

CONSERVATIVE EULERIAN-LAGRANGIAN METHODS
AND MIXED FINITE ELEMENT METHODS
FOR MODELING OF GROUNDWATER FLOW AND TRANSPORT

FINAL PROGRESS REPORT

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13. ABSTRACT (Maximum 200 words) New, improved computational methods for modeling of groundwater flow and transport have been formulated and implemented, with the intention of incorporating them as user options into the DOD Groundwater Modeling System under development at the Waterways Experiment Station. These methods, which are specifically designed to treat the difficulties of subsurface flows in porous media, yield greater accuracy with coarser spatial grids and longer time steps, making possible more detailed three-dimensional (3D) simulations than would otherwise be practical. For 3D solute transport, the methods have been implemented and perform as expected on representative test problems. Theoretical analysis that substantiates this performance has also been carried out. The method for flow equations leads to linear algebraic equations that are difficult to solve, and an efficient 3D solver that overcomes these problems has been analyzed theoretically, implemented, and shown to perform well on model problems. The 3D flow code has been extended to distorted grids, the 3D transport code has been incorporated into the USGS MOC3D codes, and the two codes are being coupled together into a flow and transport code for solute.			
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STATEMENT OF PROBLEM STUDIED

Background

The Department of Defense (DOD) has thousands of sites with subsurface contamination. The Army is charged with the responsibility of coordinating DOD's technical efforts toward cleanup of these sites. It is well understood that efficient, accurate computer models of subsurface flow and transport are vital tools in site characterization and in assessment of remediation strategies. Also important, but perhaps less widely realized, is the role that such models can be expected to play in fundamental understanding of field-scale phenomena, by numerically upscaling smaller-scale experimental results through a hierarchy of scales of heterogeneity.

The objective of this research was to design and implement new numerical techniques that will be particularly efficient and accurate for simulation of groundwater flow and transport. The prototypical problem considered was two- and three-dimensional solute transport in the saturated zone, to be followed in future research by extensions to vadose-zone transport and multiphase flow. Simultaneously, model development efforts with more conventional methods were carried forward by the staff at the Waterways Experiment Station (WES). The research of this project offers the potential of substantially greater efficiency and accuracy, but with less certainty of success owing to the newness of the approaches. The products are theoretical understanding of and practical experience with faster, better methods for flow and transport, and more tangibly, code modules (still under development) fitting into the structure of the WES model that will offer the new techniques as choices to the user.

Field groundwater modeling problems are physically three-dimensional and usually exhibit significant heterogeneity in hydraulic conductivity, porosity, and other properties. Nevertheless, models often assume that a lower-dimensional or more homogeneous representation is adequate. This is frequently the result of practical constraints, namely the inability of available software to solve the real problem accurately within available computing resources. One would like to come closer to a state of affairs in which decisions to simplify a model could be based on scientific validity rather than practical necessity.

Transport

Difficulties with Eulerian methods. Serious troubles occur in approximations of transport equations when advection dominates diffusion and dispersion. Standard Eulerian numerical methods, such as centered finite differences or Galerkin finite elements, perform well when the grid size is sufficiently small. In many practical situations, this is not feasible, and such methods produce nonphysical oscillations in concentration. The usual remedy is to remove them by employing an upstream finite difference or finite element method. Resulting concentration profiles do not oscillate, but they are seriously dispersed relative to their physical counterparts. The dilemma is a choice between spurious oscillations and numerical dispersion. In practical nonlinear problems, oscillations will cause serious distortions and cannot be allowed if accuracy is to be maintained. The same is true of numerical dispersion. Additionally, one of the principal objectives in fundamental understanding of field-scale transport is to properly upscale dispersive phenomena to account for a hierarchy of heterogeneities;

a model is clearly useless in this regard if it overwhelms physical dispersion with numerical dispersion. The dilemma is not the result of the physical process; the grid needed to avoid oscillations is at a finer scale than that of the traveling advection fronts, and other methods can be more efficient.

Advection domination also leads to large time-truncation errors for Eulerian methods. When a steep front passes by, as typically happens when advection dominates, errors will be large unless time steps are very small. A more appropriate method would reduce these errors by time stepping in a Lagrangian manner that would follow the flow, permitting larger but still accurate time steps. Thus, the methods on which almost all existing public-domain transport codes are based are ill-suited for advection-dominated transport, both spatially and temporally.

Lagrangian methods. Pure advection problems, in which diffusion and dispersion are absent, can be solved efficiently and accurately by Lagrangian schemes based on the method of characteristics. Such methods normally build on propagation of discontinuities (sharp fronts), explicitly tracking front positions. Being explicit, these methods usually require that the Courant stability condition be satisfied, and they are difficult to adapt to problems with significant dispersion. For subsurface contaminant flow and transport, fronts can be steep but will not be discontinuous because of dispersion, and advection- and dispersion-dominated regimes will both be important, often in different portions of the same computation. The research of this project combined Eulerian and Lagrangian concepts in order to obtain the advantages of both, as described in the results section.

Flow

Difficulties with anisotropy and heterogeneity. The principal challenge with flow equations is to obtain accurate fluid velocity fields (or, equivalently, accurate streamlines) when the subsurface formation is highly anisotropic and/or heterogeneous in its hydraulic conductivity, and/or geometrically irregular in its geology. This situation is typical in field cases, where a hierarchy of length scales of heterogeneity can be expected. Since desirable methods for transport should have a Lagrangian component, accuracy in transport calculations depends on accurate flow velocities as input to the transport methods.

At interfaces between geological layers or other features, large spatial discontinuities in the hydraulic conductivity are routine. Across such an interface, the pressure gradient is discontinuous, but the velocity or flux is comparatively well-behaved, having continuous normal component. Thus, procedures that solve for the flux directly, and whose errors depend on appropriate smoothness of the flux rather than the pressure, would be advantageous. Irregular (non-rectangular) geology adds another layer of complexity that typical models do not treat rigorously.

SUMMARY OF THE MOST IMPORTANT RESULTS

Formulation and implementation of transport codes

ELLAM. For transport equations, the project studied Eulerian-Lagrangian localized adjoint methods (ELLAM). These methods, which are based on space-time finite elements whose temporal faces follow space-time streamlines, generalize earlier Eulerian-Lagrangian methods and overcome their disadvantages. A major one is that such procedures are not mass-conservative, and though the errors are usually small they sometimes grow to troublesome magnitudes greater than 1%. In contaminant transport calculations, where small concentrations related to regulatory levels are important, such mass losses cast doubt on otherwise useful results. A further vexing difficulty is the treatment of backtracked streamlines that cross an inflow boundary under certain types of boundary conditions; it is not at all clear how to even formulate earlier Eulerian-Lagrangian methods under some such circumstances.

The ELLAM formulation was suggested by Celia, Russell, Herrera, and Ewing in 1990. ELLAM multiplies a conservation equation by a space-time finite-element test function and integrates over the space-time domain. The key is to choose this test function to be constant, or nearly so, on space-time streamlines, and to define space-time finite elements whose temporal faces follow streamlines. The integral formulation is naturally mass-conservative and adapts to any boundary condition in a systematic way. Prior to this project, ELLAM had been implemented and tested for model transport equations in one and two dimensions. On the theoretical side, for relatively simple one- and two-dimensional cases, Reference 1 contained convergence proofs that verified that ELLAM will preserve the efficiency and accuracy advantages of earlier Eulerian-Lagrangian methods. These proofs account for all types of boundary conditions and for temporal discretization of the outflow boundary.

Code development. For solute transport with variable velocity field in two dimensions, Reference 8 documented an implementation in the USGS code VS2D. This version is a control-volume formulation, with piecewise-constant test functions, that has local conservation properties and is well-suited for incorporation in existing finite difference codes (such as VS2D). It has performed very well in heterogeneous linear and homogeneous quarter five-spot tracer flows.

The accuracy of the method depends on the accuracy of the Lagrangian tracking algorithm that defines the space-time streamlines. The tracking algorithm developed for this code (References 12, 19, 26) is exact for velocity fields that have the lowest-order Raviart-Thomas form (x -component is continuous piecewise-linear in x and t , piecewise-constant in y ; analogous for y -component). The flow-equation methods discussed below deliver accurate velocities of precisely this form. This tracking scheme has proved to be particularly important in velocity fields in which a particle can reverse direction, where other tracking methods are prone to significant errors.

Source terms were later added to this code (References 14, 21). Then the formulation was extended to three space dimensions and implemented in the USGS method-of-characteristics package MOC3D (References 15, 22, 24, 29). The greatest difficulties lay in the integration of solute concentrations over potentially irregular regions of three-dimensional space. The ELLAM transport code was linked to the USGS MODFLOW flow code, and tested on

a suite of sample problems developed for MOC3D. The code obtains accurate results with long time steps. The velocity information provided by the flow code developed in this project is of the same form as that provided by MODFLOW, so the link to the new flow code will be a straightforward modification of the link to MODFLOW. The input data structure is compatible with MODFLOW inputs.

Computational results. In some cases the improvements over other methods were spectacular; for one sample problem, ELLAM obtained in seven time steps a solution similar to those that a standard finite-element code and earlier MOC3D codes needed hundreds or thousands of steps to compute. To summarize the results briefly, ELLAM can treat advection-dominated transport with coarser grids and longer time steps than other methods, without suffering from nonphysical oscillations in the results. Additionally, ELLAM results are relatively insensitive to the orientation of the grid with respect to the direction of the flow velocity. This means that one can obtain accurate simulations on simple rectangular grids that are much easier to handle than irregularly-shaped grids.

Theory. Advances were also made in the theoretical convergence analysis of the control-volume ELLAM. It can be viewed as a Lagrangian finite-volume element method, and the groundwork for analysis of time-dependent Eulerian methods of this type was laid in Reference 5. Reference 25, in preparation, is the first extension of these ideas to the Eulerian-Lagrangian framework.

Formulation and implementation of flow codes

Mixed finite element methods. The procedures investigated for flow equations in this project were mixed finite element methods (MFEM). The ELLAM transport algorithm depends for its accuracy on accurate streamlines. As shown by several investigators, the MFEM produces better streamlines in groundwater applications than standard approaches, particularly when hydraulic conductivity is heterogeneous.

Raviart-Thomas method. The first MFEM considered in this work was introduced by Raviart and Thomas in 1976. The fundamental idea is to decompose the flow equation into Darcy's law and conservation of mass, multiply each equation by its own test function, and solve the resulting system for the velocity (flux) and the pressure. To discretize the system, elements (rectangles, triangles, or parallelograms) are chosen and shape and test functions are specified. This is done in such a way that the velocity vector field is determined by its normal fluxes, which are continuous across edges or faces.

The advantages of this approach are considerable. The velocity field conserves mass locally, so that it can be used in the ELLAM transport algorithm, with the exact tracking used there, without creating or destroying mass. Another major advantage is that the accuracy of the approximate velocity can be shown theoretically to depend on the smoothness of the velocity, not that of the pressure. As discussed previously, in heterogeneous media this favors MFEM over standard methods and justifies theoretically the computational observations of many investigators, including some in which flow was coupled to transport. Still another advantage is that the discrete unknowns are defined as edge or face fluxes, which are finite

and bounded even as a point source or sink is approached, so that the MFEM is able to handle injection and pumping wells more accurately than other methods.

Solution of discrete equations. A major obstacle to three-dimensional applications of MFEM is the difficulty of solving the discrete linear equations iteratively. The system is indefinite, and the usual iterative methods are unreliable. The quest for efficient, reliable solvers has been active for many years. A successful two-dimensional algorithm originated by Chavent *et al.* in 1984 uses a local basis for the subspace of divergence-free functions to decompose the problem into three parts, each of which can be computed efficiently. Most of the computation is a positive-definite projection into this subspace, and the algorithm's efficiency derives in part from the fact that the subspace dimension is substantially less than that of the full velocity space.

References 9 and 17 document the theory behind an extension of this solver to three dimensions. Unlike some other algorithms, this works when the hydraulic conductivity is anisotropic, resulting in cross-derivative terms that create additional non-zero coefficients in the linear equations. Numerical results, in References 16, 17, 23, and 31, show that the convergence rate of this solver is independent of the grid size, as predicted theoretically. In a pleasant surprise, the convergence rate in most cases is also independent of the magnitude of variations in hydraulic conductivity.

Distorted grids. Another restriction on the applicability of the Raviart-Thomas MFEM described above is that, for optimal accuracy, the elements must be rectangles, triangles, or parallelograms (some of each is permissible). Existing finite difference grids and data structures are primarily based on a logically rectangular connectivity pattern. To the extent possible, it would be desirable to treat distorted logically rectangular grids, of quadrilaterals in two dimensions and hexahedra in three, designed to conform to the irregularities of subsurface geology.

Control-volume mixed finite element method. With this in mind, this project designed and implemented in two (References 7, 11, 18, 30) and three (References 13, 16, 20, 23, 31) dimensions a variant of MFEM, called the control-volume mixed finite element method (CVMFEM), that preserves optimal-order accuracy on distorted grids. In this procedure, the velocity test functions are altered from those of the MFEM, in such a way as to be distortions of piecewise constants on control volumes. The result is a discrete Darcy law for a distorted grid: the pressure difference between two adjoining cells is, instead of a multiple of the flux across their common edge or face, a linear combination of the fluxes across all of their edges or faces.

The reputation of MFEMs is that they provide more accurate velocities and streamlines in problems with heterogeneous hydraulic conductivity; for CVMFEM, Reference 7 showed this with both mathematical theory and two-dimensional numerical computations that included anisotropy and grid distortions. Other methods have particular difficulties with large discontinuous jumps in conductivity, which are of obvious importance for subsurface flow, but MFEMs do not. CVMFEM computed fluxes to the accuracy of the square of the grid size, i.e., second-order accuracy. Subsequently, similar results were found for three-dimensional CVMFEM in References 13, 20, and 31. The efficient equation solver was adapted to MFEM

and CVMFEM with distorted grids (References 16, 23, 31). The essential structure of the solver is the same as for rectangular grids, but the determination of the equation coefficients is more complicated. A CVMFEM-based flow code is currently under development in collaboration with USGS, and it may eventually become a successor to the widely-used MODFLOW.

Justification of model equations

An important issue in modeling of contaminant transport at DOD sites is justification of the manner in which the model equations represent the physical processes. Subsurface formations are heterogeneous at a multitude of length scales, including heterogeneities at scales finer than a computational grid. The effects of such properties must be represented indirectly in models, through such concepts as dispersivity in solute transport. References 3 and 10 report on a formulation, implemented with stochastic finite element methods, designed to compute effective dispersivities for real data. Such data may violate the idealized assumptions that underlie analytical approaches to this problem. Reference 2, an invited review paper, discusses the physical assumptions made by various models of multiphase multicomponent transport, with particular attention to the local equilibrium assumption and the implications for practical modeling when it is valid or invalid.

Other research

References 4 and 6 document investigations into biased interpretations of field measurements. A mathematical model consisting of a diffusion equation with a discontinuous piecewise-constant coefficient, together with analytical and numerical solutions, showed that the usual calibrations used by field scientists could be substantially in error in some cases of practical interest. Reference 27 studied operator-splitting techniques for reactive transport, delineating types of cases in which it was advantageous or disadvantageous to iterate, based on stability analysis. Reference 28 described a robust incomplete-LU (ILU) preconditioner for conjugate-gradient solution of linear equations arising from flow problems with varying anisotropy and heterogeneity. The idea was to minimize the directional sensitivity of the speed of convergence by performing the ILU decomposition in a zigzag fashion through the grid.

LIST OF PUBLICATIONS AND TECHNICAL REPORTS

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(Hence these do not cite the grant)

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SCIENTIFIC PERSONNEL

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