# Quantification of the Impacts of Subsurface Heterogeneity on Groundwater Cleanup

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***ABSTRACT***

In heterogeneous media, present numerical models are not adequate to assist the decision-maker in choosing among groundwater remediation schemes or estimating project costs, leading to expensive and ineffective remediation attempts. The U.S Army Engineer Waterways Experiment Station is engaged in a multi-scale computational project to vastly improve the Department of Defense's ability to perform engineering-scale simulation of remediation in real-world, heterogeneous soils. Pore-scale modeling is being used to guide the form of engineering-scale equations and parameters. High-resolution, field-scale modeling is employed to quantify the effects of the larger heterogeneities on flow and transport. Each of these model types requires the use of large, parallel computers. However, pore-scale modeling cannot contribute quantitatively to the larger computations without a significant overlapping of scales between each of these types of models. Simulation must proceed continuously from the pore scale to the scale of remedial assessment. These modeling strategies are discussed in this paper. These models will be fielded as part of the ongoing development of the DoD Groundwater Modeling System (GMS). Aspects of the GMS development will also be presented.

## *INTRODUCTION*

The United States (U.S.) Department of Defense (DoD) is responsible for nearly 10,000 sites on active military installations and over 6,200 sites on formerly-used installations that require some level of environmental remediation. Groundwater contamination is a primary concern for approximately 80% of these sites. Remediation of these sites is necessary either for their continued use as training grounds and facilities or to restore sites slated for realignment or closure. Funds used for environmental cleanup (estimated to have total costs of \$45 to \$200 billion with current technologies and risk assessments) are subsequently unavailable for use in training and equipping DoD personnel. Reduction of these environmental cleanup costs requires that informed decisions must be made concerning the selection, design, and operation of remedial measures.

Ongoing research at the U. S. Army Engineer Waterways Experiment Station (WES) in the development of environmental quality modeling and simulation technology is providing DoD with engineering tools with which it can confidently design more cost-

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effective and innovative cleanup technologies. These designs can also be more effectively defended to regulatory agencies, thereby providing for improved acceptance of these (particularly innovative) technologies at DoD cleanup sites. The centerpiece of the research effort is a multi-scale computational project designed to provide an ability to perform engineering-scale simulation of remediation in real-world, heterogeneous soils. This capability will be implemented directly into the DoD Groundwater Modeling System (GMS). Based on success of past GMS applications, we believe implementation of the results of this proposed project within the GMS will result in saving of approximately 10% to 20% of the total expected cost of cleanup within DoD. Such savings would be a minimum of several billion dollars for DoD sites alone. Cleanup savings at U.S. Department of Energy (DOE) and Superfund sites that could result from the use of this research could be an order of magnitude greater. Additionally, completion of this research will result in increased public goodwill (through improved remediation of contaminated military sites) at a reduced life-cycle cost associated with DoD activities.

Candidate remediation schemes must be assessed in naturally heterogeneous soils that exist at all cleanup sites. Heterogeneous soils are composed of non-uniform materials that occur in spatial patterns ranging in size from the scale of an individual soil grain to the size of the hydrologic basin. These heterogeneities compromise the effectiveness of many traditional remediation techniques such as pump-and-treat. Pump-and-treat works well in homogeneous laboratory samples and in numerical simulation of homogeneous media. However, in natural heterogeneous media, the majority of fluid flow is restricted to a limited number of paths through the medium. Contamination in less permeable regions is extracted very slowly, necessitating that remedial operations continue for a protracted time. Thus, the life-spans for pump-and-treat projects have been routinely underestimated, often resulting in large cost overruns, ineffective treatment, or both. Additionally, many proposed innovative cleanup technologies (particularly those in-situ technologies requiring additives or combinations of hydraulic control and bioremediation) will suffer similar problems in heterogeneous media.

Accurate modeling of the effects of multi-scale heterogeneity on the motion and fate of contaminants at the field scale is difficult. Macroscopic, effective flow and transport parameters can capture the effects of heterogeneity for a few idealized situations, but often prove to be inappropriate for the complex environment of real remediation. For modeling more complex conditions, it is necessary to resolve the details of physio-chemical property variation at a more fundamental scale. Additional difficulties are presented because it is impossible to completely quantify the physical structure of the soil. Therefore, any discretization of the site for numerical modeling provides only a possible realization of the actual medium. Thus, uncertainty in the soil structure must be addressed statistically.

The effectiveness of large-scale computing to predict the fate and transport of subsurface contaminants is being stretched in the research discussed herein. First, pore-scale modeling (modeling at the scale of individual soil grains) is being used to design and parameterize effective flow and transport formulations at the engineering scale. These formulations are then used in high-resolution continuum modeling to accurately model realizations of selected sites. Finally, to account for the uncertainty in the realizations, numerous realizations are being simulated and the results analyzed statistically. Each of the three modeling phases requires the accurate solution of numerical problems with millions to billions of mesh points. Calculations of this scope can only be made on scalable parallel processing computers.

## *PROBLEM STATEMENT AND TECHNICAL APPROACH*

The problem being investigated within this research is the development of an accurate methodology for modeling remediation of contaminated groundwater resources in the heterogeneous media common to DoD cleanup sites. This protocol represents use of a hierarchy of subsurface modeling technologies that lead to improved engineering-scale models. These latter models will be implemented in the DoD GMS for application at "real-world" cleanup sites. Three distinct modeling approaches are being employed and integrated:

1. ***Pore-scale models***, to provide improved understanding of fundamental flow and transport processes that control contaminant fate, transport, and remediation.

2. ***High-resolution, discrete medium models***, to demonstrate the macroscopic effects that emerge from small-scale processes. These models are applicable from the pore scale to the engineering scale. Here, they serve as a bridge between pore-scale modeling and engineering-scale modeling by revealing the 'sub-grid-scale' effects of heterogeneity to engineering-scale properties and formulations.

3. ***Engineering-scale modeling***, the decision-support tools needed to compare candidate remediation schemes, develop operational plans, and estimate project costs.

Presently, each of these modeling regimes is used independently (Figure 1). Pore-scale modeling is formulated from fundamental principles and guides the form of engineering-scale formulations, while high-resolution, field-scale modeling quantifies the effects of the larger heterogeneities on flow and transport. Each of these is useful in accurate engineering-scale modeling for remedial design and assessments and each modeling regime requires the use of large, parallel computers. However, the pore-scale modeling will not contribute quantitatively to the larger computations without a significant overlapping of scales between each of the three types of models (Figure 1).

There are three primary issues that make engineering-scale modeling of heterogeneous media difficult:

1. developing engineering-scale formulations that include the effects of 'sub-grid-scale' processes on fluid flow and contaminant transport,

2. deciding on an appropriate level of computational resolution and efficiently distributing the resolution to adequately capture the driving features of a problem without resolving basin-scale domains to the pore scale, and

3. accounting for uncertainty in the spatial distribution of heterogeneities in the medium.

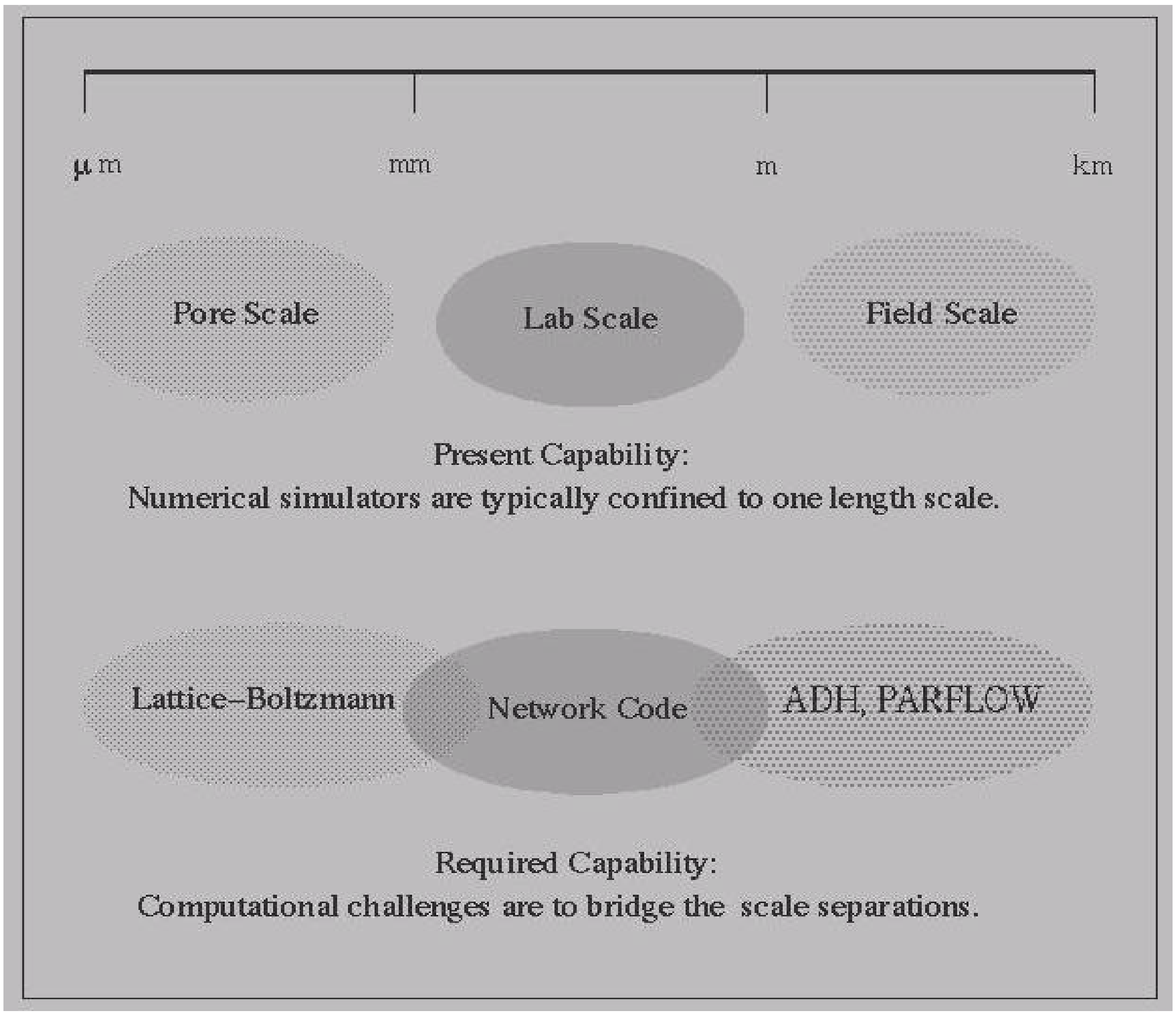


Figure 1. Relationship between Media Scales and Computational Tools

***Modeling at the Pore Scale***

Pore-scale modeling provides the testing, refinement, and parameterization of engineering-scale constitutive relationships that in effect govern the key aspect of subsurface flow and transport. These constitutive relationships are a result of averaging the pore-scale processes to obtain engineering-scale relationships. The quality of the constitutive relationships is a controlling factor in the accuracy of the results obtained by the engineering-scale model. Pore-scale modeling is used to develop these relationships. Due to the tortuous nature of the pore-scale geometry, modeling of these processes is a difficult task which requires meshes with millions to billions of grid points. These simulations require access to a parallel architecture with as much as 60 GB of memory and teraflop peak performance (***NEED TO REFERENCE THIS OR PUT SOMETHING IN HERE FROM MAIER, SUCH AS HIS FIGURE IN THE WEBPAGE, THAT SUPPORTS THIS PERFORMANCE REQUIREMENT)**.

In collaboration with DOE's Los Alamos National Laboratory, lattice-Bolzmann models are being used to simulate pore-scale phenomena. The lattice-Boltzmann method (LBM) uses a form of the discrete Boltzmann equation for particle dynamics which is designed to recover the low-Mach-number limit of the Navier-Stokes equations. Lattice methods for fluid dynamics are adaptable to complex pore-scale geometries without significant mesh generation requirements. The methods and computational scale allow for precise calculation of interfacial area between separate liquid and solid phases and improve our understanding of the effects of geometry on interfacial phenomena governing the flow, transport, and remediation of non-aqueous phase liquids, such as fuels and solvents, common to cleanup sites worldwide.

Progress to date has centered on pore-scale computations made on the CM-5 at the U.S. Army High Performance Computing Research Center (AHPCRC). These computations have explored (1) detailed velocity distributions and grid convergence at the pore scale with comparison to laboratory observations, and (2) pore-scale invasion and retreat of a dense, immiscible contaminant. Unique aspects of these simulations include the use of a single-phase version of the LB code and extremely high spatial resolution to study 3-D flows in random bead packs (which simulate actual heterogeneous porous media in an idealized manner). The calculation of a grid-convergence study of the velocity distribution in a random bead pack was a major accomplishment. (***LET'S REPLACE THE PREVIOUS SENTENCE WITH A WHOLE SECTION THAT DISCUSSES THE ACTUAL RESULTS ACHIEVED, RESULTS, RUN TIMINGS, AND WHY ALL THIS IS IMPORTANT FROM A PRACTICAL SENSE. BOB, NEED YOUR INPUT HERE. COULD BE AS STRAIGHTFORWARD AS PUTTING WORDS TO THE PICTURES YOU PROVIDED THAT ARE ON THE WEBSITE. I HAVE ALL THEM ON THE LAPTOP I'M USING NOW, SO YOU CAN JUST SPECIFY WHAT TO PUT WHERE GRAPHICS-WISE).** A technical challenge overcome was the demonstration of an out-of-core solver allowing the use of over one billion computational nodes in a flow simulation. This simulation required 14-hours on a 512-PE partition of the AHPCRC CM-5 and highlights the resource requirements associated with increased spatial resolution.

Typical simulations required between 6,000-13,000 time steps to calculate pore-scale velocity distributions. It is these velocity distributions that cause dispersion of contaminants (and therefore control contaminant spreading and remediation). Having demonstrated the ability to resolve the fluid velocity field adequately, we have begun the investigation of pore-scale transport phenomena.

Similar pore-scale calculations were conducted to compliment recently-completed centrifuge experiments of immiscible flow. Centrifuge experiments were used to separate the competing effects of gravity and capillarity in displacement of dense, non-aqueous contaminants. This is important in exploring the degree of uniformity in the displacement front and the distribution of residual contaminant. By isolating driving mechanisms, fundamental, pore-scale process descriptions that lead to appropriate engineering-scale parameters can be developed. Further, comparing our numerical models to these experiments improves confidence in our ability to simulate these phenomena while providing a "numerical laboratory" for parameter determination that cannot be obtained from most, if any, laboratory or field measurements. These computations require high resolution at the pore scale and a statistically-meaningful distribution of pore sizes, thereby necessitating millions of lattice sites. Thus far, a time-variable body force has been used to drive displacement in bead packs with 4 to 6 million lattice sites. (*****LET'S PUT A FIGURE IN ON THE CENTRIFUGE, TO GIVE IT A PLUG, AND SOME RESULTS THAT COMPARE EXPERIMENTS TO CALCULATIONS. SAYING THAT THE COMPARISONS GIVE US CONFIDENCE IS CORRECT, SO WE SHOULD SHOW SOME OF THESE COMPARISONS, IF ONLY ONE).**

***Direct Simulation at the Field Scale***

The size of military cleanup sites and the resolution required to resolve the controlling features of these cleanups dictate the use of scaleable high performance computing to adequately model the sites and provide accurate predictions for engineering decisions. If the sites were modeled entirely with a pore-scale model, then there would be no need to parameterize small-scale effects. However, because modeling at this scale is impossible for engineering applications (due to the technical and economic infeasibility of characterizing any subsurface site to the pore scale), one is left to determine how much detail in key subsurface flow and transport processes will be resolved and modeled directly, and how much will be accounted for through the averaging formulations. We are examining this question in order to establish automated procedures allowing the improved engineering-scale models to select the point at which features will no longer need to be further resolved.

To meet this goal, we must be able to use pore-scale process observations in numerical models that are much more coarsely discretized than individual pores. Discrete medium models offer the ability to simulate macroscopic behavior by providing a bridge between fundamental-scale models and engineering-scale continuum models. Examples of discrete medium modeling are highly-resolved continuum models (e.g., the PARFLOW model, developed by DOE's Lawrence Livermore National Laboratory and implemented within the GMS), macroscopic discrete network models, and particle-based transport models.

PARFLOW is a high-resolution model developed by the Lawrence Livermore National Laboratory for simulating flow and transport through heterogeneous porous media. The medium is represented by a continuous, structured finite volume computational grid. Finely-resolved velocity distributions are used to drive particle-based transport. Monte Carlo methods are integrated directly within this model as well. Discrete medium models can provide the velocity distributions necessary to simulate dispersion as an advection and mixing process. These velocity distributions may be used in the engineering-scale models to accommodate "sub-grid-scale" velocity variation that is key to dispersivity.

The Statistical Network Code (SNC), **(***NOTE HERE: WE NEED REFERENCES FOR PARFLOW, SNC, AND WHATEVER CODES COME HEREAFTER THAT ARE MENTIONED IN THIS TEXT)** developed by WES, simulates fluid flow and conservative transport through a macroscopic, discrete network representation of heterogeneous porous media. The dispersion produced by SNC agrees with data from laboratory and field tests. Very recent, unpublished investigations with this model produced relationships to relate network statistics with medium properties. **(***THIS IS WONDERFUL OPPORTUNITY TO PUBLISH THE INVESTIGATIONS, OR COMPONENTS THEREOF, HEREIN. WE HAVE TO GIVE THEM SOMETHING WITH MEAT, NOT OVERVIEW ONLY IN THIS SECTION. WHAT DO WE HAVE, STACY/JOHN?)**.

***Dealing with Uncertainty***

Fundamentally, the previously described modeling assumes that the site is fully characterized and the heterogeneity specified. This is neither practical, nor is it cost effective, for any field site and can really only be done for carefully arranged experiments. Field-scale uncertainty must be taken into account in the model of the site and the accompanying predictions. We account for this uncertainty by computing the solutions for many realizations and analyzing these statistically. A realization is a model of the site that honors the known data at the site. There is, in general, a large (and often infinite) number of these realizations as a result of sparse site information. Statistical analysis of the simulations produces a reasonable estimate of the position and extent of the contaminant as well as an estimate of the reliability of the analysis in light of the lack of more complete information. A hybrid Monte Carlo approach will be enhanced to accommodate observed data at multiple scales. In this approach, each realization is compared against a large-scale measurement (pump test or tracer test). This comparison is used to refine the parameter bounds for the fine-scale statistical properties used in the next realization.

***Models for the Cleanup Specialist***

Even though the direct simulation models operate at length scales well above the pore scale, they require more resolution than is feasible for most engineering analysis. Most engineers lack access to HPC resources required for highly resolved analyses. More important, remediation analyses must concentrate computing resources on simulation of multiple processes and cannot devote massive HPC resources to dispersion. A typical high-end engineering tool is the ADaptive Hydrology (ADH) model, a new WES development, that simulates flow and transport for hydrologic problems at the engineering scale. ADH is a finite element model which uses linear tetrahedral discretizations in space and explicit discontinuous Galerkin discretizations in time. Adaptive gridding is used to resolve dynamic and fine-grid scale phenomena. Galerkin/least squares stabilization terms are added to solve convection dominated problems. The adaptive griding of ADH is designed to optimize performance on engineering work stations such that a relatively moderate-sized simulation can still resolve features such as moving fronts typical of transport and multi-phase flow simulations. On parallel HPC architectures, ADH will allow highly sophisticated multi-process simulations. **(***DEFINITELY A SPOT WHERE WE CAN PUT MORE DETAIL, OR FOR WHICH WE NEED A REALLY GOOD REFERENCE PAPER TO ADD IN FOR THE READER WHO WANTS MORE.)**

***Spanning the Scales***

The key obstacle in applying process knowledge at the field scale that is gained from laboratory experimentation and pore-scale numerical analyses in a field-scale codes such as ADH is the difficulty in scaling information from fine to coarse scales (and vice versa). We have found a potential breakthrough for bridging the model scales for contaminant transport and remediation processes. A particle tracking analysis was endowed with the statistical representation of velocity derived from a highly-resolved discrete network model. The particle tracking procedure is ideally suited for parallel transport calculations in engineering-scale codes. The History-Dependent Dispersive Transport (HD2T) model is a WES-developed particle-based transport code designed to exploit the observation that pressure fields generated by network codes (SNC in this case) were essentially independent of degree of heterogeneity. The implication of this observation is that a pressure solution may not be needed on a highly-resolved heterogeneous medium provided the velocity statistics that drive the dispersive transport can be replicated. In HD2T, the statistical components of the particle tracking velocities are time-correlated such that they replicate those observed in the network code. In an ongoing investigation, the statistical investigation is being extended to PARFLOW to further verify results from the use of SNC. HD2T generates the same dispersive characteristics as SNC, but is driven by a mean flow field that can be driven by an engineering-scale code such as ADH. A code using time-correlated velocity distributions is presently running on the AHPCRC CM-5.

The concept that acts as the basis of HD2T is illustrated in Figure 2 which compares a plume from the SNC network model with about 10,000 connections and 50,000 throats versus an HD2T particle plume generated with a uniform velocity field. The distinctive characteristic of both plumes is the material left behind in the plumes path, a feature absent in homogeneous media. **(***NO MENTION THAT THE MEDIA HERE IS HETEROGENEOUS. ANYTHING ABOUT RUN TIMES ON THE CM-5 FOR THESE RESULTS?)**

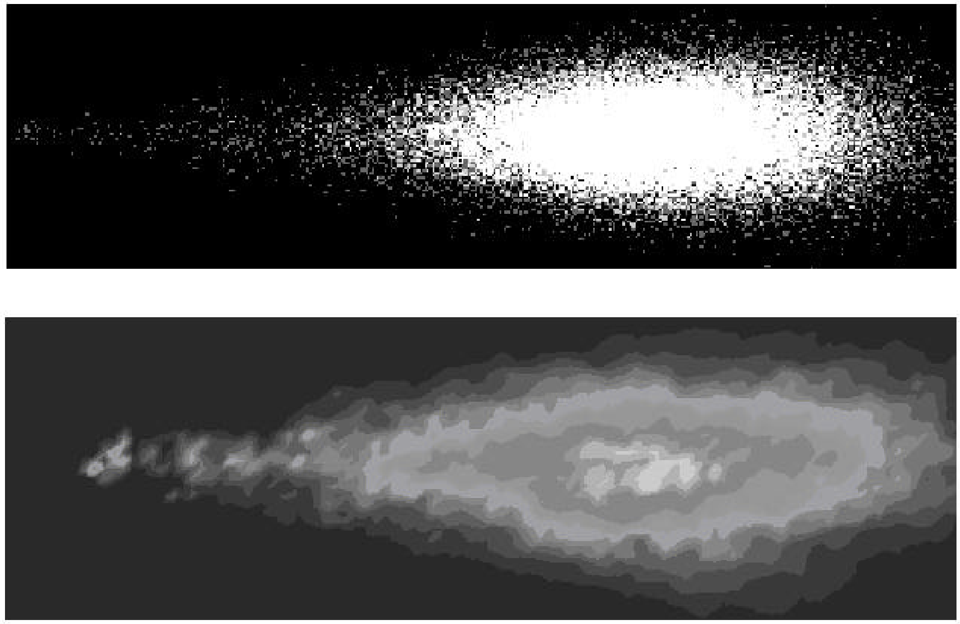

Figure 2. Particle distribution simulated by HD2T (top) and SNC concentration contours (bottom)

Application of this technology will require a concerted effort using computational models at varying scales. The LB model provides the velocity statistics for the small-scale components (spatial and temporal) in the PARFLOW and SNC simulations. For these statistics to be meaningful, the pore sizes modeled must be comparable to an actual porous media (microns to centimeters), while the domain size is on the order of a laboratory specimen (tens of cubic centimeters at a minimum). Both PARFLOW and SNC simulations must span the scales between laboratory scale and field scale (hundreds of meters to kilometers). The particle tracking code HD2T provides the means to extend the transport computations to ADH, the engineering-scale code. Therefore, HD2T must replicate the results of PARFLOW and SNC. Providing HD2T with the statistical properties derived from PARFLOW and SNC will allow HD2T to be implemented directly into ADH. This will, in turn, produce a continuum-based engineering code that replicates the same dispersion as the detailed heterogeneous media. This implementation is ongoing at the time of this printing. (*****THERE IS NOTHING HEREIN PER SE ABOUT THE THEORETICAL FORMULATION OF THE GOVERNING EQUATIONS THAT LED TO CONVOLUTION INTEGRALS, RECOGNITION OF ITS KERNEL AS A NETWORK, ETC. DO YOU, JOHN/STACY WANT TO PUT ANYOF THIS IN THE DOCUMENT?)**

### *TAKING HIGHLY-RESOLVED RESEARCH TO APPLICATION*

The research presented above will be viewed a failure unless the results of said research are implemented in actual field-scale cleanups. Our mechanism for fielding these results is to codify them in the DoD Groundwater Modeling System (GMS). WES leads a consortium of U.S. Army, Air Force, DOE, Environmental Protection Agency (EPA), and academic researchers in the development of the GMS. The GMS is an aid for site characterization, for assessing the risk of contaminant exposure to ecological and human populations, and for evaluation of the efficacy of remedial and wellhead protection actions associated with contaminated groundwater resources at DoD installations and other federal sites. The system is modular and operates across a variety of computing platforms. Version 2.0 of the GMS provides full connectivity to five subsurface flow and transport models, visualization, animation, geographic information systems, and parameter estimation under a single consistent user environment. A number of research initiatives related to characterization of the impacts of subsurface heterogeneities on remedial effectiveness, mathematical description of flow and transport processes for military-unique contaminants, optimization of remedial alternatives, and computational efficiency on multiple computing platforms, are ongoing that are producing new modeling tools. These new system components will continue to be implemented in the GMS through 2000. Major program products and milestones are presented in Table 1.

***GMS Development Partners***

The GMS is being developed through a technical partnerships between multiple agencies. These partnering agencies include: DOE's Lawrence Livermore National Lab (LLNL), Argonne National Lab (ANL), Pacific Northwest National Lab (PNNL), and Los Alamos National Lab (LANL); Air Force Armstrong Lab/EQ (AL/EQ); Air Force Office of Scientific Research (AFOSR); Army Research Office (ARO); Army Corps of Engineers Headquarters, Military Programs Directorate; Army Cold Regions Research and Engineering Lab (CRREL); Army High Performance Computing Research Center (AHPCRC); Army Environmental Center (AEC); EPA's Athens Environmental Research Lab (AERL; now a part of the National Exposure Research Lab), and R.S. Kerr Enviromental Research Lab (RSKERL; now part of the National Risk Management Research Lab); and, Cray Research-SGI. There are also over 20 academic research partners. In addition, collaboration is maintained with the U.S. Geological Survey, the Air Force Center for Environmental Excellence, and the Naval Facilities Engineering Service Center, and with the Swedish National Defense Establishment and Swedish Geological Survey. This partnering and collaboration includes technology exchanges, joint conduct/funding of research investigations, and (in several cases) nearly weekly technical contact, particularly for new model implementation into the GMS.

***GMS Status***

The GMS provides direct support to site characterization, contaminant assessment, and remedial alternative evaluation/design. The GMS technology is a dual-use development of value to both the military and civilian site cleanups. In addition to hazardous and toxic wastes cleanups, use of the GMS for several classes of civil and environmental engineering problems, including salinity intrusion, domestic use well placement and protection, design of contained dredged disposal facilities, and levee seepage, points to its ever-expanding application.

GMS v2.1 is currently being applied by over 500 DoD, DOE, and EPA users. The system is also in use through technical partnerships with the State of North Carolina, the South Florida Water Management District, and over 15 universities. Over 800 copies of the system have been sold through commercial vendors. These groups are using the system for civilian, military, and industrial cleanup design and operation activities on an international basis.

| No. | Product | Year |
|---|---|---|
| 1 | Documentation of DoD subsurface modeling requirements | FY94 |
| 2 | Initial visualization and user environment | FY94 |
| 3 | Guidance on use of existing multi-dimensional models | FY95 |
| 4 | Implementation of GMS v 1.0 with three existing models | FY95 |
| 5 | Couple GIS, DoD EQ databases w/GMS | FY95-96 |
| 6 | Add PARFLOW, NUFT3D and ADH models to the GMS | FY96-98 |
| 7 | Initial pump and treat optimization capabilities to GMS | FY96-97 |
| 8 | Add physical and hydraulic containment modules to GMS | FY96-97 |
| 9 | Subsurface conceptualization tools with uncertainty | FY96-98 |
| 10 | Add pulsed pump and treat modules to GMS | FY97 |
| 11 | Improved multiphase and cold regions algorithms in GMS | FY97-98 |
| 12 | Implementation of GMS v 2.0 w/Map Module | FY96-97 |
| 13 | Steam injection / vapor extraction modules into the GMS | FY97-98 |
| 14 | Initial soil heating modules integrated into GMS | FY97 |
| 15 | Add natural attenuation modules to GMS | FY97-99 |
| 16 | Initial in-situ bioremediation design modules in GMS | FY97-99 |
| 17 | Surface water - groundwater interaction modules in GMS | FY98 |
| 18 | Addition of bioventing and air sparging routines to GMS | FY98-99 |
| 19 | Addition of electrokinetics modules to GMS | FY99 |
| 20 | Add metals bioremediation design modules to GMS v3.0 | FY99 |
| 21 | Facilitated transport and fracture flow capabilities in GMS | FY00 |
| 22 | Demonstration of GMS components for specific sites | FY95-00 |
| 23 | Training in use of GMS products | Ongoing |

Table 1. Listing of Major Program Milestones and Products

The GMS is designed for directly analogous execution on both personal computers running Windows (3.1, 95, and NT), and for Unix workstations running X-Windows. Version 2.0 of the system supports multiple analysis tools (the reader is directed to the GMS website at http://hlnet.wes.army.mil/ for module-by-module information on the GMS's components). There are currently six flow and transport models within the system: MODFLOW, MT3D, FEMWATER, MODPATH, LEWASTE, and SEEP2D.

Several additional codes (UTCHEM, NUFT3D, PARFLOW, ADH, RT3D) are being added to the system presently, along with enhanced versions of FEMWATER and MT3D.

A key feature to the GMS is its ability to greatly enhance productivity throughout the modeling process. Resource requirements for site characterization and conceptualization, subsurface stratigraphic realization, and initial and boundary condition designation have been reduced by an order of magnitude or more through the use of the system. Much of this productivity enhancement is the result of the development of a new conceptual approach to modeling as discussed below.

***Conceptual Model Approach***

With the current state of the art in groundwater modeling, simulations are typically performed according to the following steps:

1. Develop conceptual model
2. Create numerical grid
3. Assign model parameters and boundary conditions to grid
4. Calibrate model
5. Make predictions

The first step, the development of a conceptual model, is often the most important step in the modeling process. A conceptual model is a simplified representation of the site to be modeled. As a conceptual model is developed, the modeler must make numerous assumptions and simplifications to obtain a workable model. Highly heterogeneous regions are often divided into discrete zones representing areas with similar physical properties. Average or representative property values such as hydraulic conductivity or porosity must be determined. Many physical features at the site are deemed insignificant while others are carefully measured and included in the model. Throughout this process, the modeler attempts to achieve parsimony: a balance between eliminating enough detail to make the model workable while retaining enough detail to make the model accurate and useful. If the conceptual model is not developed properly, steps 2 and 3 result in wasted effort since it will be impossible to calibrate the model in step 4. In many cases, the user must develop several conceptual models before proper calibration is achieved. This is particularly true in groundwater modeling where appropriate boundary conditions and stratigraphic representations are often difficult to determine.

Most groundwater modeling pre-processing software is designed to automate and enhance the work involved in steps 2 - 5. The conceptual model is developed independently of the modeling software. A new approach to model development has been incorporated into GMS which not only includes the conceptual model as part of the computer-assisted modeling process, but features the conceptual model as the primary focus of model generation and the data entry process. Rather than focusing the model generation and data entry on a numerical grid or mesh, the user creates a conceptual model on the computer and assigns boundary conditions and model properties to the conceptual model. The conceptual model is defined in a general purpose fashion that is independent of grid type (finite element, finite difference, etc.) and to some degree, independent of the analysis code to be used. Once the conceptual model is defined at this higher level, the numerical model is automatically generated from the conceptual model. The grid or mesh is constructed in a manner that fits or adapts the grid to the conceptual model and the boundary conditions and material properties are extracted and assigned to the appropriate cells or elements.

***Map Module***

In order to facilitate the new conceptual model approach to model design, a new module called the "Map Module" has been added to GMS. Four types of objects are supported in the Map Module: DXF objects, image objects, drawing objects, and feature objects. The first three objects: DXF objects, image objects, and drawing objects are primarily used as graphical tools to enhance the development and presentation of the conceptual model. DXF objects consist of drawings imported from standard CAD packages such as AutoCAD or MicroStation. Externally produced site drawings can often provide a useful backdrop or supplement to the graphical desktop during model construction. Drawing objects are essentially a simple set of tools that allow the user to draw text, lines, polylines, arrows, rectangles, etc., to add annotation to the graphical representation of a model. Image objects are digital images representing aerial photos or scanned maps in the form of TIFF files. TIFF files can be imported and registered to real world coordinates. Construction of the conceptual model can then be accomplished using a high resolution image in the background of the graphical desktop.

The fourth type of object, feature objects, is used to construct the actual conceptual model. Feature objects are patterned after the data model used by geographic information systems (GIS) such as ARC/INFO. The GIS data model utilizes points, arcs (polylines), and polygons to represent spatial information. For example, points represent data such as wells or point sources for contaminants, arcs represent rivers or model boundaries, and polygons represent areal data such as lakes or zones defining different recharge zones or hydraulic conductivities. Sets of points, arcs, and polygons can be grouped into layers or coverages. A set of coverages provides a complete description of the conceptual model. Since a GIS approach is used, the conceptual model can be exported to or imported from a GIS. However, the GIS is not necessary since the entire model can be constructed within GMS.

***Sample Application of Map Module***

A sample application of the new conceptual model approach to model development in GMS is shown in Figures 3 - 6. A TIFF image used to guide the construction of the model is shown in Figure 3. This image represents a portion of a USGS quad sheet that was scanned using a standard desktop scanner. Upon import to GMS, three points on the image are identified by the user and the real world coordinates of the points are used to register or map the image from image coordinates to model coordinates.

With a map of the site in the background, the next step is to construct the conceptual model using feature objects (Figure 4). The model consists of points, arcs, and polygons. Once the geometry of the objects is entered, attributes are assigned to the objects. For the case shown, the outer boundary of the model is represented by a combination of no flow boundaries and specified head boundaries. For the specified head boundaries, the head is assigned to the end points of the arcs (the nodes) and is assumed to vary linearly along the arc. The boundary arcs define a polygon representing the region to be modeled. Arcs were also used to represent several drains in the interior of the model. The drain elevations are assigned to the nodes of the arc and the conductance is assigned to the arc (the segments). Three wells with user-specified pumping rates are defined using points.

The rectangle shown with dashed lines (Figure 4) is called a grid frame. It is placed graphically by the user to surround the conceptual model and it represents the boundary of the computational grid that will be defined. The text and arrows in the figure were added using the drawing tools in the Map Module.

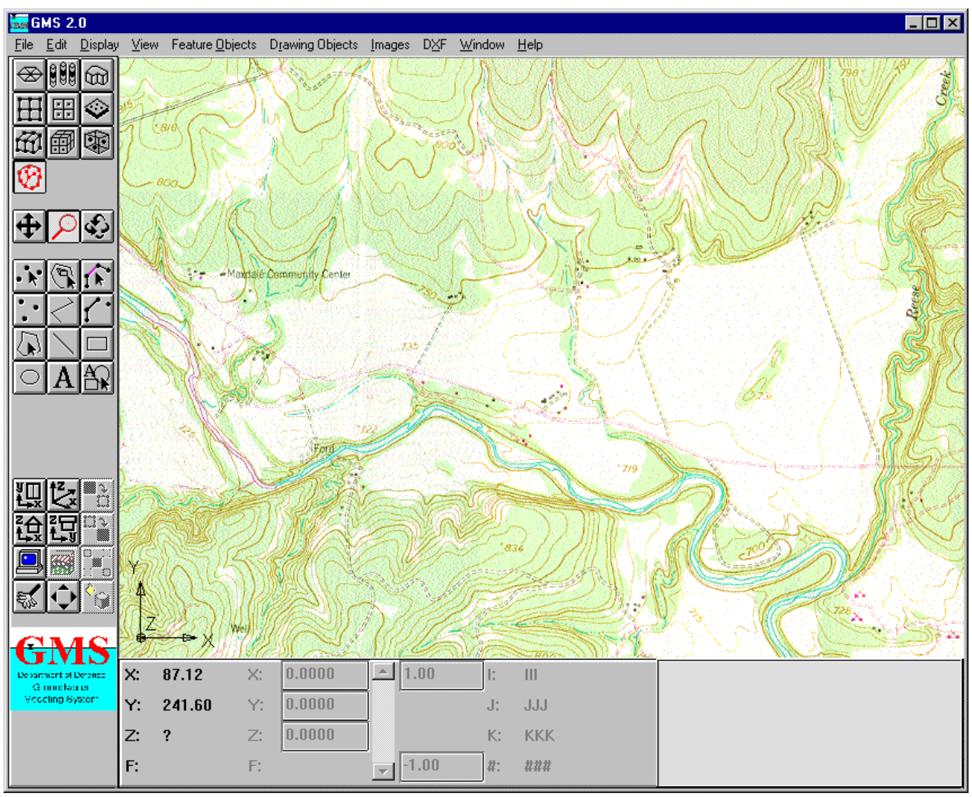


Figure 3. Desktop of the GMS with a Scanned USGS Quad Sheet Used as a Background for Developing a Conceptual Model.

Once the conceptual model is defined, the next step is to convert the conceptual model to a numerical model. Using the grid frame, the feature objects, and some cell size and refinement parameters defined at the wells, GMS automatically constructs a grid adapted to the conceptual model (Figure 5). The grid is refined around the wells and the cells outside the model boundary are inactivated. Each of the feature objects is then superimposed on the grid and the appropriate parameters are set up in MODFLOW to activate the specified head cells, the drain cells, wells, etc. Conductances for linear objects such as drains and rivers are automatically computed by GMS according to the length of the arc segments within each of the cells. At this point, the model is completely defined and no cell editing is required. If the user decides to change the conceptual model (move a boundary, add some wells, etc.) the changes can be made to the feature objects and the numerical model can be regenerated in seconds.

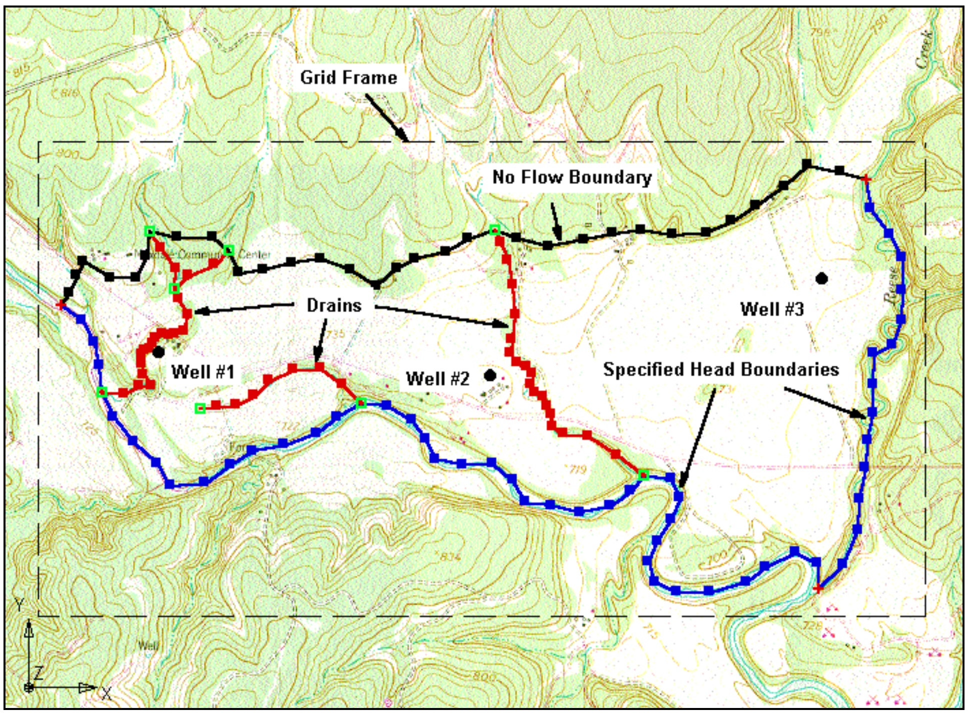


Figure 4. Conceptual Representation of a Groundwater Model Developed with GIS Objects.

The conceptual model approach can be utilized for finite element models as well. Once the conceptual model is generated, the feature objects can be used to drive an automatic mesh generator included in GMS. The resulting mesh is refined around the wells and honors all interior and exterior boundaries defined by the conceptual model (Figure 6).

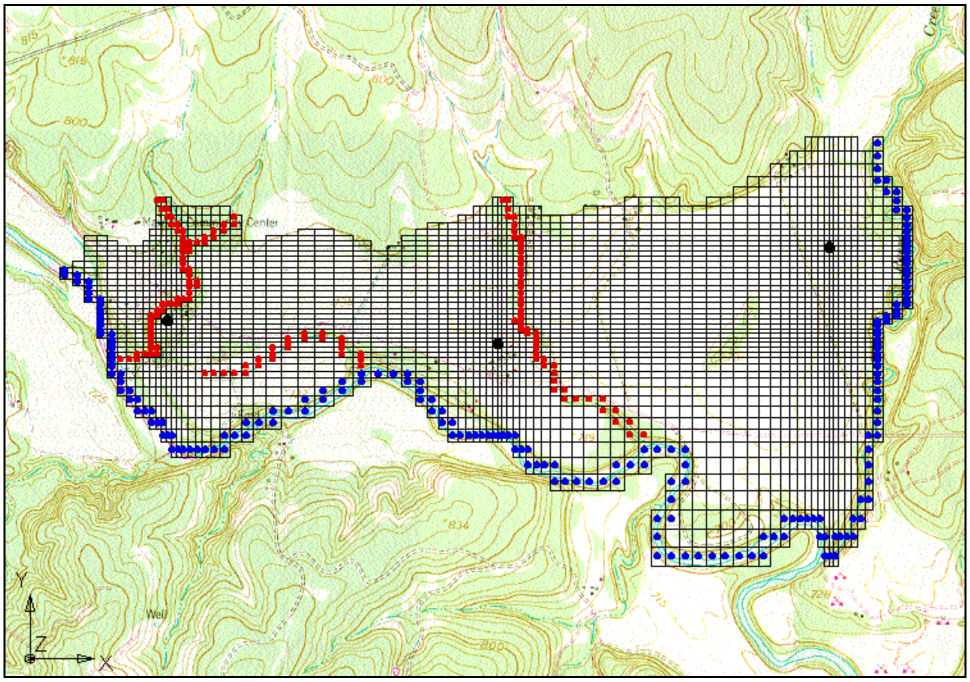

Figure 5. A MODFLOW Finite Difference Model Automatically Constructed from the Conceptual Model.

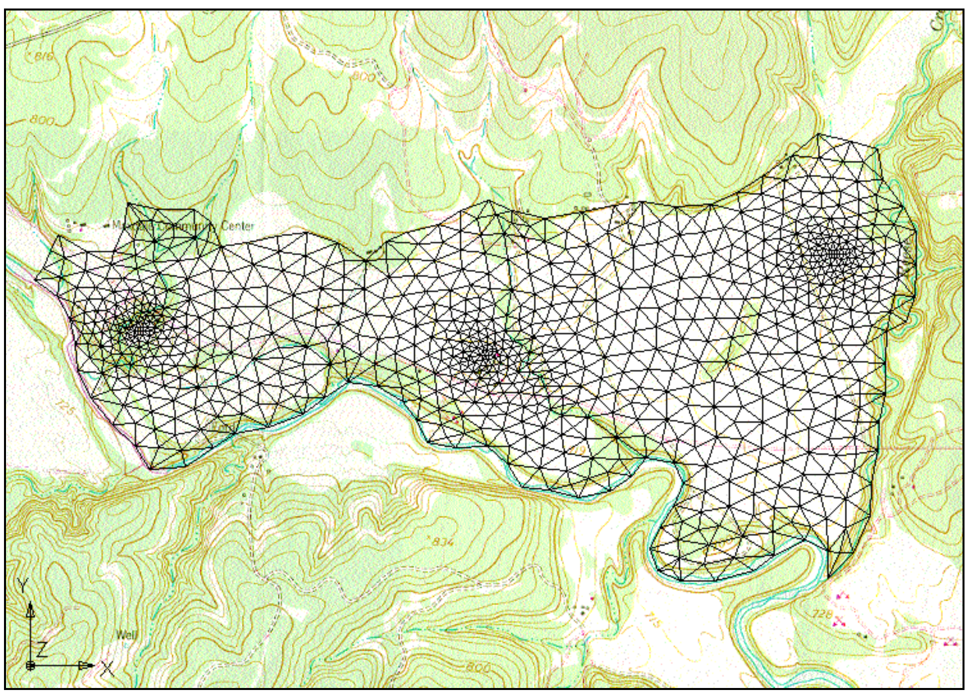

Figure 6. A Finite Element Mesh Automatically Constructed from the Conceptual Model.

In addition to the capabilities listed above, the GMS has state-of-the-art visualization, conceptualization, and parameterization capabilities on-board. Key components of these productivity-enhancing tools include GIS/CADD links, connectivity to several field data collection systems, structured and unstructured grid generators, a full geostatistical library, and AVI video file animation. Details of these capabilities are provided at the website listed above. The desktop of the GMS with a single frame of a contaminant plume conceptualization is provided in Figure 7.

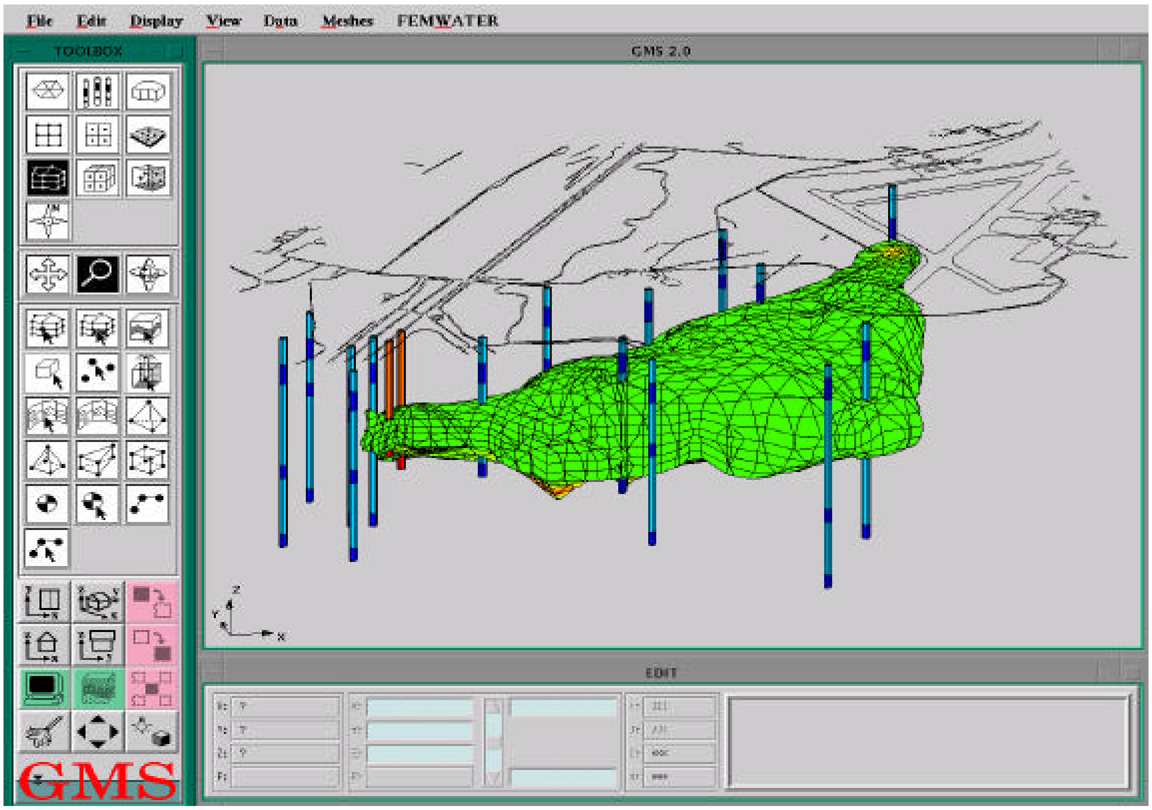


Figure 7. Desktop of the GMS with a Contaminant Plume Visualized, along with observation and recovery wells. Overlain are site surface features.

Many of the hydroenvironmental challenges facing DoD and the international community will require computational sophistication orders of magnitude beyond the current state of practice. As such, these problems will tax the full capabilities of high performance computing (HPC) resources. DoD, through its HPC Modernization Program, is leading in the effort to place the best of vector and scalable parallel computing resources in the hands of its researchers in their pursuit of DoD research concerns. One of the major efforts under the aforementioned program, the Common High Performance Computing Software Support Initiative (CHSSI), is providing DoD researchers with the opportunity to greatly enhance the productivity and efficiency (and, as such, the range of applicability and rigor) of current major software applications software on scalable parallel architectures. One of the major projects being conducted under the CHSSI program involves parallelization of the computational components of the GMS. This project was initiated in 1996 and is to be completed over the next three to four years. The products from this initiative are expected to support most of DoD's computing needs in the subsurface environmental quality modeling area. The importance of CHSSI is that it provides the focus and opportunity for vast increases in applications software execution efficiencies on near-term and future DoD computing architectures beyond those previously anticipated. Such increases will empower DoD to implement the highly-resolved, integrated subsurface models being developed by the research discussed in this paper in a comprehensive, productivity-enhancing computational framework like the GMS.

## *RESEARCH CHALLENGES TO MEET TOMORROW'S NEEDS*

Environmental quality challenges of the next decade will demand the development of integrated environmental quality modeling and simulation (EQM) systems capable of simulating surface and subsurface conditions, and the interactions there between, in a holistic framework. To this end, the following EQM activities will be the focus of WES developments over the next three to five years:

?? key basic science investigations and numerical formulations of processes associated with military-unique impacts upon the ecosystem (e.g., explosives contamination/cleanup, training impacts on the landscape, etc.).

?? coupling of surface water and groundwater modeling tools, both dynamically and passively, in two and three dimensions in support of the cleanup and conservation of natural resources (land, water, groundwater, etc.). This coupling will require development of methods for numerically handling differing time and spatial scales associated with surface water hydrodynamics, watershed runoff and erosion, infiltration, and subsurface flow and transport.

?? incorporation of uncertainty and risk into all environmental quality modeling systems to support risk-based design and environmental assessments.

?

?? coupling of three-dimensional surface water and subsurface flow and transport modeling tools with remediation alternative simulators and highly-sophisticated hydrogeochemical speciation models.

?

?? linkage of modeling and simulation tools with decision support and resource management tools to facilitate the use of modeling results by resource managers and decision makers.

?

?? linkage of hydrodynamic and hydrologic modeling tools with biological response and ecosystem modeling methodologies to augment ecosystem management strategy evaluation.

?

While not all of these items have started development, several are well into development by WES and its technical partners.

There are a number of drivers that factor into the developments envisioned above.

Both long-term and short-term periods must be simulated in environmental quality management. Hundred of thousands, or even millions, of nodes may be required for certain integrated environmental quality analyses. The simulated components, such as surface water and groundwater (or even flow and transport in a given subregion), will be modeled in a coupled fashion (rather than the generally uncoupled fashion of today). Uncertainty, associated with field-scale data collection, numerical algorithm prediction, and/or a lack of process understanding, must become an everyday component of environmental quality analysis. Visualization will be required as a real-time analysis tool rather than simply as a post-processor. High performance computing resources will be required for many of these problems, but these resources must be made transparent to DoD users (e.g., problems requiring supercomputing must be as easy to model and simulate as those on a workstation) in order to facilitate their most effective use in environmental quality management.

Given the nature of the studies envisioned over the next five years, new computational systems (their look and feel, functionality, outputs) must reach and appeal to multi-disciplinary teams and decision makers. These teams will require access to multiple conceptualization, parameterization, simulation, optimization, and visualization tools from consistent, efficient user environment. Future computational systems must stress portability (across multiple computing platforms), modularity (to allow frequent updates), connectivity (to tools within and external to the given system), and consistency (to facilitate user comprehension). Personal computer, UNIX workstation, and vector and scalable parallel supercomputing environments will all require system support. The CHSSI investigations listed above are an excellent jump-start toward meeting these goals.

## *SUMMARY*

The U.S. Department of Defense is continuing research and development whose primary goal is development of a comprehensive groundwater modeling system for use in the accurate assessment of cleanup strategies for contaminated groundwater resources at military installations. A key feature of this research and development is the investigation and development of numerical subsurface models that properly bridge the range of scales that are key to accurate modeling of flow, transport, and remediation in heterogeneous porous media. The multi-year research effort strongly leverages ongoing and near-future research through partnering with several federal agencies and universities. The integrating product from this research, the Groundwater Modeling System, represents a standardized methodology for the application and analysis of subsurface flow and transport modeling in support of site characterization, risk assessment, and remedial design. Substantial improvements in the effectiveness and defensibility of remedial actions are expected through implementation of this system, thereby resulting in significant savings in remediation costs.

## *ACKNOWLEDGEMENT*

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