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MEMORANDUM FOR: Malcolm R. Knapp, Chief
Geotechnical Branch
Division of Waste Management

FROM: Dan Goode
Hydrology Section
Geotechnical Branch
Division of Waste Management

SUBJECT: TRIP REPORT - FINITE ELEMENT CONFERENCE, June 18 - 21, 1984

Purpose: Attend 5th International Conference on Finite Elements in Water Resources in Burlington, Vermont.

Attendees: Papers were presented by authors from 20 countries. Authors included NRC and DOE contractors. No DOE personnel were in attendance.

Summary: The four day conference was conducted in an academic environment with half-hour presentation and discussion periods. Dormitory housing and common meals provided an excellent opportunity for informal discussion of finite elements and other matters. Particularly relevant papers on adjoint sensitivity, parameter estimation, 3-D flow and transport, and numerical topics are discussed below. Additional topics included sedimentation processes, surface water models, and seawater intrusion. The proceedings are available for review and the table of contents is attached.

/S/

Dan Goode
Hydrology Section
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Enclosure:
As stated

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NOTES FROM FINITE ELEMENT CONFERENCE, 18-21 JUNE 1984

Dan Goode, WMGT

Uncertainty, parameter estimation, and sensitivity

John F. Sykes (U. Waterloo, INTERA) described the application of adjoint sensitivity theory to groundwater flow simulation and presented results of a model of 2-D flow at the WIPP (DOE HLW) site. The results of this analysis are a measure of the numerical change in a model output (heads or velocities) due to a change in some system parameter (conductivity). A map was presented showing the sensitivity of head at a certain location to change in the conductivity of any of the model finite elements. This technique may be very useful to DOE in chosing new well locations in areas of maximum sensitivity. As expected, heads are most sensitive to conductivity of elements near the desired head value (the site) and of elements with high discharge. The technique can be applied to any performance measure such as head, groups of heads or velocity values, and it can be applied to the transport problem. The sensitivity is a function of the parameter field, i.e. the point on the curve at which the derivative is evaluated. Sykes did not feel that the sensitivity would change much as a function of the parameter field, within a couple of orders of magnitude. Sykes also mentioned recent application to a steady state field transport problem which indicated that solute concentrations are least sensitive to dispersion values. The numerical finite element solution for adjoint sentivity results in a matrix equation identical to the flow solution with different values in the stiffness matrix and in the forcing vector. Thus, any groundwater flow model could use its finite element grid, integration subroutines, and equation solver to solve the adjoint problem. Sykes reported an actual application in which an existing flow model was modified to also solve the adjoint problem. The primary problem (heads) cost about $2 to solve, and the adjoint problem cost about $1.5 to solve.

Lloyd R. Townley (U. Western Australia) described the effect of parameter uncertainty on calculations of piezometric head. To first order, the mean solution of a flow problem with uncertain transmissivities is equivalent to a deterministic solution using the mean transmissivities. This first order analysis is obtained by dropping higher order terms in the stochastic flow equation. When second order terms are included, the mean solution is not equivalent to the deterministic solution with mean parameters. Results were presented for steady state flow in 1-D and 2-D showing mean solutions obtained using a deterministic solution, Townley's second order mean solution, and the mean solution from Monte-Carlo simulations. In all cases, Townley's second order mean is closer to the Monte-Carlo mean solution than the first order deterministic solution. The second order technique has two major advantages over taking the mean of Monte-Carlo simulations: reproducibility, i.e. the solution is direct and involves no random number or convergence difficulties; and, computer cost. The major cost in Monte-Carlo simulation is the generation of parameter fields with the proper statistics. Using the Turning Bands Method, which is very efficient, generation of 500 fields for Townley's 2-D problems took 54 minutes of DEC-10 CPU. Solutions of the 500 resulting flow problems took 2.75 minutes. Townley's calculation of the corresponding second order mean solution took 16 seconds. In summary, Townley does not yet have a qualitative understanding of the second order effect, although he believes it will be small for most engineering problems.

Jesus Carrera (U. Arizona) described a model for parameter estimation for groundwater flow. The procedure is basically optimization or a nonlinear equation describing the least squares deviation of calculated heads and other model parameters from measured heads and prior information. The sensitivity of the solution to system parameters is used to calculate the gradient of the optimization function. This sensitivity is calculated using the adjoint sensitivity which drastically reduces computational effort. This technique was applied to a transient stream-aquifer interaction problem. This technique is a direct calibration of a model using measured values, estimated parameters, and the variance or error of those values and parameters.

3-D flow and transport

Allen M. Shapiro (Technion-Israel, now USGS-Reston) simulated steady state flow in 3-D network of fractures. Discrete fractures were modeled as 2-D flow planes and fracture intersections were modeled as 1-D tubes. This model ignored flow in the rock matrix, which is probably unimportant for steady state flow. For the transient flow problem, and for the solute transport problem, the rock matrix is likely to be crucial. Shapiro's treatment of individual fractures, as opposed to the continuum or equivalent porous media approach, may be best suited for analysis of small scale pump tests. The present restriction of steady state will probably be lifted in the future. The Boundary Integral Element Method (BIEM) is used to solve the flow equations. The governing equation within the fracture can be represented by a governing equation on the boundary of the fracture and an integral over the domain of the boundary values multiplied by shape functions. These shape functions are general solutions to Laplace's equation. By applying Green's theorem, the field problem is converted to a boundary problem. Once the boundary problem has been solved, heads and fluxes within the domain are computed using the shape functions. The limitations of this method are that the shape functions are available only for Laplace's equation, which requires constant conductivity over the domain, and for a few simply varying conductivity fields (see Cheng below). Shapiro presented results of application to a pump test problem with three fractures and one pumping well that intersected two fractures. An interative technique is used for the well boundary condition due to the nonlinear relation between the head in the well and discharge from the two (or more) fractures. Heads at observation points, a given x and y, are shown to be dependent on which fracture or what elevation is screened. This model may be useful in analyzing the anisotropy of pump test data, which may be due to fracture patterns alone, and not related to conductivity anisotropy within fractures. (Note: this work is included in WRR 19, 959-969.)

George T. Yeh (ORNL) compared four different numerical formulations of the finite element solution to the solute transport problem. The standard difficulties in solving this problem with difference-type techniques are numerical dispersion or smearing of the concentration front, and overshoot or oscillation in concentrations near the front. The latter results in negative concentrations and concentrations greater than the source. Upwinding, an attempt to overcome the latter problem, essentially uses a non-symmetric weighting in calculating concentration difference terms with more weight on the nodes upstream. Yeh compares standard Galerkin weighting, upstream weighting as developed by Huyakorn and others, a non-upstream orthogonal weighting, and orthogonal upstream weighting. In addition, these numerical formulations are solved using both a direct solver, and a successive over-relaxation iterative technique. The "best" combination of numerical formulation and equation solver is evaluated by convergence and computational effort. Unfortunately, there is no best technique for all problems, rather it is a function of the size of the problem and the relative dominance of advection over dispersion. In general, the succesive over-relaxation technique is cheaper for large problems but will converge for advection problems only when using orthogonal upstream weighting. This combination is suggested for the types of problems NRC will be solving in evaluation of radionuclide transport from HLW repositories.

D.K. Babu (Princeton U.) presented a mixed finite element - finite difference model for 3-D solute transport. To date, computational effort has been a major problem with 3-D finite element models. Not only are nodes connected to adjacent nodes, vertically and horizontally, but they are, by virtue of the integral form of the finite element technique, connected to nodes on opposite corners. For example, in a grid of quadrilateral box elements with one node at each corner, each node is connected to 26 other nodes. For a corresponding finite difference grid, each node is connected to only 6 other nodes. Babu overcomes a significant portion of this effort by using finite elements in the horizontal plane only. Vertical terms in the governing equation are treated with finite difference terms. At the beginning of each time step, the concentration field in each layer is solved independently as a horizontal system with concentrations in other layers, which contribute vertical transport, assumed equal to the values from the last time step. Each layer is solved implicitly with explicit contributions from the other layers. This results in a intermediate solution for concentration in all layers. The vertical coupling is then solved by considering only a vertical column of finite difference nodes with horizontal contributions explicitly calculated from the intermediate solution. Thus, instead of solving an (NxM)x(NxM) system of equations (N is number of nodes in each layer, M is number of vertical layers), an NxN system of equations is solved directly for each of the M layers, and then M tridiagonal equations are solved for each vertical column. The latter effort, solution of tridiagonal equations, is trivial. An example problem was presented for spherical transport to a pumping well. Model results compared well with the analytical solution. The 3-D grid was oriented along the flow paths and results would probably not be as pleasing for a more realistic application in which the grid could not be oriented along streamlines.

Allan D. Woodbury (U. British Columbia) solved the coupled saturated flow and heat transport equations using 3-D finite elements. The grid is composed of quadrilateral sided cubes which are each split into 5 linear sided tetrahedrons. This formulation allows direct integration of the finite element terms, rather than the computationally taxing process of numerical intergration. Fortunately, a pre-processor automatically breaks each user specified cube into the tetrahedrons. The flow and heat equations are seperately solved directly and the model iterates between these two solutions until the temperature solution converges at each time step. The model was applied to simulation of a hypothetical 5 kilometer deep groundwater basin to investigate the effect of groundwater flow on heat flux measurements at the land surface. In this closed basin, increases in groundwater flux increased the variability in surface heat flux from one end of the basin to the other. For advection dominated systems, heat flux at the discharge boundary of the model was over 4 times heat flux at the recharge boundary. In addition to demonstrating the tetrahedron formulation, this work may indicate a powerful investigative tool for large hydrogeologic systems: the use of surface heat flux measurements to assist in determination of regional groundwater flow rates. In the sense that this would be a remote sensing technique, it would integrate the system properties over a very large area, incorporating spatial variability. Due to this large scale, it would probably only provide data on mean flow for large areas.

Other topics

Chris Milly (Princeton U.) presented a new formulation for the specific moisture capacity (C) term in finite element models of unsaturated flow. This term represents the water storage and is a highly nonlinear function of the unsaturated pressure (matric potential). This formulation is obtained by developing the finite element equations for the spatial terms in the equation and forcing the system of equations to balance mass (volume). Over time, the change in volume of water stored in the entire system must balance the difference between the volume of water which has flowed in through the boundaries and the volume which has flowed out. This technique is shown to reduce mass balance errors significantly for an example problem of infiltration into the ubiquitous Yolo light clay. An interesting implication of this formulation is that the specific moisture capacity is not a unique function of the moisture content or the matric potential. Rather, C for the model is a function of those terms and the rate of change of those terms at a particular time. Modelers are finding that the parameters of a numerical model which should be used to generate the most accurate and realistic results are not necessarily measured values of those parameters. This is almost obvious for large scale problems where the true property field has not been identified through lab or field measurements. It is also true for the case where the property field is known exactly; there is no spatial variability and no measurement error. This use of "unrealistic" properties is required because of the numerical approximations to the governing equations. Use of the exact "real" properties in the approximate model will not yield as accurate results as use of "adjusted" parameters. What, me worry?

Myron B. Allen (U. Wyoming) discussed upwinding and demonstrated that it not only suppresses numerical oscillation for advection-dominated transport problems, but it is required for some problems for convergence to an accurate solution. In particular, Allen showed that upwinding is an appropriate term in numerical approximations to the Buckley-Leverett problem (immiscible displacement), based on the mathematics of nonlinear hyperbolic equations. It is not clear if this means that upwinding is also on sound mathematical footing for the advection-dispersion problem.

Alexander Cheng (Columbia U.) presented a boundary integral solution technique for steady state groundwater flow with variable hydraulic conductivity. A major criticism of the boundary integral method (BIEM) has been that the material properties must be homogeneous within the domain. Cheng has extended the method to domains which have properties which vary according to certain shape functions. Unfortunately, these shape functions must also have Green's function solutions, thus limiting the technique to very special cases. Cheng did present certain shape functions which could approximate linear variations, a common conceptual model. This may be useful in conjunction with the fracture system model of Shapiro above.

Informal discussion

The following notes are not organized; I can provide a more thorough report verbally. In any case: Several researchers commented to me on the relative strengths of NRC's modeling capabilities. No one was particularily supportive of SWIFT. Many of the alternatives can be used only under propriety license, which may or may not be prohibitive for NRC's use. NRC's simpler codes are probably adequate; technology has not advanced significantly. A hot problem now is tricks to make simulation in three dimensions feasible. These concerns are even more important for unsaturated flow which is nonlinear. The coupling of a multi-dimensional transport model with a chemical speciation model does not appear computationally feasible given current technology. An alternative approach (G. Yeh) is to simulate transport and chemical evolution of a small set of chemical controllers, say pH and TDS, and then to adjust geochemical parameters like dispersion and retardation for each solute of interest, based on the value of those controllers at each location at each time step. Graphic data presentation and pre- and post-processing are absolutely vital to effective modeling, especially for 3-D systems. In terms of pratical applications, these tools trail far behind numerical development. Trailing even further behind is data collection and experimental verification.

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