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Hierarchical modeling of a groundwater remediation capture system

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SUMMARY

In this paper, we present a real-world demonstration of a generalized hierarchical approach for modeling complex groundwater systems, the hierarchical patch dynamics paradigm (HPDP). In particular, we illustrate how the HPDP approach enables flexible and efficient simulation of a complex contaminant capture system at one of the largest groundwater pump-and-treat remediation operations in Michigan. The groundwater flow system at the site exhibits a multi-scale pattern that is difficult to simulate using standard modeling tools because of the complex interaction between ambient hydrologic stresses and on-site remediation operations. The hierarchical modeling system was calibrated to water level measurements collected from 208 monitoring wells located both on-site and in its immediate proximity and flux measurements from 6 trenches on-site. Systematic hierarchical simulations, including forward and reverse particle tracking as well as integrated water budget analyses, were performed to study the on-going remediation. The hierarchical modeling results show that some contamination leaked off-site because of small-scale inefficiencies in the design of the remediation system. Thus, the HPDP approach provides an opportunity to analyze complex hydrological field environments in a pragmatic, time-efficient manner.

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1. Introduction

In many groundwater systems, complex configurations of stresses and the hydrogeological environment leads to multi-scale variability of the flow field in space and time. Characterizing such complexity is critical for evaluation of groundwater management, especially pollution control and remediation (Afshari et al., 2008). In such circumstances numerical models are used to simulate the groundwater system and predict solute transport, using many discrete cells to represent the aquifer system and the head values at model nodes to estimate the velocity field. Generally, real-world problems extend over large geographic areas, requiring that the model utilizes numerical cells with large spatial dimensions and large time-steps relative to the small-scale variability (e.g., injection/extraction wells with rapid head variability in space and time). This is necessary to avoid (a) computational costs that are prohibitively expensive or (b) ill-posed matrices that are result of using a single numerical representation of a complex system (Li et al., 2006). The resulting simulated heads from a regional model in close proximity to point sources or sinks are generally bad approximations, despite correct predictions of head further from the well (Anderson and Woessner, 1992). Alternatively, if one simulates local- or site-scale models independently, they may misrepresent the regional processes and thus lose the ability to accurately analyze the impact of regional variations (e.g., seasonal irrigation) on the groundwater management strategies.

Modeling across multiple scales while ensuring computational practicality and absence of numerical problems has thus become an important issue in groundwater modeling over the past few decades. The challenge of multi-scale modeling has been addressed in several different ways, including (1) local grid refinement (Fung, 1992; Gable et al., 1996; Heinemann et al., 1983); (2) local analytical correction (Prickett, 1967; Peaceman 1978; Pritchett and Garg, 1980); (3) local nested numerical correction (Ward et al., 1987; Efendiev et al., 2000; Mehl and Hill, 2002); (4) the hierarchical patch dynamics paradigm (HPDP), more recently developed and verified with a handful of synthetic examples (Li et al., 2006; Afshari et al., 2008). In this study, we present one of the first field applications of HPDP by simulating multi-scale flow and transport dynamics associated with an extensive pump-and-treat remediation operation. First, we review the advantages and disadvantages of the various multi-scale approaches.

1.1. Local grid refinement

Local grid refinement is the process of subdividing relatively large-sized cells in a numerical model into cells of smaller spatial

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dimensions in the areas of interest. This results in a more accurate estimation of hydraulic gradients at the well-scale (Fung, 1992; Gable et al., 1996; Heinemann et al., 1983; Matott et al., 2006; Sutradhar and Paulino, 2004). Applications for simple or small-scale problems provides solutions quickly while maintaining consistency between the regional and local areas around while. However, for large-scale regional groundwater models, where there may be a significant increase in the number of nodes (e.g., millions rather than thousands), the cost of computation increases exponentially and the process can become very expensive in terms of time and computer resources required.

1.2. Local analytical correction

An approach for representing detailed well dynamics in a regional model has involves a local analytical correction within the cell containing the well based on the steady-state Thiem equation (Thiem, 1906; Anderson and Woessner, 1992). Trescott et al. (1976) systematically evaluated the performance of local analytical correction and showed that corrected drawdown is approximately applicable if the following assumptions are satisfied: (1) flow to the well is within a square finite-difference cell and can be described by a steady-state equation with no source term except for the well discharge, (2) the aquifer is isotropic and homogenous in the well cell, (3) only one well, located at the cell center, is in the well cell, and (4) the well fully penetrates the aquifer. Pritchett and Garg (1980) provided formulas for analytical correction for grid cell geometries other than square. Our own empirical experience shows that local analytical correction can lead to problematic flow patterns around the wells although the corrected drawdown is reasonably accurate.

1.3. Local numerical correction

Nested grid modeling, or "local numerical correction", is a more general approach for modeling well-scale processes within a regional model. This approach utilizes grid-dependent information from the regional model to construct a separate model with finer grid spacing around the area of interest to resolve more details (Ward et al., 1987; Efendiev et al., 2000; Mehl and Hill, 2002). Often called the "submodel", "Local model", or "Patch model", the finer grid model derives its initial and boundary conditions from the parent model (Townley and Wilson, 1980; Ward et al., 1987; Buxton and Reilly, 1986). The boundary conditions can be either interpolated heads or fluxes, constraining the finer grid to then perform as an independent model. Thus, the original problem of solving a very large matrix system (encountered with local grid refinement) is avoided by converting the problem to one that requires solving a multitude of much smaller matrix systems.

In nested grid modeling, the interaction between the parent and local models depends on the offline analysis and processing of model modifications or simulation results from the parent model to obtain the boundary and starting conditions for the local model. This represents a major bottleneck in implementing this approach because making modifications to models or processing simulation results for use in different scales can be very time consuming. This is especially the case for transient flow problems and flow simulations coupled with solute transport (Li et al., 2006). When offline conceptual changes must be made iteratively in more than one model, the effort involved may become impractical (Li and Liu, 2006a,b). Additionally, a feedback loop is needed to account for potential significant two-way interactions between the parent and its nested submodels. Therefore, applications of the nested grid approach are often implemented with little flexibility to just a few sub-models.

1.4. The hierarchical patch dynamics paradigm

The hierarchical patch modeling approach was introduced by Li et al. (2006) to overcome the limitations of local numerical correction through the use of dynamic coupling between the parent and submodels. All patch models are integrated at the end of each time step during a simulation so that any changes or results (e.g., boundary conditions) to or from the parent model automatically propagate to all submodels in the model hierarchy. This is made possible by the fact that HPDP is supported by the Interactive Groundwater modeling environment (Li and Liu, 2006a,b). This environment enables the creation of submodels without the need for offline-post processing; the modeler can insert interactively and recursively a hierarchy of submodels throughout the simulation process. The results are continually displayed at the end of each time step, allowing for conceptual changes and analysis without forcing the modeler to wait until the entire simulation is complete.

Li et al. (2009) provided a detailed overview of the approach and demonstrate its potential through a synthetic exercise involving 30 wells and 20 surface water features. They simulated an *in situ* bioremediation operation using HPDP to study the effects of seasonal irrigation and simulate the biocurtain evolution. Although the predicted breakthrough curves matched well with observed tracer tests, the modeling application lacked calibration targets or regional data to characterize the long-term regional processes. Afshari et al. (2008) applied HPDP to a suite of synthetic examples of complex wellfields, including a 2D simulation of a confined aquifer containing several wellfield clusters. The simulated drawdowns were consistent with the analytical solution, i.e., the superposition of the Theis solution (Theis, 1935). A 3D transient example showed that submodels used in the hierarchical approach could reproduce drawdown results from a single fine-grid model, but at a fraction of the computational costs. Additional advantages highlighted were (a) HPDP eliminated the restrictive assumptions inherent in the analytical correction approach; (b) HPDP eliminated the data input and output difficulties in the traditional numerical correction approach; and (c) HPDP allowed for simulation of detailed well dynamics in a large regional model without solving a large matrix system. Liao et al. (in press) applied HPDP to a lake augmentation project including several surface water bodies and an extraction well. Mathematical models for surface and groundwater interactions and hierarchical parameter estimation were incorporated into HPDP. While these studies presented clear advantages of the HPDP, there is still the need for a complex field application of the approach that demonstrates the high level of detail with which design performance can be evaluated.

1.5. Study objectives

In this paper, we simulate a complex flow-field that is a result of many (>50) point source and sinks used in a pump-and-treat remediation operation. The specific objective of the study are to (1) verify that hierarchical patch dynamics modeling can capture small-scale dynamics at various well locations while honoring the long-term regional flow patterns predicted from a reasonable and data-intensive hydrogeologic framework, and (2) demonstrate the detailed evaluation of design performance made possible when applying HPDP to simulate a groundwater remediation system.

2. Real-world example

In this section, we introduce a large groundwater pump-and-treatment remediation operation in Michigan. At this