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Abstract

In this paper, we present a hierarchical patch dynamic paradigm for modeling complex groundwater systems across multiple scales – one that has the potential to substantially alleviate the infamous “curse of dimensionality” and the associated computational bottlenecks in large-scale groundwater modeling. The new modeling paradigm is inspired by the observations on how biological systems have been doing a great job coping with complexity, especially on their ability to process far more information than their limited bandwidths allow. Specifically, the new modeling paradigm takes advantage of hierarchy theory, mimics how biological systems “divide and conquer” complexities, and decouples scale-dependent subsurface dynamics hierarchically. The result is a systematic framework that allows converting a large problem into many smaller sub-problems and thus enables modeling complex groundwater systems in high resolution without having to solve large, ill-posed matrix systems. We illustrate the basic concept and the effectiveness of hierarchical modeling with a simple example. In part 2 of this paper series [Li et al., to submit], we address practical implementation issues and present an integrated, object-oriented, computational steering environment to specifically support hierarchical patch dynamic modeling. We demonstrate the power of the hierarchical modeling environment by applying it to solve a large, complex groundwater problem across multiple spatial scales.

Introduction

Despite the exponential growth of computational capability over the last two decades – one that has allowed computational science and engineering to become a unique, powerful tool for scientific discovery [Moravec, 1998] — our ability to model large complex groundwater systems is still severely limited because of the following tough computational challenges:

1. The Machine Bottleneck. The computational cost in large-scale groundwater modeling, analysis, and visualization increases exponentially with the domain size and the level of details simulated and quickly becomes prohibitive for large problems. This is especially the case for multi-scale modeling, coupled processes modeling, inverse modeling, uncertainty analysis, iterative hypothesis testing, and data sufficiency evaluation. Modeling and visualizing a highly discretized transient system (e.g., 500,000...
nodes or more) of flow and transport processes often brings conventional workstations to a near standstill.

The Numerical Algorithmic Bottleneck. Large-scale groundwater modeling based on a single numerical representation of a complex, heterogeneous, and multi-scale system faces an algorithmic bottleneck. The high dimensionality, especially when combined with highly distorted grids representing strong heterogeneity, anisotropy, multitude of scales, complex aquifer structure, and singular stresses, translates into highly “ill-conditioned” or “stiff” matrix systems and causes a host of tough numerical problems, including extremely slow convergence, unphysical oscillations, and total solution failure.

In this paper, we address systematically these fundamental computational difficulties in large-scale groundwater modeling using an interdisciplinary approach. In particular, we explore ideas and theories which allow us to move beyond evolutionary advances to innovations that promise much higher speeds and allow solving much larger, more complex problems than traditional approaches currently permit.

Biological Inspirations

Our approach to modeling of large, complex groundwater systems is inspired by the observations on how nature has been doing a great job maintaining life and coping with complexity for millions of years (Shadbolt, 2004; Milewski, 2001). In particular, our approach to modeling complex groundwater systems is motivated by the following observations made by Milewski (2001) on how human beings and biological systems in general are able to process far more information than what their limited bandwidths allow through a set of fundamental strategies.

In our immediate memory we can deal only with a finite and rather small number of objects—whatever type they are, ideas, images, words. To deal with complexity, we have long been employing (perhaps subconsciously) a highly effective strategy—the “divide-and-conquer” method. The method is based on imposing a tree-like structure on top of a complex problem. The idea is that at every node of the tree we have to deal with only a small number of branches, within the limits of our immediate memory. The traversal of the tree leaf-to-root or root-to-leaf requires only a logarithmic number of steps—again, presumably within the limits of our immediate memory. For instance, the body of academic knowledge is divided into humanities and sciences (branching factor of 2). Sciences are subdivided into various areas, one of them being Hydrological Sciences, and so on. To understand Freeze and Cherry’s book on Groundwater Hydrology [Freeze and Cherry, 1979], the hydrological science student needs only very limited education in humanities. On the other hand, to write a poem one is not required to know how to model groundwater flow and contaminant transport. The tree-like subdivision of human knowledge not only facilitates in-depth traversal and search, it also enables division of work between various teams. We can think of the whole humanity as one large team taking part in the enormous project of trying to understand the World.

Biological Systems as Metaphors

Use of biological systems as metaphors can potentially lead to highly efficient computational and information system technologies. At the system level, biological and computational systems are fundamentally similar. They both involve processing data and facing the challenge of having to deal with a large amount of complex information with a limited system capacity. Although biological systems are often slow, they can solve problems that are far larger than what their system capacities allow. Biological systems appear to be doing a masterful job in coping with complexity and information overload—they seem to scale, to be robust and inherently adaptable at the system level (Shadbolt, 2004). Although computational systems are very fast, they are often inflexible, unrobust, and inherently limited by their system bandwidths. An ideal “data” processor or information system would be a hybrid one that allows combining the best advantages of computational and biological systems—a system that offers a flexible, robust, and high-speed solution to large, complex problems without being bottlenecked by the system capacity.

A Hierarchical Patch Dynamic Modeling Paradigm

We present in this paper such a flexible and high-speed computational system for large-scale groundwater modeling. In particular, we present a biologically motivated, “hierarchical” and “patch” dynamic framework for modeling complex groundwater systems across multiple scales. The basic idea is to move away from developing a single monolithic system that would solve a large, ill-conditioned, and complex problem, and to employ a population (hierarchy) of simpler sub-systems that cooperatively solve the problem. In such a hierarchical system, each sub-system is simpler and
easier to solve than the monolithic system. The integrated system based on the whole population can generalize better than any single subsystem in the hierarchy.

Directly mimicking the way a biological system functions and deals with complexity, we represent a large complex groundwater system hierarchically, systematically breaking it “vertically” into many levels and “horizontally” into many patches or clusters/subareas of interest (figure 1). The patch dynamics in different subareas at different levels are related efficiently to each other through a hierarchical patch structure (figure 2).

![Figure 1 – Recursive hierarchical patch decomposit](image)

A complex groundwater system can be recursively broken into many smaller patches or clusters.

The patches at higher levels are used to simulate slower and larger-scale groundwater dynamics whereas nested patches at lower levels are used to simulate faster and smaller-scale flow and transport processes. The upper level exerts constraints (e.g., as boundary conditions) to the lower level, whereas the rapid dynamics at lower level can be used to provide aggregated “feedback” to the upper. The patches at the same level interact with each other indirectly, through their common ancestors (at higher levels).

The conceptual basis for the new modeling paradigm emerges from hierarchy theory (Simon, 1962, 1973; Cushman, 1990) and a diversity of studies in various disciplines, including management science, economics, psychology, biology, ecology, and system science. The hierarchy theory has been significantly refined and expanded in the context of evolutionary biology and ecology [Allen and Starr, 1982; Salthe, 1985; Ahl and Allen, 1986; Wu, 2001; Wu and David, 2002].

According to hierarchy theory [Simon, 1962, 1973], complexity frequently takes the form of hierarchy, whereby a complex system consists of interrelated subsystems that are in turn composed of their own subsystems, and so on. Such complex systems are nearly completely decomposable (or nearly decomposable) systems because of their “loose vertical coupling”, permitting the distinction between levels, and “loose horizontal coupling”, allowing the separation between patches or subsystems at each level.

### Hierarchical Groundwater Equations

Mathematically, the new, nature-inspired modeling framework involves solving a set of hierarchically formulated groundwater equations (see table 1). These equations describe the space-time patch dynamics at a typical level \(l\) defined on \(\Omega^l\) and their interaction with the dynamics in the parent patch (defined on \(\Omega^{l-1}\) at level \(l-1\)) and in the various daughter patches (\(\Omega^{l+1}_k\), \(k=1,2,\ldots\) at level \(l+1\)) (see figure 3). The notations \(h\), \(u\), and \(c\) are respectively the hydraulic head, seepage velocity, and solute concentration; \(n_o\), \(S_o\), \(R\), \(K_{ij}\), and \(D_{ij}\) are respectively the effective porosity, specific storage coefficient, retardation factor, hydraulic conductivity tensor, and dispersion coefficient tensor; \(\varepsilon\) and \(r\) are the water
and solute source/sink term; \( n_i \) is the unit normal vector for the patch boundary. These equations are based on the assumption that 1) the fluid in question is incompressible, homogeneous, and isothermal, 2) the porous medium is saturated, non-deformable, and nonfractured, and 3) the contaminant considered is soluble.

The governing patch dynamic equations are standard groundwater flow and transport equations, except that the boundary and initial conditions [Eqs. (1-3), (1-4) and (1-6), (1-7)] are formulated in a special way to take advantage of the scale dependent correlation dynamics. Specifically, the patch boundary and initial conditions at level \( l \) are lagged by one scale or imposed in terms of (or interpolated from) the coarser parent dynamics at level \( l-1 \), implicitly assuming that the patch boundaries are selected in such a way that they are located in the area where the coarser parent dynamics are already accurate and thus any error introduced at the patch boundaries is small or exerts little influence on the internal dynamics in the area of critical interest. The scale lag introduced at the patch boundaries simplifies the numerical solution of the groundwater equations. It allows systematically decoupling a large complex problem into many smaller problems that can be solved sequentially. In particular, hierarchical decoupling makes it possible to solve the governing groundwater equations over a large area across multiple scales (for \( l=0,1,2,... \)) based on a scale-dependent discretization. Successive solution of (1) down the entire patch hierarchy, beginning at the highest level on a coarsest grid/timestep, provides an approximation of the complete system dynamics and a mechanism to pass systematically field information and regional influence from higher levels to lower levels.

The detailed dynamics at lower levels can also be used to improve the higher-level dynamics. This can be achieved through a systematic “upscaleing” process that involves re-solving in a reverse sequence the same groundwater equations “conditioned” on the known finer-scale dynamics. In this paper, we focus on the important process of “downscaling” and will discuss the issues of two-way scale interactions across multiple scales in future publications.

### Advantages of Hierarchical Patch Dynamic Modeling

The hierarchical patch dynamic approach significantly alleviates the computational bottlenecks facing large-scale groundwater modeling. Specifically, the new hierarchical patch dynamic approach:

- allows modeling and visualizing a large system in high resolution without having to solve large matrix systems and thus substantially alleviate the infamous “curse of dimensionality” or the machine bottleneck.
- allows modeling heterogeneous dynamics incrementally (one scale at a time) and thus obviate the need to use highly distorted grids representing multiple scales of variability, and substantially alleviate the stiff matrix problem - the algorithmic bottleneck.
- provides a “scaling ladder” to relate groundwater equations across different scales.

The hierarchical patch dynamic approach represents a powerful generalization of the popular “telescopic approach” used in computational fluid dynamics, climate modeling, and groundwater modeling [Ward et al., 1987; Mehl and Hills, 2002; Miller et al 1987; Anderson and Woesnner, 1992]. It represents a marriage of hierarchical modeling and patch dynamics [Allen et al, 1982; Cushman, 1990; Cushman et al, 2002; Wu and Loucks, 1995; Wu, 2001; Wu and Levin, 1997] to address the fundamental bottlenecks in groundwater modeling. The hierarchical patch dynamic approach also shares some of the distinct features of the innovative Analytical Element Methods (AEM) that make it possible to include distant hydrogeologic boundaries and at the same time allows for local detail without the excessive computational effort that would be required with the traditional finite difference method [Haitjema, 1995; Hunt et al., 1998; Bakker et al., 1999]. The new hierarchical patch dynamic approach represents “in spirit” an major extension of the AEM to allow modeling general heterogeneity, general

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**Figure 3 - A typical model patch and its interaction with the parent and daughter patches.**
nonlinear dynamics, and general 3D unsteady flow and transport. Finally, the hierarchical patch modeling approach complements, and can be combined with, the recent exciting developments in parallel computing [Chung et al, 1992; Cliffe et al, 2000; Yevi et al, 1998; Wu et al 2002] that has enhanced our ability to solve large-scale modeling problems. Parallel computing by itself does not directly address the algorithmic bottlenecks in large-scale modeling and is still be limited by the machine bottlenecks.

<table>
<thead>
<tr>
<th>Table 1 – Governing patch dynamics equations.</th>
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<tbody>
<tr>
<td>Governing Eq.</td>
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<tr>
<td>Flow</td>
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<td></td>
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<td></td>
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<tr>
<td>Initial Cond</td>
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<tr>
<td>Governing Eq.</td>
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<tr>
<td>Transport</td>
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<td></td>
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<tr>
<td>Initial Cond</td>
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We feel that the hierarchical patch dynamic approach is essential to modeling and understanding complex subsurface processes. It is hardly justifiable theoretically and overwhelmingly difficult technically to translate information directly between two distant levels (or corresponding scales), when ignoring intervening levels that are relevant to the phenomenon under study. Although it may be possible to scale down from the regional scale to detailed processes at a site or localized hot spots of critical interest, successful approaches most likely have to be hierarchical. A hierarchical patch dynamic approach is probably the only way one can hope to model and freely explore fine-scale processes in a large, regional system under general conditions.

An Illustrative Example

In this section, we use an example to illustrate the basic concept of the hierarchical patch dynamic approach and its implications for large-scale groundwater modeling. Our example considers two dimensional, steady state groundwater flow in a regional wellfield system.

![Diagram](image.png)

**Figure 4 – Conceptual definition sketch for the example problem**
Table 3 – Pumping rates used in the example problem

<table>
<thead>
<tr>
<th>Well ID</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pumping Rate x 1000 (m$^3$/day)</td>
<td>2</td>
<td>2.5</td>
<td>1.5</td>
<td>0.7</td>
<td>1.5</td>
<td>1.8</td>
<td>1.5</td>
<td>0.5</td>
<td>1.0</td>
<td>2.5</td>
<td>0.2</td>
<td>2.5</td>
<td>0.6</td>
<td>0.7</td>
<td>0.7</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 2 - Aquifer properties and boundary conditions for the example problem

Figure 4 presents a conceptual definition sketch for the problem. Tables 2 and 3 present the physical parameters defining the problem. We are interested in modeling the regional dynamics as well as the local wellfield system and the detailed flow patterns around local well-clusters and selected individual wells. We demonstrate the effectiveness and advantage of the multi-resolution, hierarchical patch dynamic approach by comparing the hierarchical solution with a high resolution, single model solution.

Under the new, hierarchical patch dynamic paradigm, we model the region incrementally. We begin with modeling the system using a coarse grid and then successively make localized corrections by adding model-patches or patches in a patch in areas where we believe the solution is inaccurate and we are interested in knowing more details. The modeling patches are defined interactively based on a visual examination of the parent dynamics so that the patch boundaries are located where the parent solution is judged to be adequately resolved.

Actual implementation for the example is carried out in a general purpose, object-oriented computational environment called Interactive Ground Water (IGW) [Li and Liu, 2003; Li and Liu, in review]. IGW supports incremental hierarchical modeling and is designed such that a modeler can insert interactively and graphically, at any time, 1) one or multiple model patches, 2) patches in a patch, or more generally 3) a hierarchical network of patches into a parent model in order to provide greater detail where it is required, while dynamically coupling the various scales of flow and transport modeling, visualization, and analysis. Hierarchical modeling within IGW becomes essentially a process of successively and visually zooming into more and more details of interest. We will discuss in detail IGW’s hierarchical modeling capability in part 2 of this paper series [Li et al., to submit].

Results

Figures 6 through 11 present the hierarchical modeling results for the example problem and a systematic comparison with the standard single model solution. Figure 5 shows the hierarchical patch network used to solve the problem and to link the solutions in nine different patches and at five different scales. The symbol $M^i_{jk}$ represents a typical patch model within the overall hierarchical network. The indices define the hierarchical relationships of the different modeling patches; $i$ denotes the model level or “generation”, $j$ the parent index, and $k$ the children index.
Figure 6 shows the coarsest model solution that provides the general dynamics for the entire region. Figure 7 presents the same regional solution with a modeling patch in the general wellfield area and three sub-modeling patches providing more details around each of the three well clusters. The coarsest model has a grid resolution of 50 m, the wellfield modeling patch has a resolution of 25 m, and the three submodeling patches, covering much smaller areas, have a resolution of respectively 12.5 m.

Figure 6 – Hierarchical patch solution (level 1, coarsest grid 50m) for the example problem. Boxed areas (around the wellfields) are where the spatial dynamics are rapidly varying.

Figure 8 presents the single model solution with a uniform resolution of 12.5 m for the entire region. A comparison of Figures 7 and 8 clearly shows that, despite the decoupling, the hierarchical solution matches well with the single model solution.

Figure 9 further compares the hierarchical and single model solutions along a representative cross-section (the A-A cross-section). The plot shows the local patch solution in $M_{11}$, represented by a solid circle, virtually collapses into the solid line representing the single model solution.

The most important advantage of the hierarchical modeling approach lies in that it allows zooming “indefinitely” into details (as long as the governing equations still hold at the scale of interest) within an areally expansive model. Figure 10 shows two additional levels of local patch solutions at a resolution of respectively 6.25 m and 3.125 m. These patch solutions accurately and efficiently resolving the detailed local stresses, the locations of the wells, and provide a highly detailed description of local well dynamics in the regional system.
Figure 7 – Hierarchical patch solution (level 1 to 3) for the example problem. The head distribution in the wellfield area is locally corrected with a modeling patch of a resolution of 25 m. The wellfield patch is further corrected with three additional subpatches around the well clusters. The grid resolution of the subpatches is 12.5m.
Figure 8 – Single model solution with a uniform resolution of 12.5 m for the entire region. The boxed areas are where the spatial dynamics are rapidly varying. The head contours are plotted in such a way that they are directly comparable with the hierarchical patch solution. Note the hierarchical solution matches well with the single model solution.
Figure 9 – Comparison of the hierarchical and single model solutions along the A-A profile in the submodel area $M_{11}^1$. The location of the A-A profile is defined in Figure 4. Note the hierarchical solution at level 3 (solid circle) virtually collapses into the single model solution (the solid line).
Figure 10 – Hierarchical patch solution (level 3 to 5) for the example problem. The patch solution for the west subwellfield is further corrected with two additional nested patches (at level 4) improving the flow description around two individual wells. The patch dynamics around the individual wells are again patched at level 5. The model resolutions, from level 3 to 5, are 12.5 m, 6.25 m, and 3.125 m. Note the submodel at level 5 allows resolving more accurately the locations of the individual wells.
Summary and Conclusions

The example confirms the potential of using the new hierarchical patch dynamic approach as a general framework for large-scale groundwater modeling. In particular, the solutions show that hierarchical patch predictions are able to reproduce the single model solution and allow capturing large-scale regional dynamics and at the same time resolving local details and the rapidly varying drawdown dynamics in the immediate proximity of individual wells without having to solve large, ill-conditioned matrix systems.

In part 2 of this paper series [Li et al., to submit], we will address important practical implementation issues. In particular, we will present an object-oriented, computational steering environment to specifically support general, hierarchical patch dynamic modeling. We will demonstrate the power of the new hierarchical steering environment by applying it to the modeling of flow and solute transport in a large, complex, heterogeneous groundwater system across multiple spatial scales – a problem that is difficult to solve using traditional modeling approaches.

Acknowledgments

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