A Real-Time, Interactive Steering Environment for Integrated Ground Water Modeling

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Abstract

We present in this note an innovative software environment, called Interactive Ground Water (IGW), for unified deterministic and stochastic ground water modeling. Based on efficient computational algorithms, IGW allows simulating three-dimensional (3D) unsteady flow and transport in saturated media subject to systematic and “random” stresses and geological and chemical heterogeneity. Adopting a new computing paradigm, IGW eliminates the fragmentation in the traditional modeling schemes and allows fully utilizing today’s dramatically increased computing power. For many problems, IGW enables real-time modeling, visualization, mapping, and analysis. The software environment functions as a “numerical laboratory” in which an investigator may freely explore the following: creating visually an aquifer system of desired configurations, interactively applying stresses and boundary conditions, and then investigating and visualizing on the fly the geology and flow and transport dynamics. At any time, a researcher can pause to interact dynamically with virtually any aspects of the modeling process and then resume the integrated visual exploration; he or she can initiate, pause, or resume particle tracking, plume modeling, subscale modeling, stochastic modeling, monitoring, and budget analyses. IGW continually provides results that are dynamically processed, overlaid, and displayed. It dynamically merges modeling inputs and outputs into composite two-dimensional/3D images—integrating related data to provide a more complete view of the complex interplay among the geology, hydrology, flow system, and transport. These unique capabilities of real-time modeling, steering, analysis, and mapping expand the utility of models as tools for research, education, and professional investigations.

Introduction

Despite an exponential growth of computational capability over the past decades—one that has allowed computational science and engineering to become a powerful tool for scientific discovery—the cost of ground water modeling continues to limit its use. This occurs, in many cases, not because the problems we are solving today are simply too large, the computers available are too slow, the solvers used in the software are inefficient, the graphical interfaces for individual models are still too difficult to employ, or the utility programs for postprocessing are still not sufficiently sophisticated. This is so often because the way we model is too fragmented to take full advantage of recent developments in computer, communication, graphic, and visualization technologies.

In this note, we present a new computing paradigm and a sophisticated environment for integrated ground water modeling—one that eliminates the fragmentation in the modeling process and allows capitalizing on the rapidly increasing computing power. The new environment, called Interactive Ground Water (IGW), utilizes a powerful “parallel computing” methodology as well as novel computing concepts including computational steering and dynamic visualization. The term “parallel computing” used in this note does not mean modeling on parallel machines but, rather, a new way of structuring computation—one that allows efficient data routing and dynamic integration of flow and transport modeling, data processing, analyses, geographical information system (GIS) mapping, and three-dimensional (3D) visualization.

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IGW Overview

A single object-oriented application program forms the core of IGW. It employs multiple modeling tasks to rapidly integrate complex data in a sophisticated graphical format. IGW permits the modeler to pause program execution and rapidly explore and edit, on-line, any aspect of the modeling process. It permits the modeler to insert submodel regions into a parent model, in order to provide greater detail where it is required, while numerically coupling the two scales of modeling. It permits the modeler to produce on-the-fly sophisticated two-dimensional (2D)/3D displays of spatial, time-varying information. It permits the modeler to steer the modeling process. Modeling under the new paradigm continually displays results that have been intelligently processed and overlaid. It dynamically merges heterogeneous geospatial data into graphical

Figure 1. Real-time hierarchical modeling. IGW allows modeling a complex ground water system hierarchically, converting a large problem into a cascade of smaller problems. The user can zoom incrementally into more details with automatic and dynamic multiscale coupling and on-the-fly integrated visualization.
images—integrating related data to provide a more complete view of complex interrelationships. It provides a quick connection between modeling concepts/assumptions and their significance/implications.

We developed this general-purpose, integrated problem-solving environment for research, educational, and professional pursuits by taking advantage of the recent advances in software component technologies, image processing, 3D visualization, GIS technologies, as well as research in geostatistics, stochastic subsurface hydrology and modeling, hierarchical modeling, and numerical modeling techniques. IGW consists of eight dynamically embedded modeling, analysis, and visualization engines: (1) 3DFLOW for incremental flow modeling; (2) 3DTRANS for incremental transport modeling; (3) MATSOLVE for iterative solution of sparse matrix systems; (4) UNCERT for first-order stochastic flow modeling; (5) GSLIB for variogram modeling and stochastic simulation; (6) OLECTRA CHART for 2D visualization; (7) GIS MAP-OBJECTS for geospatial mapping; and (8) VTK for 3D visualization. A trial version of IGW can be downloaded from http://www.egr.msu.edu/igw.

The New Computing Paradigm

The parallel paradigm allows us to couple the various models and solve them for conditions one time step forward from the current time. This allows us to restructure the computations and modeling tasks into a single application program—one that permits the modeler to visualize the model’s behavior at every time step and evaluate its adequacy, so that we can interrupt the computations, alter the model in significant ways, and restart computations as we deem necessary.

The basic concept is simple. Instead of treating flow and transport separately, we model them concurrently. Instead of treating flow modeling, transport modeling, subscale modeling, particle tracking, and budget analyses as different phases in a sequential process, we couple the multistaged processes and model them simultaneously. Instead of relegating the analysis and presentation of results to “postprocessing,” at the end of a time-consuming sequence of many steps, we incorporate them into a single program along with the simulation, to permit the interpretation of results as soon as they become available, at the end of each time step. To accomplish this, we adopt the following new computing paradigm:
At a discrete time level $t = t_n$ (the $n$th time step)

1. Flow modeling
2. Subscale flow modeling, if subarea(s) of interest is specified
3. Particle tracking, if particles are released
4. Plume modeling, if contaminant(s) is introduced
5. Subscale transport modeling, if subarea(s) of interest is specified and contaminant(s) introduced
6. Data and output processing/analysis, solute/water budget analyses
7. Integrated visualization/presentation
8. $t_{n+1} = t_n +$ time step
9. Repeat steps 1 through 8

Real-Time Modeling

IGW provides an interactive environment for defining the aquifer framework, for inputting parameters, properties and stresses, for changing grid resolution, matrix solvers, numerical schemes, and interpolation methods, for controlling program execution, and for integrating, overlaying, and visualizing data and results.

We have taken advantage of object-oriented programming and designed IGW so that modelers can, at any time, pause to interact with virtually any aspects of the modeling process. At any time, the modeler can initiate, stop, and edit particle tracking, plume modeling, and subscale modeling. At any time, modelers can see the current results presented in a meaningful way, no matter how preliminary the assumptions are. The results displayed on the screen can then be used as starting conditions for continued incremental improvement. An incremental capability proves useful for ground water modeling because of its inherently uncertain nature.

Modeling within IGW becomes a process of high-level conceptualization, as if one is drawing a picture of the site and iteratively improving the representation. It becomes a process of iteratively making sense of the results and solving integrated problems. By pointing and clicking the mouse, the modeler can delineate areas of interest (e.g., the spatial extent of the aquifer and its materials and properties, the spatial coverage of rivers and wetlands, and contamination sources) and quickly visualize the integrated dynamics. The user is always in control throughout the problem-solving process.

Specifically, IGW allows an investigator, during the modeling process, to pause program execution and do any of the following:

- To modify the conceptual model. The modeler can edit boundaries, structures, properties, and stresses. These changes can be imposed over any areas or 3D volumes, independent of the space-time discretizations. Data describing aquifer parameters at scattered locations can be analyzed using advanced regression, interpolation, and geostatistical techniques. The conceptual model can be converted on the fly to integrated numerical models.
- To modify the numerical representation. The modeler can change numerical parameters such as time step and grid spacing, the number of computational layers in a geological layer, the discretization schemes, solution methods, and spatial-interpolation techniques.
- To initiate particle tracking and/or transport modeling. The modeler can interactively release particles at scattered points, along polylines, over polygons, or around wells and track forward/backward their migration. The modeler can also simulate the migration of plumes from many sources, including polluted rivers/lakes, recharge, waste well injections, as well as instantaneous/continuous spills with a time-dependent loading rate.
- To develop hierarchically nested submodels of flow and transport. The modelers can define incrementally a hierarchy of submodel regions within a larger model. Submodels can span one or more geological layers and run in parallel within the parent. They are solved right after the parent solution is obtained for each time step. Initial/boundary conditions for the submodels are extracted dynamically from their parent at every time step. The hierarchical modeling approach reduces a complex problem into a cascade of smaller problems with fewer degrees of freedom (Li et al. 2006). It alleviates the infamous “curse of dimensionality” in 3D modeling, decreases the CPU time, and improves the robustness of the solution process, especially
for strongly heterogeneous/anisotropic systems under “tough” stresses.

Figure 1 presents an example of on-the-fly, integrated hierarchical modeling of a complex ground water system across multiple scales.

- To examine the impact of unmodeled heterogeneity. The modeler can perform a stochastic analysis or Monte Carlo simulation (MCS) to quantify uncertainty caused by subgrid heterogeneity. IGW MCS permits any spatial parameters to be modeled as a random field and temporal stresses as a one-dimensional (1D) stochastic process characterized by any of a variety of statistical models. When MCS is selected, flow and transport simulations are automatically “recomputed” for the various property and/or stress realizations. The most recent realization is used as it becomes available to generate point statistics (e.g., probabilities at monitoring wells) and spatial statistics (means and uncertainty) that are dynamically visualized as the simulation proceeds. Best-available probabilistic characterizations are presented and recursively updated live with each additional realization.

Figure 2 shows an example of real-time, integrated stochastic modeling with on-the-fly recursive probabilistic analyses.

- To present model characteristics and results and customize the presentation. IGW allows (1) dynamic presentation of flexible combinations of data and model inputs/outputs for 1D, 2D, and 3D displays; (2) computing and displaying solute/water fluxes and/or budgets over specified zones or along “compliance surfaces”; (3) computing and displaying heads and concentrations as a function of time at monitoring wells.

Figure 3 presents examples of integrated modeling with live-linked, 3D visualization of aquifer and plume dynamics, as well as the scattered data, geologic framework, and monitoring network.

The IGW Web site (http://www.egr.msu.edu/igw/under Case Studies) presents a real-field application illustrating some of the capabilities and advantages of the new modeling environment. In particular, the Web site describes a 3D flow and transport modeling effort for a contaminated aquifer at the Schoolcraft site in western Michigan. The ultimate goal is to design a broadly applicable “biocurtain,” which will be applied to remediate this site using a periodic recirculation well gallery installed normal to ground water flow. The project takes advantage of IGW’s real-time and hierarchical modeling (Li et al. in press) and visualization capability for iterative conceptualizations, data sufficiency evaluations, hypothesis testing, and remediation design.

Real-Time Steering

Real-time modeling makes the modeler an equal partner with the computer in maneuvering the visual presentations of the modeling results. It allows the investigator to interactively steer the computation, to control the program execution, to guide the evolution of the aquifer dynamics, to control the visual representation of data during processing, and to dynamically modify the computational process during its execution. Such a sophisticated navigation process would be a valuable tool for understanding fundamental processes and for practical investigation.

To maximize the system’s flexibility, we have further designed IGW to allow the modeler to adjust the degree of steering at any time, from extremely fine to coarse. Specifically, IGW is designed such that an investigator can

- Visually step through the “inner iterations” or matrix solution process. This provides an intuitive feel for the convergence rate and solver performance. In many cases, this pinpoints visually the cause of common numerical problems (e.g., slow convergence or divergence caused bybad inputs, singular characteristics, or extreme heterogeneity).
- Visually step through the “outer iterations” or the process of solving the nonlinear equations (e.g., for unconfined aquifers). This is useful for helping a scientist to obtain an intuitive feel for the nonlinear dynamics. This also helps pinpoint visually possible sources of common numerical problems associated with nonlinear iterations (e.g., solution divergence or slow convergence caused by highly nonlinear, locally desaturated dynamics).
- Visually step through the hierarchical modeling process. This provides an intuitive feel for the connection among flow and transport processes at different scales.
- Visually step through time increments. This is the default steering mode. It allows modelers to visualize “instantly” aquifer dynamics in a naturally animated fashion. This also provides flexibility and efficiency in flow and transport simulations and allows cutting adaptively the time step when the simulation becomes difficult (e.g., when a plume moves close to a localized heterogeneity or an area in which sharp changes in the velocity occur) and increasing it when the difficulty passes.
- Visually step through stochastic realizations. This allows modelers to visualize how heterogeneity translates into uncertainty because of data limitation and plausible realizations of flow and plume dynamics. The dynamic recursive analysis significantly decreases the long turnaround time in integrated stochastic modeling. An investigator is able to visualize quickly probabilistic characterizations that are updated with each additional realization.

Summary

We have presented a parallel computing paradigm and a real-time steering environment for integrated ground water modeling. The new paradigm provides seamless data routing and dynamic fusion of flow and transport modeling, visualization, GIS mapping, analyses, and enables one to capitalize on the recent dramatic technological revolution.

With 4-GHz desktops available now, 10-GHz microprocessor technology in the labs and faster than 20-GHz technology clearly in sight, actively visualized aquifer dynamics incorporating live-linked component technologies promises potentially significant scientific and economic benefits. Combined with the hierarchical modeling...
methodologies, IGW allows, for many problems, real-time modeling, visualization, and mapping analysis. The new paradigm eliminates the fragmentation in the modeling process and narrows the gap between what is technologically possible and what is practically implementable. Our actual ability to model, to investigate, and to discover may increase in pace with the rapidly advancing computer technologies. We envision that, with the parallel computing paradigm and possible realization of a 100 to 1000 GHz capability in ~5 to 10 years, modelers may soon be able to investigate in real time 3D flow and transport dynamics and complex interactions with fewer assumptions and in greater details.

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