivates the concept of multiscale hybrid models, which seeks to combine microscale and macroscale simulations in such a way as to reduce the amount of microscale computation necessary, either by restricting the spatial domain over which microscale simulation is performed and coupling with a macroscale model in other portions of the domain (concurrent methods) or by restricting the period of time over which microscale simulation is performed and extrapolating on time with a macroscale model (hierarchical methods). The intent of the MAP described in the remainder of this article is to present a variety of multiscale hybrid modeling approaches in the context of more traditional multiscale modeling methods, and structured in terms of the characteristics of problems to which they are well-suited.

Multiscale Analysis Platform

Leading experts in the field of multiscale mathematics and simulation have recently pointed out the need for a unified framework for multiscale simulation that can provide guidelines regarding how to utilize various multiscale simulation approaches and develop and apply new methods (e.g., E et al. 2003). Hydrogeologists might reasonably ask questions such as “What are the differences between various multiscale simulation methods?”, “Which method is best suited to my problem?”, and “What tools are available to help me apply this approach?” Over the past several years we have devoted significant effort to development and application of hybrid multiscale models of reactive transport phenomena (Tartakovsky et al. 2008a, 2008b; Battiato et al. 2009, 2011; Battiato and Tartakovsky 2011; Boso and Battiato 2013), and have extensively wrestled with these questions. Over the course of that process, and with the input of multiscale researchers in other disciplines, we have developed a framework for analysis of multiscale problems that we call the “multiscale analysis platform” or MAP. The MAP is based on the concept that various multiscale simulation methods that can be classified into a set of motifs, each of which is applicable to problems with specific characteristics. The MAP consists of a series of questions that, when answered with a specific application in mind, will lead a modeler to a particular multiscale motif and the associated methodologies and tools. Generally speaking, these questions address the central issues of spatial and temporal scale separation and the degree of coupling between microscale and macroscale processes. Figure 3 shows the MAP in flowchart format. In the remainder of this section we discuss the questions that drive one to a particular motif (green circles in Figure 3) and provide a brief description of each motif (blue rectangles in Figure 3) with references to available methods, literature, and tools.

The starting point for the MAP is denoted as Question 0 (Q0), which prompts us to define our “best” (most fundamentally sound) model of the problem under consideration. This model is considered to be

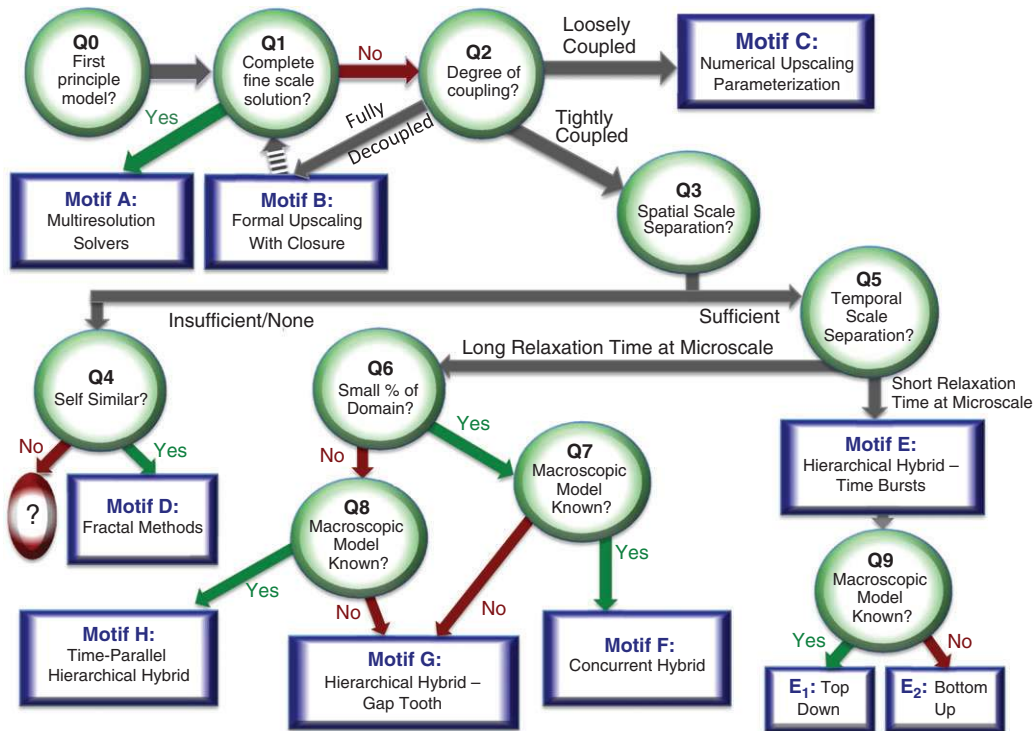


Figure 3. Multiscale analysis platform (MAP) flowchart.

the most complex and most highly resolved in space and time, and in the terms of multiscale simulation serves as our “microscale” model. As an example, in subsurface transport modeling we might propose as our microscale model a pore-scale simulation based on three-dimensional pore geometry measured with X-ray microtomography, with flow represented by the Navier-Stokes equations, transport mechanisms consisting only of pore-scale advection and molecular diffusion, and reactions defined by fundamental reaction rate models based on fully-mixed batch reactor studies.

Motif A: Multiresolution Methods

Given a particular microscale model, we move to the first question (Q1), which asks whether we are able to solve our microscale model directly over the spatial and temporal domain of interest. In our example, it is clearly not currently feasible to either measure pore geometry or computationally solve the Navier-Stokes equations at the pore scale over any practical field-scale domain. However, depending on what we are willing to accept as our microscale model, there may be situations where we can affirmatively answer this question. For example, many simulations assume validity of the ADE if geological heterogeneity can be resolved at a fine scale. As an example, Ramanathan et al. (2010) and Guin et al. (2010) describe a stochastic model of braided gravelly aquifer stratigraphy with resolution as fine as centimeters over a domain of kilometer extent. In such a case, containing trillions of grid cells, we may consider this model to capture most important heterogeneous features. However, we would currently be computationally forced to average

or upscale the local permeability values onto a coarser grid in order to obtain an approximate solution. Methods in Motif A are intended to avoid such approximations by providing computationally efficient ways of obtaining a complete solution on the fine grid. These methods are multiscale in the sense that they use approximate upscaled (coarse) grids in intermediate steps to facilitate efficient computation of the microscale solution, and are referred to by E et al. (2003) as “traditional” multiscale methods. Specific examples of multiresolution methods include multigrid solvers and preconditioners (e.g., Wesseling 1992; Trottenberg et al. 2001), multiscale finite element (FE) methods (e.g. Hou and Wu 1997; Jenny et al. 2003; Aarnes et al. 2005), and multiscale mimetic methods (e.g., Lipnikov et al. 2008). We consider further the example of Aarnes et al. (2005), who combined a coarse solution for pressure and velocity with a streamline method to simulate two-phase fluid transport on a fine-scale subgrid, using a mixed multiscale finite-element method. They demonstrated the method using a three-dimensional benchmark model containing over 1 million grid cells (Christie and Blunt 2001), and showed that their method allowed direct solution of this high-resolution problem as a robust alternative to conventional upscaling-based simulation methods.

Motif B: Formal Upscaling with Closure

In most cases we are not able (or not willing even if we are able) to solve our system with complete microscale resolution, and the answer to Q1 is “No.” The situation in which we consider a pore-scale simulation to be our microscale model, is clearly such a case. Q2 then asks,

“What is the degree of coupling between microscale and macroscale models?” Here we refer to coupling in the sense of the degree to which macroscale phenomena depend explicitly on microscale processes (as opposed to algorithmic coupling of two simulation codes, which is addressed in specific hybrid multiscale methodologies).

Although upscaling involves some formal averaging procedure to link the scales of interest, the actual reduction in degrees of freedom occurs through the conceptual or mathematical assumptions or approximations (scaling laws) that are inherent. Wood (2009) states that upscaling inherently involves imposition of one or more “scaling laws” (closure approximations) that allow one to represent microscale details in terms of some representative macroscale equations and parameterizations. Solving the system requires a constitutive equation for each of the constitutive independent variables to close the system (i.e., the need to have the same number of equations as unknowns). Typically, one variable is not included in the system, and herein lies the closure requirement (Boure 1987). This arises from the homogenization of the microscopic geometry, and generally is present in all upscaling techniques. A scaling law is an axiomatic statement about the essential character of the microscale system (Wood 2009) that allows reduction of the number of degrees of freedom and closure of the macroscopic equations. Typical scaling laws include assumptions about the statistical structure of microscale variables (e.g., statistical homogeneity, stationarity, and ergodicity), separation of scales, the magnitude of local fluctuations, and the nature of boundary conditions (e.g., infinite or periodic). Wood (2009) and Wood and Valdes-Parada (2013) point out that the actual methodology used for upscaling (e.g., volume averaging, homogenization, and mixture methods) is perhaps of less importance than the scaling laws that are imposed in any methodology. Beven (2006) offers the opinion that the search for appropriate closure approximations (i.e., scaling laws) is “A Holy Grail” of hydrology, a grand challenge critical to practical application of hydrologic models and worthy of significant effort even if it proves an impossible quest. When necessary closure approximations are valid, the microscale and macroscale models can be completely decoupled, and valid macroscale models and parameters can be defined which eliminate the need for any explicit microscale knowledge. Methods in Motif B address this situation and provide formal tools for developing macroscale models and parameters. Assuming that microscale and macroscale systems can be effectively decoupled, upscaling involves transforming equations and parameters from the microscale to the macroscale for use in macroscale simulation, without the need for further explicit consideration of microscale processes.

While there does not exist yet a rigorous and general means of quantifying the degree of coupling between microscopic and macroscopic models, we can provide an example in which a rigorous answer has been developed. Battiato and Tartakovsky (2011) and Boso and Battiato (2013) analyzed a mixing-controlled precipitation reaction problem and determined combinations of dimensionless

numbers (Peclet and Damkohler numbers, Pe and Da) under which the assumptions necessary to obtain a closure to upscale pore-scale processes to the Darcy scale were met (and conversely those combinations under which their assumptions were not met). Figure 4, reproduced from Battiato and Tartakovsky (2011), graphically denotes the domains in which closure approximations are valid and invalid. In the gray region, a macroscale model written in terms only of macroscopic variables is well defined (macroscale and microscale models can be fully decoupled). Outside the gray region, microscale (pore-scale) information must be explicitly considered (macroscale and microscale models are tightly coupled). The analysis of Battiato and Tartakovsky (2011) effectively defines conditions under which the scaling laws used to derive macroscale (upscaled) equations for their problem are valid or invalid.

A number of excellent reviews of upscaling techniques with a focus on solute transport through porous media have been published recently (Cushman et al. 2002; Gray and Miller 2005; Fripiat and Holeyman 2008; Wood 2009; Dentz et al. 2011). Cushman et al. (2002) discuss several different categories of upscaling techniques that have emerged in the literature. Since these reviews are already available, we will not further discuss specific upscaling methods here. We note that in situations where Motif B applies, the macroscale model that results from the upscaling analysis effectively becomes our new microscale model; that is, we accept it as being a fundamental description of system behavior. An example is the use of Navier-Stokes equations to perform direct numerical simulation of pore-scale flow. Although Navier-Stokes is itself an upscaled representation of molecular-scale interactions, with effective parameters such as viscosity and density, it has proven to be robust under most conditions of practical interest and therefore can usually be assumed to be valid as a microscale model. In such a case, one might then return back to Motif A to seek computational methods for solving the upscaled model with high resolution (as indicated by the dashed arrow from Motif B to Q1 in the MAP).

Motif C: Numerical Upscaling/Parameterization

In some cases there exists a loose coupling between microscale and macroscale models. For fully decoupled systems the effective parameters at the macroscale, derived from microscale properties using upscaling methods, are assumed to be independent of the local boundary conditions or history. For example, in porous media flow, saturated hydraulic conductivity is usually assumed to be an intrinsic property of the medium and the fluid, and not dependent on specific boundary configurations or history. However, the nonlocal nature of the flow and transport in strongly heterogeneous porous media leads to violation of this assumption and introduces a loose form of coupling. Numerical upscaling methods for highly resolved heterogeneous hydraulic conductivities to compute effective hydraulic conductivities for coarser blocks must often account for the effects of local boundary conditions on

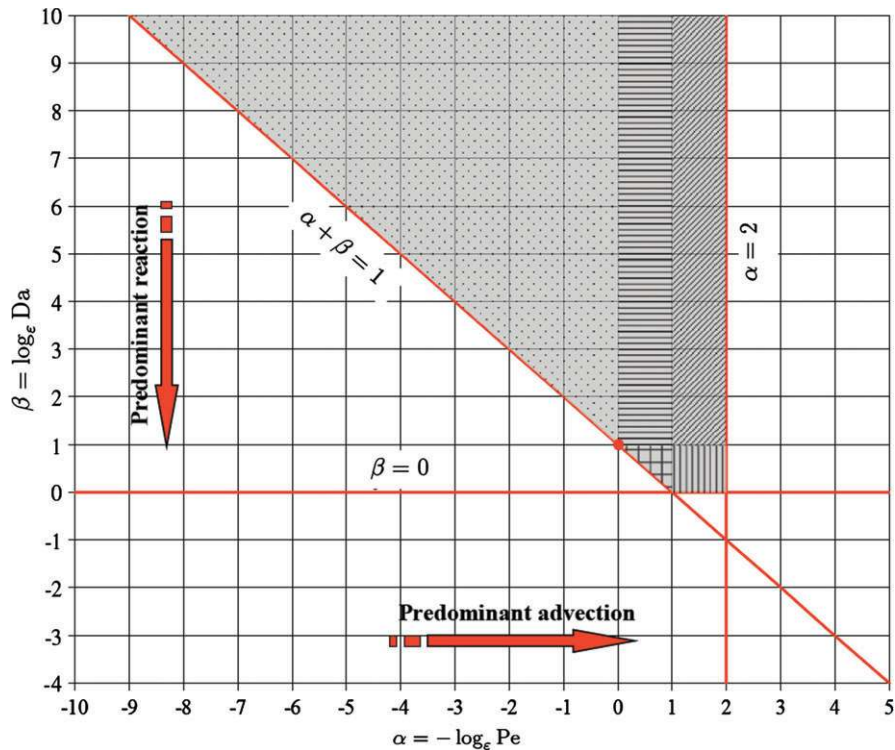


Figure 4. Graphical representation of nondimensional parameter space in which a valid Darcy-scale representation of a mixing-controlled reaction can be defined (gray regions). Outside the gray regions, pore- and Darcy-scale models cannot be fully decoupled and a general upscaled representation cannot be obtained. The location of the red dot denotes the point where advection, diffusion, and reaction time scales are of the same order of magnitude. Reproduced from Battiato and Tartakovsky (2011); see that work for specific definitions of hatched subregions within the gray region.

effective parameters (e.g., Chen and Durlofsky 2006; Wen et al. 2006; Sun et al. 2012a, 2012b). This is particularly the case when heterogeneous structures are correlated at the scale of the averaging volume; Zhang et al. (2006) showed that effective permeabilities were not dependent on boundary conditions when correlation lengths of permeability were relatively small. A form of loose coupling may also exist for multiphase flow systems, in which macroscopic parameterizations depend not only on local boundary conditions and configurations of heterogeneous media, but also on the history of wetting and drying (Miller et al. 1998). Numerical upscaling is commonly used to account for the loose coupling between macroscale and microscale models when it is not computationally feasible to directly solve the microscale model over the full domain. In the problems described by Chen and Durlofsky (2006) and Wen et al. (2006), a high-resolution model of spatial permeability variations is available (e.g., a realization from a conditional stochastic simulation method), but cannot be solved directly. The domain is broken up into several subdomains, and a fine-scale solution is obtained on each small domain (computationally feasible) using assumed boundary conditions. Effective parameters computed from the fine-scale results are then used to compute a global solution on a coarser grid, which provides updated estimates of boundary conditions for the local subdomains. This process is then iterated until a consistent solution is obtained at both scales. Note that

in this case the microscale and macroscale models are the same—continuity equations and Darcy’s law—but effective parameters of the coarse model depend on specific configurations of fine-scale permeability and the local boundary conditions. These examples use a form of the conventional numerical method of domain decomposition in which the problems on each subdomain are solved at full resolution independently but then coordinated globally by obtaining an approximate solution to a coarsened problem.

Numerical upscaling can also be used in cases where microscale and macroscale models can be fully decoupled but the formal closure problem is too complex for general solution. An example of this is the work of Rhodes et al. (2008, 2009), who propose a “pore-to-field” numerical upscaling approach for solute transport based on the continuous time random walk (CTRW) particle tracking method. They start with a pore-scale model formulated using a pore network modeling approach (Rhodes and Blunt 2006), with the network topology prescribed from X-ray microtomographic observations of pore geometry. A simulation of solute particle movement through the network provides computed statistics of particle transition times (e.g., from one pore to the next) that are needed for the macroscale representation (CTRW). While the parameters of the CTRW (state transition time distributions) would be difficult to directly derive from properties of the pore network, the numerical

upscaling approach provides a mean of computing them for a given pore network geometry. A similar approach can be used at larger scales if the spatial distribution of geological material classes with characteristic pore network topology (i.e., lithofacies) can be specified either deterministically or stochastically, with the combination of multiple CTRW models giving rise to parameters of a new CTRW model applicable at the aquifer scale.

Another example of numerical upscaling is the use of cloud-resolving models within individual elements of global circulation models (GCMs) used to predict future global climate. Traditional GCMs are computationally limited to earth-covering grids with elements that are too large to directly resolve cloud processes and features, but these processes nevertheless are known to play a significant role in global circulation processes. Therefore, many GCMs use a parameterization approach that is a form of upscaling with closure (Motif B). However, because the local processes (e.g., cloud formation) depend on larger-scale driving forces, there is a loose coupling between the scales which often invalidates the closure approximations intrinsic to the parameterizations, motivating alternative approaches. While extreme-scale computation is currently opening doors to direct resolution of some cloud features in GCMs, (e.g., Palmer et al. 2011), some effects of features that remain too small to be directly resolved (e.g., subgrid-scale features) must still be accounted for (Moeng et al. 2010). Grabowski (2001) and Randall et al. (2003) advocate the use of a “super-parameterization” approach in which a subgrid model that explicitly resolves cloud physics is embedded in each grid element of a coarse GCM (i.e., a “super-GCM”). Rather than a fixed parameterization, summary statistics are computed from the subgrid cloud physics model at each GCM time step, effectively providing a superparameterization that responds to changes in global forcings and accounts directly for subgrid-scale physics. Because the subgrid model only simulates a portion of the GCM grid space (typically with lower dimensionality, e.g., a two-dimensional cloud model within a three-dimensional GCM grid element), it represents only a statistical sample of subgrid behavior. However, this methodology provides loose coupling between models with different physics and defined on different time and spatial scales, and therefore offers a natural segue to the fully coupled (hybrid) multiscale simulation methods described in the following sections.

Introduction to Hybrid Multiscale Simulation Methods (Motifs D to G)

The case where microscale and macroscale models are tightly coupled (e.g., the white region in Figure 4) motivates hybrid multiscale methods, in which microscale and macroscale simulations are explicitly coupled together. Hybrid multiscale simulation methods as defined here are those that combine two or more models defined at fundamentally different physical length scales within the same overall model spatial and temporal domain. In most 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 FE) simulations at larger scales. Here we use the term “hybrid multiscale simulation” as that seems to us to be the clearest descriptor of this concept. However, the terms “adaptive algorithms,” that is, the use of different model algorithms at different scales in a manner analogous to adaptive mesh refinement (e.g., Garcia et al. 1999; Alexander et al. 2002, 2005), and “multiphysics modeling,” that is, the simultaneous use of multiple fundamentally different process representations in a single model (e.g., Michopoulos et al. 2005; Tartakovsky and Alexander 2005), have also been used to describe the same concept. Keyes et al. (2013) provide a thorough review and discussion of the relationship between multiscale and multiphysics models and methods for coupling. Published reviews of hybrid multiscale modeling concepts are provided by Michopoulos et al. (2005), Oden et al. (2006) and Rabczuk et al. (2006). One may consider that hybrid multiscale approaches are applicable to problems for which there exist a limited form of spatial scale separation that allows us to define distinct microscale and macroscale models but the degree of spatial scale separation is insufficient to fully decouple the microscale and macroscale system behaviors (macroscale behavior depends explicitly on microscale variables and vice versa). To begin to identify which hybrid multiscale approach is best suited to the problem at hand, we now turn to the question of temporal scale separation.

Motif D: Hierarchical Hybrid Multiscale Methods Using Short Microscale Bursts in Time

The first critical question in defining the type of hybrid multiscale method to be used asks to what degree there exists temporal scale separation (Q3). The question may also be posed as: “Do microscale conditions rapidly equilibrate to changes in macroscale conditions?” If the answer to this question is “Yes” (strong temporal scale separation exists), then we can take advantage of this feature of the problem to reduce the amount of required microscale simulation. Typically, microscale simulation is more computationally intensive than macroscale simulation (requires higher spatial and temporal resolution), so a significant reduction in the amount of microscale simulation will have a strong effect on the overall computational demands of the simulation. Methods within Motif D utilize a hierarchical approach in which the macroscale simulation domain overlies one or more microscale simulation domains, and microscale simulation is periodically performed in short bursts of time (using a small time step) to inform macroscale simulations over the full simulation time period (using a large time step), as shown schematically in Figure 5. Two submotifs are defined here, depending on whether or not formal equations are defined at the macroscale (Q4).

Methods such as the heterogeneous multiscale method (HMM; E et al. 2003, 2007), the seamless

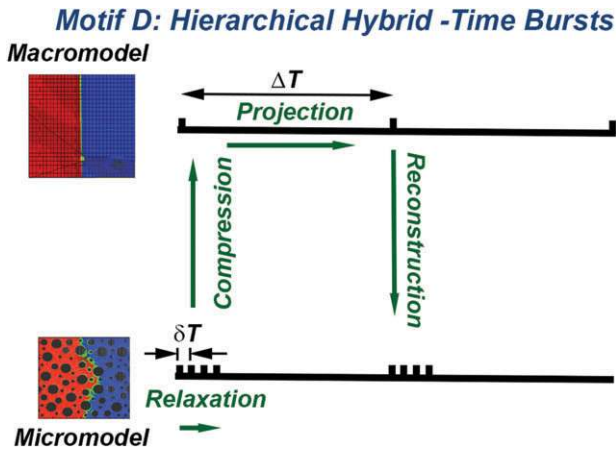


Figure 5. Schematic diagram showing the concept of the hierarchical hybrid - time bursts approach. The micromodel is solved for a short burst of micromodel time steps (relaxation), then information is appropriately averaged and passed to the macromodel (compression). The macromodel is then advanced a large time step (projection), thus bypassing many micromodel time steps. When macroscopic conditions change sufficiently, the micromodel must be re-initialized (reconstruction) and run for another short burst of time to update the macromodel parameterization. This process is repeated as many times as necessary until the end of the overall simulation period.

method (E et al. 2009), and the Dimension Reduction with Numerical Closure (DRNC) method (Tartakovsky and Scheibe 2011) address the case where formal model equations can be defined at both the macroscale and the microscale. These methods are called “Top-Down” (Motif D₂), because the macroscale system is used to drive short bursts of microscale simulation that in turn provide updated parameters for the macroscale system. The HMM is designed for scenarios where a macroscale process is of interest, but the macroscale model is not valid in all parts of the domain. However, a microscale model is applicable everywhere. The HMM works by filling in whatever macroscopic knowledge is missing via a series of brief runs of a microscopic model. The HMM comprises three parts: a macrosolver, a microsolver, and a data estimator. Data from the macro model is used to force the micro model. Using micro time steps, the micro model is evolved until relaxation (which because of time scale separation is short relative to the macroscopic time step), and then the data estimator is employed to calculate the data missing in the macro model from micro model runs. The newly informed macro model then proceeds forward one macro time step. An HMM iteration ends as the current state of the macro model is set forward one step, and new macro data is used to force the micro model. There are a large variety of applications for the HMM (Oden et al. 2006). However, to our knowledge, few studies have been published applying the HMM to subsurface hydrological problems.

The seamless method (E et al. 2009) is similar to the HMM in that a top-down approach is applied such that data needed for the macro model is derived from the

micro model. The difference between the two methods is the need for reinitialization of the micro model. For the HMM, the micro model reinitializes after every macro time step. This is not the case for the seamless method. An iteration of the seamless method begins with the current state of both the macro and micro models. The microscale simulation evolves one time step, with a step size appropriate for the micro model. The macro model also advances, with its own appropriate time step. Data are exchanged between micro and macro models at each step. Both models are set forward and the process repeats. Because data are interchanged at every step, the macro model runs more slowly (shorter time steps) than it would if not linked to the micro model, thus the seamless method is more computationally costly than HMM. However, the attraction of the seamless method is the elimination of the need for microscale model reinitialization, which can provide an overall decrease in runtimes and improved accuracy, despite the need for an increased number of time steps at the macro level. Strictly speaking, the seamless method does not fit within this motif since it performs microscale simulation over the complete time period, but is included here because it is closely related to the HMM.

A third example of a top-down multiscale approach is the DRNC method (Tartakovsky and Scheibe 2011; Tartakovsky et al. 2011), which can also be considered a variant of the HMM. This technique provides average solutions of microscale equations to approximate macroscale behavior. The idea is that macroscale equations based on direct numerical averaging of microscale states can take larger time steps with fewer variables as compared to the original microscale equations, thus providing significant computational savings. Like the HMM, the DRNC method relies on quick relaxation of the microscale model to accomplish computational closure. The DRNC method is made up of two iterated processes. The first is execution of a short burst of the microscale model and calculation of effective parameters for the macroscale model by averaging the microscale states. Tartakovsky and Scheibe (2011) provide an example of how microscale reaction rates are averaged to produce effective macroscale rates. The second is execution of the macroscale model for a period of time followed by re-initialization of the microscale model to accommodate changes in macroscale conditions. These two steps are iterated repeatedly, with bursts of microscale simulation used to update macroscale parameters on regular intervals.

The case where formal equations describing the physics and chemistry exist only at the microscale motivate the equation-free method (EFM) (Kevrekidis et al. 2003; Kevrekidis and Samaey 2009) and its variant the patch dynamics method (Hyman 2005). These methods are called “Bottom-Up” (Motif D₁), because macroscale projections in time (EFM) or time and space (Patch Dynamics) are performed based purely on microscale simulation results without reference to any closed-form macroscale equations. This is accomplished by extracting

macroscopic information from short bursts of appropriately initialized microscale simulations. EFM is built upon a coarse time-stepper, which progresses a time step of the unavailable macroscopic model in three steps: (1) lifting, which maps the coarse variable to consistent distribution of fine-scale variable and is used to create initial conditions for the microscopic simulations; (2) evolve, which uses the microscopic simulator to evolve the fine-scale variable over a short time interval; and (3) restriction, which transforms the evolved fine-scale solution to the coarse-scale solution, that is, coarse time-stepper solution. The simulation can be accelerated over large time steps through coarse projective integration, which extrapolates the time derivatives calculated from consecutive short bursts to larger time steps.

Patch dynamics (Hyman 2005) is an EFM variant that combines the coarse projective integration in time and its spatial analogy, the gap-tooth scheme (discussed further below under Motif F). It thus enables the exploration of “large space, large time” tasks through “small space, small time” (i.e., patch) simulations. The simulated patch dynamics are extrapolated in time using the coarse projective integration and interpolated in space using the gap-tooth scheme. Although an explicit closed-form coarse-scale model is not required to use EFM, more information about the nature of the coarse equation, such as the order or character (parabolic, hyperbolic) of the unavailable equation, could help to capture the coarse dynamics more accurately or help to design the lifting or restriction strategies. A strategy to obtain such information, also using only appropriately initialized simulations with the fine-scale model, is the baby-bathwater scheme (Li et al. 2003).

Motif E: Concurrent Hybrid Multiscale Methods

If the microscale simulation behavior equilibrates (relaxes) slowly relative to time scales over which macroscale conditions change, then it is not possible to restrict the time duration of microscale simulation. In this case, one might then ask whether it is possible to restrict the extent of the spatial domain that must be simulated at the microscale (Q5). If the conditions necessary for decoupling microscale and macroscale models are violated only within a small fraction of the overall simulation domain, for example, at a precipitation reaction front as in Tartakovsky et al. (2008a), then it may be computationally feasible to perform microscale simulation over the full simulation period (with small time step) but over only a small spatial domain, coupled to macroscale simulation over the remainder of the spatial domain. This situation motivates concurrent hybrid multiscale methods that perform simultaneous microscale and macroscale simulations over different spatial subdomains and link them through a “handshake” at the region boundaries or in some overlapping subregion, as shown schematically in Figure 6.

Several concurrent hybrid methods are aimed at coupling mesh-free particle methods at the microscale with mesh-based continuum macroscale models; a review

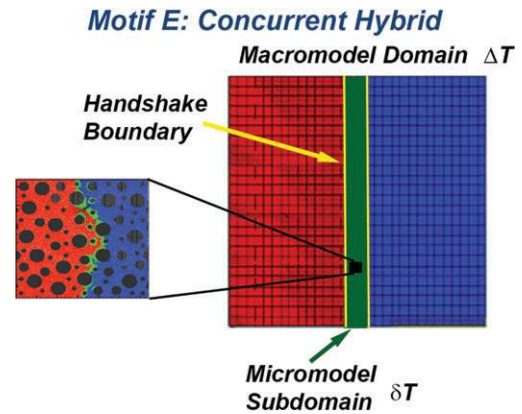


Figure 6. Schematic diagram showing the concept of the concurrent multiscale hybrid approach. The micromodel is defined only on some subset of the overall model domain, and the micromodel and macromodel are run independently on different time steps, with synchronization through the boundary condition “handshake” at selected time intervals. Here the boundary is shown as a sharp entity dividing the two model subdomains, but in many methods this is actually an overlapping region where both models are executed.

is provided by Rabczuk et al. (2006). For example, the “bridging scale method” (BSM) is a concurrent method for multiscale coupling of atomistic (MD) and continuum models, developed by Wagner and Liu (2001, 2003). Atomistic simulation tools are limited in application because of restrictions on the length or time scales that can be feasibly simulated, and by themselves they are not sufficient for several important problems in computational mechanics. This has motivated the integration of atomistic simulation tools with continuum simulation approaches using the BSM (Liu et al. 2004). Several recent reviews of BSM provide details and applications (Liu et al. 2004, 2006, 2010; Farrell et al. 2007). The BSM uses MD simulations to enhance the accuracy of continuum simulation results in local areas of interest where atomistic scale resolution is needed. The coupling is based on the projection of the MD solution onto the coarse scale FE shape functions. This projection, or the bridging scale, represents the portion of the domain that is solved concurrently using both methods (Wagner and Liu 2003). The decomposition of scales is achieved by subtracting the bridging scale from the total solution. The basic idea of the method is in the decomposition of the total displacement field into separate coarse and fine-scale contributions (Liu et al. 2010). A beneficial result of this projection operator decomposition is that it decouples the kinetic energy of the two models, which allows for concurrent simulations with a separation of time scales. Thus, the coarse and fine scales operate on separate time scales, and the coarse scale progression is not limited to the time scale of the atomic vibrations of the fine scale (Wagner and Liu 2003; Liu et al. 2010). Additionally, during the simulations, both simulations run simultaneously with dynamic information exchange, and the high-frequency signals simulated from the fine-scale model are removed using lattice impedance

techniques (Liu et al. 2006). The BSM procedure has also been applied to a larger-scale application (termed mesoscopic bridging scale or MBS) that coupled a mesoscale discrete particle model and a macroscale continuum model of incompressible fluid flow (Kojic et al. 2008). The FE macroscale model solves Navier-Stokes and continuity equations, and the internal nodal FE forces are evaluated using viscous stresses derived from the mesoscale model, which uses the dissipative particle dynamics (DPD) method for the discrete particles. Belytschko and Xiao (2003) and Xiao and Belytschko (2004) developed another method for coupling atomistic and continuum simulations using a bridging domain. In their approach, the Hamiltonian in an overlapping region (bridging domain) between the continuum and molecular domains is taken as a linear combination of the continuum and molecular Hamiltonians. Compatibility of the two domains is enforced through a Lagrangian multiplier or augmented Lagrangian method. They demonstrate that the bridging domain approach can reduce problems with artifacts such as nonphysical wave reflections that often occur at molecular/continuum interfaces.

Mortar methods utilize a FE space of reduced dimension and a Lagrange multiplier approach to compute matching boundary conditions for two adjacent model regions (Bernardi et al. 1994; BenBelgacem 1999; Peszynska et al. 2002; Pichot et al. 2010) in which concurrent computations are performed. For example, to compute consistent boundary conditions (e.g., to ensure flux matching) for volumetric elements in two separate three-dimensional domains, a mortar with planar elements would be utilized. Mortar methods can be used to compute boundary conditions for nonmatching grids of the same type or mixed grids of different type (multinumercs, e.g., Peszynska et al. 2000a), grids representing different physical systems (multiphysics, e.g., Peszynska et al. 2000b), and/or grids with different resolution or different scale representations (multiscale, e.g., Arbogast et al. 2007). Mortar methods allow partial differential equations on the boundary (mortar) and internal nodes in each connected domain to be formulated into a consistent single matrix solve in a fully implicit manner. However, mortar methods may not be well suited for connecting particle-based methods with grid-based methods. Although mortar methods are a general means of connecting different model domains of various types, they can be used in a hybrid multiscale sense to connect models with different resolution scale and physics. Application of mortar methods for hybrid multiscale simulation of subsurface processes has been pioneered by (Balhoff et al. 2008; Sun et al. 2012a, 2012b).

Boundary condition matching between model subdomains with different scales can also be implemented through an iterative approach (e.g., Battiato et al. 2011). In this approach, an initial guess of the boundary condition for a boundary between two different domains (e.g., pore- and continuum-scale domains) is specified and then solutions are iteratively updated in each domain until a consistent solution is achieved. While this approach is

Motif F: Hierarchical Hybrid - Spatial Projection

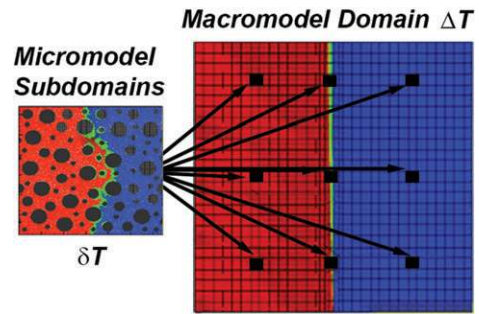


Figure 7. Schematic diagram showing the concept of the hierarchical hybrid spatial projection approach. Several local patches of microscale simulation are defined (typically corresponding to macromodel mesh elements or nodes), and the results of microscale simulation are extrapolated to the rest of the macroscale domain on a larger time interval.

less direct than the mortar method, it is also more flexible and could be used for mixed particle- and grid-based methods.

Motif F: Hierarchical Hybrid Multiscale Methods—Spatial Projection

An alternative to concurrent methods for the situation where time-scale separation is insufficient to allow short bursts of microscale computation is the so-called gap-tooth method (Gear et al. 2003; Kevrekidis et al. 2003). This method is based on the EFM (described above) but performs macroscale projection in space from small spatial patches of microscale simulation (e.g., around each macroscale node) to the full macroscale domain as shown schematically in Figure 7. A limited form of time-scale separation is required in that the boundary conditions on the microscale domain are assumed to be constant over a single period of microscale simulation.

The gap-tooth method covers the entire spatial domain with teeth and gaps between teeth. The microscopic simulations take place in the interior of each tooth with appropriate boundary conditions constructed from the coarse solution at the edges of each tooth. The compression-projection-reconstruction procedure transfers information between the coarse- and fine-scale variables, followed by interpolation of the localized coarse solution to the entire domain. The gap-tooth method enables “large space, small time” simulations through “small space, small time” simulations. An extra advantage of the gap-tooth and patch dynamics scheme is that the microscale simulations in teeth and patches are independent, and thus they can be performed in parallel to significantly reduce the wall-clock computational time.

We note that, although the Gap-Tooth approach as derived from the EFM is designed for cases where no macroscopic equation exists, a similar approach can be used when the macroscale equation is known, and in fact the macroscale projection operation is likely to be more accurate in such a case.

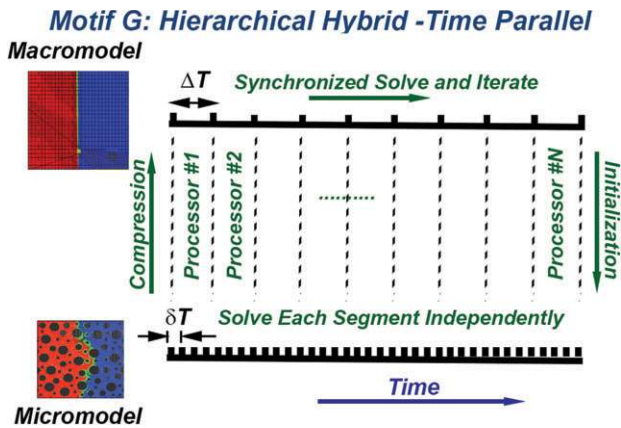


Figure 8. Schematic diagram showing the concept of the hierarchical hybrid time parallel approach. This approach deconstructs the complete microscale solution into many smaller time periods, each of which is solved independently in parallel. Since the initial conditions for one time period strictly depend on the result of the previous time period, this independence is achieved by making an initial guess of initial conditions for each time period based on a coarse macromodel solution. The micromodel results are then used to improve the macromodel parameterization (compression), which in turn provides a better guess of initial conditions to each microscale time period (initialization). The process is iterated until a converged solution is obtained.

Motif G: Hierarchical Hybrid Multiscale Methods—Time-Parallel Formulation

The most challenging multiscale situation is that in which the microscale simulation domain cannot be restricted either in time or space, but must be performed over all time and space. In such cases, it may be possible to take advantage of parallel computing through space- or time-domain decomposition as shown schematically in Figure 8. In Motif G we focus on a time-parallel multiscale/multiphysics framework (Baffico et al. 2002; Farhat and Chandesris 2003; Garrido et al. 2006; Mitran 2010; Young and Mitran 2011) that is based on the parareal algorithm (Lions et al. 2001; Bal and Maday 2002). The time-parallel method couples different but consistent governing equations at different scales. Assuming the coarse trajectory is less expensive to compute, the time-parallel method divides the overall simulation time interval into smaller subintervals and computes the fine trajectory on each of the subintervals in parallel (on different computer processors) with initial conditions generated by the coarse propagator. The fine solution in each subinterval is then used to iteratively correct the coarse trajectory (i.e., initial conditions for fine propagator) over the entire time interval until convergence. If the coarse propagator is inexpensive and it converges to the fine propagator rapidly, significant computational gains can be achieved by the time-parallel method.

In cases where the high-frequency fine-scale simulations in each subinterval become computationally prohibitive, wavelet-based methods can be combined with the time-parallel method to alleviate this problem as proposed by Frantziskonis et al. (2009). Using the composite

scheme called tpCWM, the fine-scale trajectory is only simulated for a portion of each subinterval, then this fine solution is used to correct the coarse trajectory using a compound wavelet method operator (Frantziskonis and Deymier 2003; Frantziskonis et al. 2006; Mishra et al. 2008; Muralidharan et al. 2008).

Model Adaptivity, Error Estimation, and Uncertainty Quantification

The concept of model adaptivity in the context of hybrid/multialgorithm models often refers to methodologies/tools (Oden et al. 2006) that allow one to compare models and to adapt features of different models so that they deliver results of a target accuracy sufficient to capture essential features of the response. This may be achieved with algorithms which estimate modeling error, and control modeling error through model adaptivity, such as Goals Algorithms (e.g., Bauman et al. 2009).

Since the proposed MAP serves a similar purpose of selecting appropriate models depending on the degree of coupling between the fine- and coarse-scale models, we will focus on a rather different aspect of model adaptivity, that is, the ability to dynamically track spatial and temporal locations where a finer-scale model needs to be solved. A desirable feature of hybrid/multialgorithm models is their ability, based on coarse-scale model evaluations, to track where and when to use pore-scale simulations. This is crucial to achieve optimal performances while containing the high computational burden due to fine-scale component of the hybrid algorithm. While still an open question in the computational hydrology community, recent theoretical (Battiato et al. 2009; Battiato and Tartakovsky 2011) and computational (Boso and Battiato 2013) works suggest that a priori estimates of continuum scale quantities/parameters might be employed as adaptivity criteria. These include evaluation of gradients of continuum-scale quantities (Battiato et al. 2009; Kunze and Lunati 2012) and time- or space-dependent macroscopic dimensionless numbers (Boso and Battiato 2013).

Another important consideration when designing hybrid algorithms is how the coupling of two different types of solvers impacts the accuracy of the individual methods. The concept of model adaptivity is strongly related to that of error estimation and accuracy. Any upscaled (Darcy-scale) model represents pore-scale dynamics up to a certain, controlled, accuracy. When a specific physical process does not satisfy dynamical constraints imposed by the upscaled model (e.g., processes whose parameters fall into the white region of Figure 4), then its accuracy cannot be guaranteed, and a finer-scale representation must be employed. Parameter spaces as the one depicted in Figure 4 can be therefore interpreted as maps of accuracy/error for any given macroscopic model. Studies on accuracy of multiscale hybrid models include Alexander et al. (2005a, 2005b), Leemput et al. (2007), and Zagaris et al. (2009). Yet the development of robust error estimation tools for hybrid models in porous media is still at its infancy. In Leemput et al. (2007), a closed form expression for the spatial

discretization error of a hybrid lattice Boltzmann/finite difference model for one-dimensional reaction-diffusion system was derived. Alexander et al. (2005a, 2005b) discuss the effects, both positive and negative, of statistical fluctuations on hybrid computational methods, focusing on schemes that combine a particle algorithm with a partial differential equation solver.

Most natural systems are inherently uncertain and, because of this, uncertainty quantification has become an important research area in recent years. Uncertainty in transport models can be present on all scales. Some sources of uncertainty, such as deterministically unknown initial and boundary conditions, are common to all scales (e.g., pore and Darcy scales). Other sources of uncertainty are specific to each scale: at the pore scale, the possible sources of uncertainty are unknown pore geometry and rate constants; at the Darcy scale, uncertainty can be due to variable properties of porous media (e.g., permeability, porosity, dispersion coefficients) and insufficient data. As a result, uncertainty can be present in each component of a multiscale model. It is common to treat uncertainty in probabilistic terms, that is, to represent unknown parameters and initial and/or boundary conditions as random variables with statistics obtained from available measurements. Random parameters render governing equations stochastic, and in the probabilistic framework uncertainty quantification is equivalent to solving stochastic equations. A number of methods have been developed for uncertainty quantification at a given scale including sampling methods (Minasny and McBratney 2002), Polynomial Chaos (PC; Lin and Tartakovsky 2009, 2010), probability density function (PDF; Tartakovsky and Broyda 2011), cumulative density function (CDF; Wang and Tartakovsky 2012), and moment equation (ME; Tartakovsky et al. 2002, 2003) methods. Sampling methods such as Monte Carlo and Latin Hyper Cube are robust but have slow convergence rate and, given high complexity of the governing equations, may be prohibitively expensive. PC methods rely on a Karhunen-Loeve expansion to approximate correlated random inputs. The number of random dimensions in Karhunen-Loeve expansion increases with decreasing correlation length of the random inputs. In turn, the computational cost of PC methods increases exponentially with the number of random dimensions and the PC methods become inefficient for Darcy models where parameters, such as permeability, often have correlation length that is much smaller than the size of the computational domain. The dimension reduction methods, such as PDF, CDF, and ME methods, rely on closures to derive closed form deterministic equations for PDF, CDF, or leading statistical moments of the state variables. These closures are usually accurate only for small variances of the stochastic inputs. Several approaches have been recently proposed to increase the range of applicability of these methods including analysis of variance (ANOVA) decomposition for PC methods (Foo and Karniadakis 2010) and Random Domain Decomposition for both PC and the dimension reduction methods (Lin and Tartakovsky 2010).

Uncertainty quantification (UQ) in multiscale methods is a less mature area. UQ in a multiscale model has the same challenges as UQ in a single-scale model and the added complexity of multiscale models presents additional challenges. One possible approach for UQ in multiscale systems is to utilize a multiscale operator decomposition (MOD) that has been developed in context of a posteriori and a priori analysis of multiphysics systems (Estep et al. 2008). In the MOD approach, a multiphysics problem is split into components involving simpler physics over a limited range of scales, and the solution of the entire system is found via iteration of solutions of the individual components. When applying such approach to UQ in multiscale systems, special care should be taken with regard to stability and accuracy of solution of the stochastic equations, as the interactions between different scales have been discretized.

Applications of Hybrid Multiscale Simulation

Hybrid multiscale modeling methods have been most widely applied in the fields of materials science and chemical engineering, in which atomic-scale models of MD have been linked to continuum-scale models of material deposition, strength, deformation, and failure. Recent reviews of multiscale methods applied to materials science are given by Curtin and Miller (2003), Csanyi et al. (2005), and Wang and Zhang (2006). Two important application areas are stress-induced defects and brittle failure of materials (e.g., Abraham et al. 1998; Abraham 2000) and formation of thin films in micromanufacturing (e.g., Vlachos 1999). Hybrid MD/continuum models can be traced back to the early 1970s (Gehlen et al. 1972) and have become widely used in the past decade. The recent expansion of interest in multiscale modeling methods is also reflected in the launching of two new journals, *Multiscale Modeling and Simulation* (published by the Society for Industrial and Applied Mathematics [SIAM]) and the *International Journal for Multiscale Computational Engineering* (published by Begell House), both of which published their first volume in 2003. We note that these journals, and multiscale mathematics and modeling, include a broad range of methods in addition to the hybrid multiscale methods of focus here, including but not limited to multigrid, multiscale variational, adaptive mesh refinement, homogenization, and others. However, several articles appearing in these journals do specifically address hybrid multiscale methods (e.g., Kroger et al. 2003).

In chemical engineering, catalysis and reactor processes have also been the subject of significant multiscale modeling efforts (e.g., Raimondeau and Vlachos 2002; Vlachos et al. 2006). While aimed at process engineering applications, it is likely that these could also be applicable to surface geochemistry processes of interest in subsurface reactive transport applications. A review of multiscale approaches in chemical engineering is provided by Ingram et al. (2004). The life sciences are another discipline in which hybrid multiscale methods have been

extensively applied. The first 2005 issue of *Multiscale Modeling and Simulation* (volume 4, number 1) contains a special section on *Multiscale Modeling in Materials and Life Sciences*. Some interesting examples of multiscale hybrid modeling in the life sciences include Quarteroni and Veneziani (2003), Villa et al. (2004), Setayeshgar et al. (2005), and Ayati and Klapper (2007).

More closely related to subsurface porous media applications are a number of studies that have applied hybrid multiscale methods to problems in liquid or gas hydrodynamics (e.g., O'Connell and Thompson 1995; Hadjiconstantinou and Patera 1997; Li et al. 1998; Garcia et al. 1999; Nie et al. 2004; Sun and Candler 2004; Wijesinghe et al. 2004; Werder et al. 2005; Ren and E 2005; Koumoutsakos 2005; Bergdorf et al. 2005; Fyta et al. 2006), diffusive transport (e.g., Flekkoy et al. 2001; Alexander et al. 2002; Bergdorf et al. 2005; and Xiu et al. 2005), and colloid transport and deposition on a two-dimensional surface (Magan and Sureshkumar 2004, 2006). Koumoutsakos (2005) provides a review of particle and hybrid methods applied to fluid dynamics simulations.

Although hybrid multiscale techniques have been developed and applied in a number of other science and engineering disciplines, they have to date only been applied to subsurface water flow and reactive transport to a limited extent. To our best knowledge, the first published example is given by Balhoff et al. (2007), who describe a hybrid model that utilizes a pore network model to simulate pore-scale water flow in a sand-filled fracture linked with a continuum-scale FE model of flow in a porous rock matrix. Tartakovsky et al. (2008a) presented a hybrid multiscale model of a diffusion-reaction (mineral precipitation) system in porous media with pore and continuum subdomains, and demonstrated equivalence of the hybrid multiscale simulation with a simulation resolved fully at the pore scale. Both of these early applications utilized a concurrent hybrid approach (Motif E), in which the pore- and continuum-scale domains occupied separate regions of the overall model system and were run simultaneously with boundary condition coupling. In both examples, the boundary coupling was accomplished using an approach specific to the particular model types utilized (i.e., particle models or pore network models). A more general boundary coupling approach was presented by Battiato et al. (2011), who studied the problem of fracture flow and reactive transport (a solute that reacts with the fracture walls). That work used an iterative method to converge on a solution for which the macroscale and microscale solutions were consistent at the boundary, and demonstrated the accuracy of the method by comparison to a full microscale simulation. Another recent concurrent hybrid application was presented by Sun et al. (2012a, 2012b), who simulated flow near an injection well by coupling thousands of small pore-scale subdomains near the well with a single continuum domain away from the well using a mortar coupling method. They demonstrated that, for the selected problem, the hybrid multiscale method provided a significantly improved result in comparison to a model using numerically upscaled permeabilities for

each of the pore network model domains. An example of a HHM (Motif D) is given by Tartakovsky and Scheibe (2011), who coupled a particle-based pore-scale simulation of a mixing-controlled precipitation reaction with a continuum-scale simulation. We found concurrent coupling of particle- and grid-based methods challenging when including advection, because of difficulty in matching boundary conditions; the hierarchical approach was much better suited to this problem and was shown to provide a highly accurate solution while significantly reducing computational requirements. Sheng and Thompson (2013) describe a concurrent hybrid method to couple pore- and continuum-scale simulations of steady or transient multiphase porous media flow using a dynamic pore network model; they noted that allowing the microscale simulation to evolve to steady state at each time step helped to reconcile the large time scale differences between the pore- and continuum-scales. Although most of these examples focus on flow through granular porous media rather than fractured porous media, there is no general reason why multiscale hybrid methods (and the MAP) cannot be applied to fractured systems. In fact, incorporation of coupled flow and geomechanical processes in fractured media into subsurface models may be an excellent application for hybrid methods.

Concluding Remarks

We have reviewed a wide range of approaches that can be brought to bear on the challenging problem of multiscale process modeling in heterogeneous porous media. A MAP is presented that classifies these approaches into a number of motifs to provide guidance on their applicability to different types of problems. Although some of the methods presented do not fall neatly into one category alone, MAP is intended to be a dynamic community resource used to gain insight into some of the key issues surrounding multiscale simulation. We have found MAP especially useful for transferring methodologies developed in one discipline to a completely different application area. To this end, MAP is a Wiki-based website (<https://kef.pnnl.gov/map>) where community members can contribute or draw information. In addition to descriptions of the MAP and its component Motifs, the site provides a repository for relevant literature, more detailed descriptions of methods within each Motif, and, depending on availability, links to open-source software that can be used to implement specific methods.

Multiscale hybrid simulation is a highly complex modeling approach that requires significant computational, theoretical, and data resources. It is our hope that this article has provided a context for scientists and engineers to begin to understand the methodologies, and more importantly to gain insights into the nature of multiscale problems and the various solution approaches (including hybrid multiscale). Some problems will require this level of complexity in order to achieve a truly predictive capability, such as coupled flow and geomechanics (e.g., hydrofracturing and gas recovery),

multiphase fluid flow with density instabilities (e.g., geological carbon sequestration), and effects of microbial cells on subsurface reactions (e.g., bioremediation). All of these problems involve processes that are fundamentally controlled by small-scale (pore-scale and smaller) features of the medium, and in many cases we have not yet discovered adequate upscaled representations. For such problems, we envision that hybrid multiscale simulation methods, enabled by continued advances in computational and characterization technologies, will become a powerful tool for gaining critical understanding and predicting the outcomes of complex interactions.

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