Workshop on Simulation and Optimization
April 28-30, 2003

ABSTRACTS

Steven F. Carle, Roger Aines, Bill Hanley, Robin Newmark, John Nitao, and Abe Ramirez
Geoscience and Environmental Technologies
Lawrence Livermore National Laboratory

TITLE: "Environmental Applications of the Stochastic Engine"

The Stochastic Engine (SE) is a flexible computational tool for inversion or optimization of large non-linear or underdetermined problems with non-unique solutions. Such difficult problems are common to environmental applications. The SE uses Bayesian inferencing to incorporate prior information into a Metropolis-type search algorithm that efficiently samples a multi-dimensional solution space. For imaging problems in environmental applications, the SE approach enables: (1) incorporation of hard or soft data as prior information, (2) estimation of probability distributions for lithology types at a grid of locations, and (3) preservation of geologic realism in multiple solutions consistent with data. The SE offers flexibility because forward calculations are used to drive the solution search algorithm, and different forward models can be plugged into the SE. The SE uses a staged approach, whereby the SE is run successively using forward models of increasing complexity and! computational intensity (e.g, lithology>flow>transport). The staged approach enables consideration of multiple processes in determination of the solution space, while weeding out unlikely solutions using less computationally intensive forward models at early stages. Environmental applications of the SE thus far have focused on determination of the spatial distribution of lithology types given prior geologic knowledge, electrical resistance tomography data, geophysical logs, and flow measurements. The code "TSIM" is used for the initial lithology generation stage to generate geologically plausible realizations. TSIM has been modified to control stepsize in the Metropolis search by controlling how similar a new realization is to a previous lithologic configuration. In these environmental applications, the SE finds lithologic configurations that are consistent with prior geologic knowledge and available direct and indirect data on lithology.

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Clint Dawson
Department of Aerospace Engineering and Engineering Mechanics
University of Texas at Austin

TITLE: "Discontinuous Galerkin Methods for Convection-Diffusion Problems"

Discontinuous Galerkin (DG) methods have attracted much interest recently as a means for solving a variety of problems, most notably, elliptic flow problems and convection-diffusion systems. These methods have become popular because of their ability to use very general, even nonconforming meshes, general approximating spaces, adaptive grids, and because they satisfy local mass conservation. Several variants of the DG method have been proposed. In this talk, we will focus on DG methods for convection-diffusion problems. Methods based on both primal and mixed formulations will be discussed, and numerical results for geoscience applications, including contaminant transport and shallow water equations, will be given. Issues related to local and global mass conservation, and why it is important, will also be discussed.

John Dennis
Mark Abramson, USAFIT,
Charles Audet, Gilles Coutour, Ecole Polytechnic Montreal
Andrew Booker, Evin Cramer, Paul Frank, Boeing Phantom Works
Department of Computational and Applied Mathematics
Rice University

TITLE: "Constrained Optimization of Expensive Functions Using Surrogates"

ABSTRACT:
Many engineering design problems are governed by coupled systems of partial differential equations, table lookups, and who knows what. It is common in these problems for the governing simulations to return no value for a high proportion of feasible points. This talk is a hurried introduction to the filtered direct search method incorporated into the current Boeing Design Explorer release and the public domain NOMAD code. This talk goes quickly over the algorithmic and theoretical details to save time for supporting numerical results. Technical reports giving the omitted details are available from www.caam.rice.edu and www.crpc.rice.edu.

Darinka Dentcheva
Department of Mathematical Sciences
Stevens Institute of Technology, New Jersey

TITLE: "Stochastic Programming Approach to Uncertainty and Risk"

ABSTRACT:
Stochastic programming provides a methodology for optimization in the presence of uncertainty and risk. We shall discuss some basic modeling approaches and formulate the most popular models in stochastic programming. Two-stage and multi-stage models, as well as problems involving probability functions will be presented. Brief overview of their main structural properties will be given. Fundamental ideas of numerical methods for solving stochastic optimization problems will be presented. We shall discuss also how limited information about probability distributions can be used in optimization models. At the end of the talk we shall suggest approaches to modeling risk. Several examples will illustrate the concepts and ideas.

William G. Gray, Cass T. Miller, UNC
Department of Civil Engineering and Geological Sciences
University of Notre Dame

TITLE: "On the Governing Equations of Flow in Porous Media"

ABSTRACT:
In the subsurface environment, the presence of a solid phase provides a tortuous network through which a fluid must flow. This network imposes challenges on efforts to model the flow that are different from those encountered in modeling surface or atmospheric processes. If models are to be successful in accounting for heterogeneities, simulating flow of multiple fluid phases, and providing information on contaminant transport, they must be built on sound theoretical principles as well as effective and efficient numerical techniques. The purpose of this presentation is to indicate some of the shortcomings of the theoretical foundation. In particular, it is noted that a hunt for appropriate parameters to complete a model is unsatisfactory if those parameters merely support governing equations that do not properly account for the physical processes of importance. The suggestion is made that improvement is needed in the forms of the governing equations as well as the coefficients in those equations.

Stacy Howington, Charlie Berger, Jennifer Tate, Jackie Hallberg, Alex Carrillo[1], Joe Schmidt[2], Lea Jenkins[3], Katie Kavanagh, Tim Kelley[4], Bob Maier[5], Jeff Hensley[6]
US Engineer Research and Development Center
Waterways Experiment Station

TITLE: "The Department of Defense's ADaptive Hydraulics/Hydrology Model (ADH)"

ABSTRACT:
The Department of Defense is responsible for cleaning up groundwater contamination at present and formerly-used defense sites. Common contaminants include solvents, metals, and explosives. The DoD relies on numerical modeling to help assess the extent of contamination, identify the source of contamination, estimate the future threat, and design remedial measures. Computational domains often are large to include known boundary conditions. However, fine resolution is needed to describe geologic variability, to capture flow fields in the vicinity of wells, drains, trenches, or where groundwater and surface water interact, and to resolve contaminant plumes. The resulting computational meshes typically range from 500,000 to millions of elements. The DoD's Corps of Engineers also has responsibilities in surface water for maintaining navigation, flood control, and environmental quality. These require the use of numerical models to simulate hydrodynamics and sediment and constituent transport.

A new model is nearing completion in response to several needs not met by present simulation tools. Among these needs are dynamic mesh refinement and coarsening, efficient distributed computing, and multi-physics coupling. The ADH (ADaptive Hydraulics/Hydrology) model is a multi-dimensional, continuous finite element code that simulates partially saturated groundwater flow, shallow overland flow using either diffusive wave or full St. Venant equations, hydrostatic or non-hydrostatic Navier-Stokes equations, and constituent and non-cohesive sediment transport. The model is written in the C programming language and permits only simplex elements (tetrahedra, triangles, and lines). The computational mesh adapts during the simulation in response to error indicators. As the mesh adapts, the computational load is redistributed among processors.

A central idea in the development of this code is reuse of investment in parallelism, adaption, solvers, and preconditioners. Thus, the computational engine forms the center of the code to which many equation sets are 'strapped'. At present, the model is being extended to permit coupling among different flow physics and to include a multiple-continuum transport scheme and more efficient methods for simulating flow over initially dry ground. For the future, we want to make use of available computational power to automate model calibration and sensitivity analysis and to optimize remedial design in uncertain geology.

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[6]University of Texas at Austin, stationed at Vicksburg, MS

Lea Jenkins
Department of Mathematical Sciences
Clemson University

TITLE: “Non-Newtonian Fluid Flow Through an Extrusion Filter”

ABSTRACT:
In this talk, we discuss the flow of a non-Newtonian fluid through an extrusion filter. The problem is important in the fiber industry, where companies are interested in extending filter lives. Debris is deposited as the fluid moves through the filter, which changes the flow velocities. Darcy's equation, modified by a power law, is used to model the fluid velocity. We discuss previous three-dimensional models for the filter medium, and we also discuss our efforts to model the medium using partial differential equations. We present our method of handling the nonlinearities, and our finite element formulation.

Kathleen Kavanagh
Department of Mathematics
North Carolina State University

TITLE: “Optimal Design for Groundwater Flow and Remediation Problems”

ABSTRACT:
Recently a set of optimization problems was proposed in the environmental engineering literature for benchmarking purposes. We present a subset of these problems, describe some implementation approaches, and provide numerical results for a well-field design problem and a hydraulic capture problem. Both of these applications lead to objective functions that are nonsmooth and have local minima, hence making them challenging problems for traditional, gradient based optmization techniques.

C. T. Kelley
Department of Mathematics
North Carolina State University

TITLE: “Implicit Filtering”

ABSTRACT:
Implicit filtering is a sampling method that uses difference gradients in a projected BFGS iterations. The size of the difference increment is reduced as the optimization progresses. In this talk we will discuss implementation decisions, similar decisions that must be made in all sampling methods, and the theoretical support for those decisions.

Alex Mayer, Tim Kelley, and Casey Miller
Department of Geological and Mining Engineering and Sciences
Michigan Technological University

TITLE: "Optimization of Engineering Design of Subsurface Environmental Remediation Systems- Development and Testing of Community Benchmark Problems"

ABSTRACT:
The U.S. EPA has estimated that remediation of contaminated soil and groundwater will cost on the order of tens of billions of dollars. Application of optimization has the potential to provide more efficient engineering solutions for remediation systems. Much work has been accomplished in the area of optimization of subsurface remediation systems in the last two decades. A wide range of optimization techniques- from traditional, gradient-based techniques to evolutionary algorithms- have been applied. However, one of the roadblocks to further success in the field is that there is little uniformity in the composition of the problems that are used by researchers when testing their optimization technique of choice. The consequence is that it is difficult to compare the results of different studies, and ultimately, to recommend the best optimization techniques to be used for a given type of problem.

In an attempt to overcome this difficulty, we have designed a set of systematic test problems to be attacked by the engineering and mathematics community, as a means for benchmarking and comparing optimization approaches. The test problems pose many of the difficulties anticipated in solving real-world problems such as (a) mixed continuous and integer, nonlinear objective functions, (b) the combination of boundary conditions and system parameters gives rise to complex relationships between the objective function, the decision variables, the constraints, and the state variables, (c) evaluation of the objective function is based on solving model equations that are difficult to solve accurately and quickly; and (d) the number and range of decision variables is potentially enormous. Furthermore, the problem specifications have been designed to encourage, not restrict, innovation in optimal design and subsurface science. This talk will describe the design and execution of the test problems.

Dennis McLaughlin
Department of Civil and Environmental Engineering
Massachusetts Institute of Technology

TITLE: "New Models for New Times: Remote Sensing, Data Assimilation, and Coupled Problems"

ABSTRACT:
Environmental simulation models have long been used mostly to investigate the future consequences of alternative design and management options. Such models are generally intended to be faithful reproductions of reality and are based on abstract fundamental principles. Measurements of predicted variables are included in the modeling process primarily as aids to calibration. Recent developments in ubiquitous sensing (both remote and in situ) have opened up new possibilities and challenges for hydrologic modeling. The vast amounts of data becoming available are likely to reveal processes and behavior not previously observed or predicted. This has already occurred in oceanography and other earth sciences. New data sources may eventually make it possible to monitor the planetary environment in real time, at high resolution. Such developments suggest that environmental models can be viewed as data processing tools, useful primarily for extracting information from measurements. This viewpoint has significant implications for model design. In particular, the modeling process needs to be enlarged to consider the nature of the measurements and the scale of the problem as well as the physical/chemical/biological principles thought to govern the observed system. This will be illustrated with a few examples.

Cass T. Miller, C. Pan, H. Li, K.A. Culligan, D. Adalsteinsson, and W.G. Gray
Department of Environmental Sciences and Engineering
University North Carolina-Chapel Hill

TITLE: "Pore-Scale Modeling for Closure of Multiphase Models Derived Using Thermodynamically Constrained Averaging Theory Approaches"

ABSTRACT:
Traditional models for multiphase flow in porous media are closed using empirical, ad hoc approaches. Evolving approaches are based upon a rigorous set of conservation principles and thermodynamically constrained closure approximations. These new models require new types of closure approximations. We explore the use of Lattice-Boltzmann models as a means of simulating multiphase models. Aspects considered include model forms, pore morphology, pore-scale simulation, pressure-saturation-interfacial area, curvatures, and viscous coupling.

Shlomo P. Neuman and Ming Ye
Department of Hydrology and Water Resources
University of Arizona

TITLE: "A Highly Efficient Conditional Moment Algorithm For Transient Flow In Random Porous Media"

ABSTRACT:
We present a highly efficient parallel computational algorithm for transient flow in random porous media of finite extent subject to uncertain forcing terms. The algorithm combines finite elements with numerical Laplace transform inversion to solve recursive approximations of otherwise exact nonlocal equations for the mean and variance-covariance of hydraulic head and flux. The random head and flux are nonstationary in space-time due to arbitrary forcing and conditioning on measured values of hydraulic conductivity at discrete points in space. Recursive approximation is carried to second order in log hydraulic conductivity conditional standard estimation error. The conditional moment solution compares well with "ground truth" Monte Carlo simulations of superimposed mean-uniform and convergent flows in a rectangular domain when log hydraulic conductivity exhibits large random fluctuations. The algorithm requires much less computer time than is needed for Monte Carlo statistics to stabilize, regardless of whether both solutions are computed sequentially or in parallel. The computational advantage of the parallel moment algorithm over parallel Monte Carlo simulations becomes more pronounced as grid size increases. Another computational advantage of the moment algorithm is that it allows analyzing a variety of flow scenarios by modifying forcing term statistics without recomputing Green's functions as long as the boundary configuration remains unaltered.

Linda Petzold
Department of Mechanical and Environmental Engineering
University of California Santa Barbara

TITLE: "Adaptive Numerical Methods for Sensitivity Analysis of Differential-Algebraic Equations and Partial Differential Equations"

ABSTRACT:
Sensitivity analysis of differential-algebraic equation (DAE) systems generates essential information for design optimization, parameter estimation, optimal control, model reduction, process sensitivity and experimental design. Recent work on methods and software for sensitivity analysis of DAE systems has demonstrated that forward sensitivities can be computed reliably and efficiently. However, for problems which require the sensitivities with respect to a large number of parameters, the forward sensitivity approach is intractable and the adjoint (reverse) method is advantageous. In this talk we give the adjoint system for general DAEs and investigate some of its fundamental analytical and numerical properties. We describe our new adjoint DAE software and outline some issues which are critical to the implementation.

Defining the adjoint sensitivity system and writing the appropriate software to describe it can be a very challenging problem for large-scale engineering systems, particularly when it comes to finding appropriate boundary conditions for the adjoint partial differential equation (PDE) system. Therefore our goal for both DAE and PDE systems has been the development of methods and software in which generation and solution of the sensitivity system are transparent to the user. This has been largely achieved for DAE systems. We will propose a solution to this problem for PDE systems solved with adaptive mesh refinement.

Thomas F. Russell
Department of Mathematics
University of Colorado at Denver

TITLE: "Annoying Issues in Numerical Simulation of Subsurface Transport"

ABSTRACT:
It is an empirical fact that most practical numerical simulations of subsurface transport processes are carried out with "old" or "crude" discretization techniques. Most prominent among these is first-order upstream finite differences. When such methods are used in an inner simulation loop, their inaccuracy limits the usefulness of outer-loop optimization procedures. The persistence of these old techniques, despite their drawbacks, is largely due to the difficulty of formulating better methods that are robust, fast, and accurate. The presentation will outline the attributes of various old and new methods for transport, and will speculate on how optimization might be used in the design of better inner-loop transport-simulation methods.

Christine Shoemaker, Joseph P. Ripley Professor of Engineering
School of Civil and Environmental Engineering & Center for Applied Mathematics
Cornell University

TITLE: "Groundwater Optimization: Advantages and Disadvantages of Derivative-Based, Heuristic and Surface Approximation Methods"

This talk will review applications of a variety of optimization methods to groundwater remediation optimization, including a description of side-by-side comparisons of 7 alternative methods on a bioremediation problem that involves finite difference solution to a system of highly nonlinear partial differential equations.

I will also discuss our current research project on the use of surface approximation methods in combination with other optimization techniques. Such methods can significantly improve computational efficiency of algorithms for the optimization of a continuous function *f(x)* that is costly to evaluate. In groundwater remediation this function *f(x)* is the objective function that requires solution of the partial differential equations describing groundwater hydrology, reactive transport and microbe population growth. A nonlinear surface approximation *R(x)* is a continuous nonlinear multivariate approximation to *f(x)* based on evaluations of *f(x)* at a limited number of values of *x.* I will show that *R(x)* can be used as part of optimization algorithms in order to reduce the number of points at which we compute *f(x),* and thereby reduce computational cost. I will discuss the use of augmented radial basis function surface approximation methods to solve nonconvex deterministic optimization problems. The optimization search done on the response surface to select the next point *x* for evaluation of *f(x)* can then be based on a number of methods, including modern heuristic or gradient-based search procedures. Numerical results will be presented for nonconvex deterministic optimization in serial and parallel algorithms on test functions.

Mary Fanett Wheeler
Center for Subsurface Modeling
Texas Institute for Computational and Applied Mathematics

TITLE: “Advanced Modeling Techniques for Numerical Simulation of Complex Subsurface Hydrosystems”

ABSTRACT:
We describe a methodolgy for simulating coupled flow, transport and reaction processes over large space and time scales in subsurface hydrosytems. As the relevant processes strongly differ in the various subdomains of a subsurface hydrosystem, different model concepts must be chosen for the subdomains, and special coupling methods must be applied to account for the interaction processes between these subdomains as well as for moving subdomain boundaries. Important examples include natural attenuation which is used in tens of thousands of contaminated sites in the United States in place of or in conjunction with engineering remediation systems, migration and storage of carbon-dioxide in the subsurface and atomic waste disposal sites.

Computational results demonstrating this methodolgy for multiphase flow and reactive transport are presented. In addition, current efforts in developing a posterioi error bounds are discussed.

Pamela J. Williams and Monica L. Martinez-Canales
Computational Sciences and Mathematics Research
Sandia National Laboratories

TITLE: "Using Nonlinear Interior Point Methods for Optimal Groundwater Contamination Containment"

ABSTRACT:
The design of optimal groundwater contamination containment strategies have received increased interest over the past decade as decision makers consider trade-offs between preventing further contamination through short-term containment strategies or adopting the wait-and-see approach while seeking complex long-term bioremediation strategies. Many researchers have used active-set methods, which are combinatorial in nature, to identify and analyze containment strategies. We propose the use of a nonlinear interior-point method to determine the optimal groundwater contamination containment strategy. An advantage of an interior-point method is that estimation of active inequality constraints is unnecessary. In our implementation, we have developed techniques to speed-up time to solution and to incorporate parameter sensitivity information into the finite-difference gradient calculations.

We will discuss the problem formulation, aspects of the interior-point method, and the interface to the groundwater flow and contaminant transport models. In addition, we will present numerical results and outline directions of future research.

Carol S. Woodward
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory

TITLE: "Nonlinear Solution and Sensitivity Methods for Variably Saturated Flow"

ABSTRACT:
Simulation of water resource management problems often requires the solution of large problems with many spatial zones. In addition, effective use of simulation solutions requires knowledge of the uncertainty introduced into the solution by variances in problem data. Current techniques for obtaining this information can require many runs of the simulation code and can be very time-consuming, especially for large-scale problems. In this two-part talk, we will look at both solution methods for these problems as well as uncertainty quantification based on sensitivity analysis.

In part 1, we present nonlinear solvers for variably saturated porous media flow problems. In particular, we consider the set of nonlinear equations arising from a finite difference discretization of the time-dependent Richards' equation. The solvers make use of multigrid methods in various forms. We first consider solvers which use a Newton-Krylov approach for handling the nonlinearities, and apply multigrid as the linear system preconditioner. Multigrid is used in an attempt to achieve scalability. We compare the effectiveness of two multigrid preconditioning algorithms in the context of large-scale, three-dimensional domains with heterogeneous, discontinuous permeability fields. We will also present recent work on the development of nonlinear multigrid methods for similar problems.

In part 2, we will look at sensitivity analysis for these problems. Sensitivity analysis techniques give a way to compute solution uncertainties by using information on the sensitivities of the solution to various parameters. These sensitivities are just the solution derivative with respect to the parameter in question, and equations for them can be derived by differentiating the original model problem. The resulting sensitivity equation is linear and can be solved in tandem with the model equations. First order estimates of solution uncertainties can be developed from these sensitivities with a straightforward additional calculation.

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

William W-G. Yeh
Department of Civil and Environmental Engineering
University of California, Los Angeles

TITLE: “The Inverse Problem of Parameter Structure Identification”

ABSTRACT: This research proposes a combinatorial optimization scheme for solving the inverse problem of parameter structure identification. Identification of distributed parameters invariably involves a large number of unknowns. Because of data limitation, the formulated inverse problem is inherently non-unique and unstable. Parameterization reduces the degrees of freedom of the unknown distributed parameter and defines the spatial attributes of a distributed parameter in terms of parameter dimension, parameter pattern and parameter values. Traditional parameterization methods include zonation, finite element, as well as other interpolation schemes. In this research, we demonstrate the use of Voronoi tessellation for parameterization. Accordingly, the inverse problem seeks to identify the number and locations as well as the values of the basis points associated with the Voronoi tessellation. We first use a genetic algorithm to search for the near-optimal parameter pattern and values. We then use grid search and a quasi-Newton algorithm iteratively to improve the GA solution. We use either the sensitivity equations or the adjoint state equations to calculate the gradient vector. We also discuss a proposed universal parameterization scheme that unifies various continuous and piece-wise constant (zonation) structures. Numerical experiments are conducted to demonstrate the proposed methodology.

James V. Zidek, hu D Le, BC Cancer Agency, and Li Sun, Edmunds.com, Inc.
Department of Statistics
University of British Columbia

TITLE: "Optimal Designs for Monitoring the Extremes of Environmental Processes"

ABSTRACT:
The Np hard problem of combinatorial optimization confronting the designer of an environmental monitoring network is very computationally demanding. Add to that the special technical and conceptual problems arising in the of measurement of extremes and one has a very challenging optimization problem indeed.

In this talk, we describe methods for augmenting an environmental monitoring network, in particular, one that uses entropy to sidestep the pervasive problem of ill-defined objectives. We demonstrate that approach by showing how to extend a monitoring network in Vancouver, that measures hourly small particulate airborne concentrations. Our approach uses a hierarchical Bayesian spatial predictive distribution for potential sites, conditional on all available data. We indicate how, in constructing that distribution, we over the challenges presented by high strong autocorrelations and incomplete data, that available having a staircase pattern due to different start times of existing network stations.

How well would that design solution work if site extremes such as the yearly 98th percentile of daily average levels were the metric of interest? Our predictive distribution allows us to explore that issue through simulation of the concentration field and discover difficulties, depending on how the assessment is made. We will propose a design strategy for extremes that gets around some of these difficulties along with an exact branch and bound algorithm for finding the optimal design.