

Statement of Research Experience

Background and Interests. I have my feet in many camps, and this makes me difficult to categorize. I was trained in numerical analysis in one of the best pure mathematics departments (Chicago); my thesis and many of my subsequent papers contain complicated theoretical error estimates with little relation to practical computations on real-world problems. Some of my later research is primarily mathematical but more in the nature of the observed efficiency and accuracy of new numerical methods for partial differential equations; this might best be put in the world of scientific computing. After my Ph.D., I went to work in the oil industry on reservoir simulation; I continued my research on numerical methods as a sideline, but my top priority was development and implementation of models for practical problems. I developed a strong interest in the physics of flow in porous media and in working with scientists and engineers on these problems, to the point where I could pass for an engineer. It was eye-opening to formulate mathematical models and to be concerned with the validity of these continuum equations, as opposed to simply trying to solve them mathematically. When I returned to academia after seven years in industry, I expanded into environmental problems of groundwater contamination, which are physically and mathematically similar to petroleum recovery, but with some fundamental differences. Finally, over the years I have come to understand the importance of uncertainty in models of subsurface flow, due to the lack of data and also due to the impracticality of direct representations of small-scale heterogeneities, which can be random when viewed from a larger scale, in large-scale models. This raises questions of upscaling of models and is causing me to consider modeling with stochastic processes, and the study of associated numerical procedures. Depending on one's point of view, my field could be considered to be some combination of numerical analysis, scientific computing, mathematical modeling, petroleum engineering, groundwater hydrology, and stochastic processes.

Perhaps the most appropriate overall characterization of my work is that it is problem-driven research. Throughout my career I have been concerned with numerical methods for convection-dominated diffusion equations, motivated by their importance in applications to subsurface flow. In practice, the accuracy of these methods depends on the accuracy of the velocity field that drives the convection. This velocity comes from a potential equation with a conductivity that can be anisotropic and highly heterogeneous, with discontinuities along geometrically irregular subsurface features. Thus, I have been led to study methods designed for these difficulties. From the standpoint of mathematical modeling, the validity of these macroscopic continuum equations depends on upscaling of smaller-scale models, in such as way as to account for microscopic properties that are uncertain or too fine to represent directly in a practical computation. My training and outlook had always been deterministic, but two of my Ph.D. students have helped me begin to enter the domain of stochastic modeling [14, 35, 36, 37, 38], and in September 2002 I received a large NSF grant to pursue this work.

Numerical Methods for Transport Equations. For convection-diffusion equations, my work began with the modified method of characteristics (MMOC), which was introduced in my Ph.D. thesis [46] and in a paper with Jim Douglas, Jr. [18] This was one of the first Eulerian-Lagrangian methods, in which an Eulerian (roughly speaking, fixed-grid) finite-difference or finite-element treatment of diffusion is combined with a Lagrangian (using characteristics or streamlines) treatment of convection. Some other researchers proposed similar ideas at about the same time, and these methods have become widely used under a variety of names (characteristic Galerkin, semi-Lagrangian, Arbitrary Lagrangian-Eulerian, Lagrange Galerkin, etc.) for Navier-Stokes equations, atmospheric modeling, and other applications. My early work on MMOC proved optimal-order error estimates that placed the approach on a sound theoretical footing, and implemented it for a coupled system that modeled enhanced oil recovery by miscible displacement [47, 48, 13]. The efficiency and accuracy of the procedure were excellent relative to other methods available at the time; its principal drawbacks were that it did not conserve mass, and that its formulation for certain types of boundary conditions was not obvious.

In the late 1980's, Michael Celia, Richard Ewing, Ismael Herrera, and I found that MMOC could be generalized in a manner that would overcome these drawbacks. The new procedure was named the Eulerian-Lagrangian localized adjoint method (ELLAM) [7, 50, 33, 56]. The formulation involves space-time finite elements, oriented exactly or approximately along streamlines. Similarly-oriented space-time test functions w are chosen such that the adjoint L^*w vanishes locally, hence the name of the method, where L is the hyperbolic part of the differential operator. The convection-diffusion equation is multiplied by such a test function and integrated over the spatial domain and over a time step. The resulting discrete weak form conserves mass as long as the integrals are evaluated in a consistent manner [62], and general boundary conditions are handled systematically via integrals. In certain simple cases with particular choices of numerical integrals, ELLAM reduces to MMOC.

ELLAM provides a sound framework within which to design efficient, accurate methods that perform well in both convection-dominated and diffusion-dominated regimes. In later years, the approach has been extended to variable velocity [62], nonlinear flux (unsaturated or two-phase flow) [12], degenerate diffusion, reactive flow [70], and three space dimensions [30, 31]. A finite-volume version (FVELLAM) has also been developed [27, 28, 29, 54], in which the test functions are characteristic functions of space-time subdomains oriented along streamlines; this yields local conservation in a Lagrangian sense and is more compatible with existing finite-difference codes than the original ELLAM was. Error estimates have been proved for some relatively simple cases [69]; the analysis is complicated because of special space-time elements near inflow and outflow boundaries. Numerical results are comparable in accuracy to MMOC where both methods apply. Mass is conserved, and arbitrary boundary conditions are treated. A recent review paper [56] summarizes research in this area.

Recently, two U.S. Geological Survey scientists, one of my Ph.D. students, and I implemented FVELLAM in the USGS suite of method-of-characteristics codes known as MOC3D [30, 31, 59, 60]. This code is now available at <http://water.usgs.gov/nrp/gwsoftware/> as

Version 3.5 of MOC3D. It performed well in all of the standard USGS test cases, including one in which it obtained an accurate solution in seven time steps, while a benchmark finite-element code took 4000 time steps to reach the same simulated time. The hope is that this code, or an improved version (next paragraph), will be widely used in the groundwater modeling community. As a follow-up to funding over the past several years from the U.S. Army Waterways Experiment Station and the Terrestrial Sciences (TS) Program of the Army Research Office (ARO), we intend to transfer this technology to the Department of Defense's Groundwater Modeling System (GMS) as well. The principal drawback of the existing code is that solutions can show non-physical oscillations when the grid is too coarse. A possible joint project has been discussed with Chunmiao Zheng, the principal author of the well-known groundwater transport code MT3DMS [75]. By adapting some flux-based Eulerian-Lagrangian concepts of Roache [45], this work would incorporate total variation diminishing (TVD) flux limiters into the ELLAM formulation, in order to avoid non-physical oscillations. A colleague at the University of Heidelberg, Germany, has done some similar work for classical finite-volume methods, where numerical diffusion is more of a problem, and we have had preliminary discussions on a collaboration to apply this to FVELLAM, which produces sharper fronts that are closer to physical reality.

Other future plans for research on ELLAM, to be coordinated with the TVD work, include theoretical analysis of FVELLAM, improved numerical integration techniques in the three-dimensional code, and extensions to more complex physical problems. Starting from an analysis of the same type of method without the Lagrangian component [63], a convergence analysis with Martin Stynes for a simple case of FVELLAM is nearly complete, with some delicate stability questions yet to be resolved [32]. Numerical integration is crucial in these methods; essentially, the mass at the previous time step must be integrated over irregular regions of space that correspond to tracebacks along velocity streamlines of regular elements at the new time level. One of our USGS collaborators plans to extend the variably-saturated two-dimensional code VS2D, which currently contains a version of FVELLAM for saturated (single-phase) flow and transport, to three dimensions (VS3D); this will involve extensions of FVELLAM to unsaturated (two-phase) flow, and we intend to consider nonlinear reactions as well. Extensions to multiphase multicomponent systems began during my sabbatical visits to INRIA (Rocquencourt, France, fall 2002), the University of North Carolina (April 2003) [25], and the University of Bergen (Norway, spring 2003) [61]. An adaptive-lumping approach to avoiding oscillations, which could be an alternative to the TVD methods discussed above, was started during my sabbatical visit to the University of Newcastle (Australia, winter 2003) [55]. Another Heidelberg colleague is exploring an artificial diffusion term for a similar purpose, and is interested in collaborating on that as well as on implementations for unstructured grids and higher-order discontinuous basis functions. All of these future plans raise a host of theoretical and practical questions.

Numerical Methods for Flow Equations. Methods with a Lagrangian component depend for their accuracy on an accurate velocity field, and the Eulerian-Lagrangian meth-

ods in my research are no exception. Thus, I have been interested for a long time in velocity methods that can deal with the difficulties of subsurface flow: strong heterogeneity, anisotropy, and geometrically irregular interfaces for the conductivity coefficient \mathbf{K} in a prototypical flow equation $\nabla \cdot \vec{v} \equiv -\nabla \cdot (\mathbf{K}\nabla p) = q$. Mixed finite element methods (MFEM) are well-suited for at least the first two of these difficulties, and in conjunction with many colleagues I have been investigating and using them since early in my career. These methods solve simultaneously for pressure and velocity, representing each unknown with its own space of trial functions. In heterogeneous media, the computed velocities are substantially more accurate than those obtained from standard methods that do not represent the velocity directly [8, 40]. Coupled to MMOC for transport, we theoretically analyzed and implemented MFEM for flow [22, 23, 65, 24], and subsequently combined this with local grid refinement [21, 19, 20]. More recently, we have tackled the question of how best to solve the discrete equations arising from three-dimensional MFEM; it turns out that a particularly efficient algorithm can be based on a decomposition of the discrete velocity space, using a computationally convenient basis for its divergence-free subspace [5, 6]. This leads to a symmetric positive-definite system of smaller dimension than the velocity space, which can be solved by conjugate gradients with an overlapping domain-decomposition preconditioner, such that the condition number is independent of the mesh size. We have also investigated analytical particle-tracking procedures [58], given a velocity of MFEM type, to enhance the accuracy of transport calculations.

In the early 1990’s, colleagues in the petroleum industry were seeking rigorous discretizations for irregular cell-centered finite-difference grids. There was an acknowledged need for more accurate representations of subsurface geological features, along with a desire to conform to the accustomed logically rectangular conceptualizations of flow between finite-difference cells. Formulations in commercial codes, going by names such as “corner-point geometry,” were mathematically inconsistent and subject to serious errors in practice. MFEM, which had a well-established theoretical basis, constituted a promising methodology within which to attack this problem.

After some time, we came to a formulation that we called a control-volume mixed finite element method (CVMFEM) [4]. This differs from a standard MFEM in that the velocity test functions are not the same as the trial functions. On a rectangular grid, the usual lowest-order Raviart-Thomas (RT₀) [44] elements are used as trial functions, but the test functions are vector characteristic functions of subvolumes centered around edges of the grid. This yields algebraic equations that represent a discrete Darcy law on each edge-centered subvolume, similar to an engineer’s conception of a laboratory tank. Unlike the trial functions, these test functions do not have continuous normal components at edges. On distorted grids, as with MFEM, the elements are determined by a Piola transformation [3]. This can lead to a mildly nonsymmetric mass matrix, but it has the advantage that the Lagrange multipliers required by MFEM to maintain accuracy on distorted grids [2] can be eliminated through a flexible choice of the test function. An independent investigation [26] has found CVMFEM to be “quasi-optimal” in the sense of having relatively small error in

the spectral (frequency) domain for the whole range of error components. Other independent investigations have demonstrated convergence of the pressure and velocity on rectangular [9] and quadrilateral [10] grids, though no one has proved the robust second-order convergence of velocities (fluxes) that has been observed in numerical experiments [4, 26] whenever the exact solution is not singular. It is this feature that makes CVMFEM particularly attractive in computing velocities for use in FVELLAM simulations of transport equations. We have a second-order proof in preparation that applies to rectangular grids [66]. We have studied to some extent the relationships between CVMFEM, MFEM, and other methods (e.g., the support operators method [34]) that have been proposed for this problem [52, 39].

All of the work in the preceding paragraph is two-dimensional. The situation in three dimensions is considerably more complicated, as has been revealed in work with a USGS colleague [41, 42, 43]. Unlike a bilinear image of a square (a quadrilateral), a trilinear image of a cube need not have flat faces. In two dimensions, the Piola-transformed RT_0 vector fields include the constants, but in three dimensions, they do not [53, 42]. This makes the choice of test and trial functions less clear, as the finite elements do not necessarily pass the classical “patch test” [68]. Our test functions [4], as modified by Garanzha and Konshin [26], appear to be the best choice [41], but the details of the trial functions are still being investigated [42, 43]. With the trial functions in use now, and regular asymptotic refinement in the reference space of the trilinear mapping, robust second-order convergence of fluxes has been observed, as in two dimensions. With random refinement, where angular distortions do not decrease asymptotically, these trial functions yield observed first-order convergence, whereas Piola trial functions do not converge at all [42, 43]. The efficient divergence-free-based solver and another multigrid solver for three-dimensional MFEM are also being adapted for CVMFEM [72, 73, 71].

Future plans for research on CVMFEM begin with the determination of the trial functions and the adaptation of the solver. In its current form, the code handles distorted grids but not the full-tensor conductivity coefficient that results from anisotropy; anisotropy will require no new structure in the code, but more complicated equations to generate the matrix. Another step is the theoretical analysis of convergence of the solver; with a nonsymmetric mass matrix, this will require some tools different from those of the previous analysis. Another analytical task is to generalize the second-order velocity convergence [66] to more general grids in two and three dimensions. For MFEM, algorithms for local refinement and non-matching grids are already known [1, 74]; because the matrix structure of CVMFEM is the same, but with different coefficient values, these techniques should be adaptable to CVMFEM. The formulation and analysis of this for non-matching rectangular grids has begun [67].

Scientists at INRIA (fall 2002 sabbatical visit) are implementing these ideas in their flow codes, and the visit to Bergen (spring 2003) started a collaboration to extend this work. There is also significant interest in the applications communities. USGS has committed and is continuing to commit a substantial effort. The hope is that this code will evolve into the replacement for MODFLOW, the old USGS model that has been the standard groundwater flow code for decades. Having USGS personnel involved in the development makes this a

real possibility.

Upscaling and Stochastic Processes. Upscaling, or the derivation of effective or averaged macroscopic models from possibly different microscopic models, is a fundamental issue in many areas of applied science, and particularly for flow in heterogeneous porous media. This understanding should take the form of mathematical models that are valid at multiple scales. Theories developed up to now have generally depended on restrictive idealized assumptions, such as periodicity, small variance in hydraulic conductivity, ergodicity (small correlation scale of conductivity relative to the scale of transport), single-scale (exponentially decaying autocorrelation) or fractal (polynomial decay) correlation, and near-uniform flow. One of our approaches is to use numerical methods, instead of analytical derivations, to obtain upscaled dispersivities for use in transport calculations. This flexible framework need not be subject to restrictive global assumptions; instead, assumptions can be made at the scale of a grid block [57]. A Lagrangian stochastic approach, similar to a formulation of Dagan [11], tracked ensembles of particles through realizations of multi-scale heterogeneous media, computing scalable dispersivities by integrating hydraulic conductivity covariances along streamlines. Good comparisons of upscaled transport calculations to laboratory experimental data were made [57, 16, 17]. So far, this work has involved conventional Galerkin finite element methods. With the heterogeneous medium and the Lagrangian tracking, this is a natural fit with CVMFEM and FVELLAM, and these connections will be made in future research. Efficient, accurate numerical schemes for three-dimensional stochastic differential equations will also be studied.

An alternative approach for upscaling is to seek moment differential equations that can be solved deterministically for macroscopic statistical information about a contaminant plume. For single-phase flow, starting from a microscopic Wiener process, this can be done with the Itô theory via the conditional probability density function [14, 16, 15, 17]. A major question for future research is whether more general semi-martingales can be used in an analogous way to obtain other macroscopic models of interest, such as two-phase flow. If this could be done, then these models could be simulated at any scale by methods for stochastic differential equations, without the usual closure problem for moment equations. The theoretical framework is in place to explore a variety of formulations, and this will be done. A joint proposal with hydrologist Tissa Illangasekare of the Colorado School of Mines was funded in September 2002 by the NSF CMG program (Opportunities for Collaborations Between the Mathematical Sciences and the Geosciences). This involves numerical and experimental validation of stochastic upscaling procedures for two-phase transport of immiscible contaminants in heterogeneous media. A key theoretical component of this is the use of stochastic processes with jumps to model multiphase interfacial phenomena.

This is still speculative at this point, and a more conventional perturbation formulation of two-phase moment equations has also been investigated [35, 36, 37]. For the classical Buckley-Leverett problem without capillary pressure, which is hyperbolic, in one space dimension the system of second-order moment equations reduces to a hyperbolic system for

the mean saturation and the saturation variance. Assuming a unique solution, which existing theory for systems of conservation laws is insufficient to prove, the resulting saturation profile is bimodal, with two shocks between rarefactions or quiescent regions. In two dimensions, even with the assumption that the saturation equation can be decoupled from the pressure equation (i.e., that the total-mobility coefficient in the pressure equation depends weakly on the saturation and can be assumed to be independent of it), the reduction of the moment-equation system is not possible and it cannot be rigorously classified as hyperbolic, but qualitative numerical results are similar. Comparisons to Monte Carlo simulations are good, with Monte Carlo averages being smoother and shock-free. Approximate statistical information can be obtained much more efficiently from moment equations than Monte Carlo simulation, at least in this case. Closure of the system is a major issue, as the results do not support a multivariate Gaussian assumption.

In future work, we will attempt to extend this moment-equation formulation to include capillary pressure, to allow coupling to the pressure equation, and to consider higher-order moments. It is not clear how far it can be extended within practical limitations. Capillary pressure, with its diffusive character, could make a rigorous uniqueness argument possible in one dimension. The goal of the research to this point has been a qualitative assessment of the merits of the approach, which has had a positive outcome; numerical techniques were chosen on the basis of convenience of adaptation from existing codes, rather than efficiency or accuracy. Future work will delve into the theoretical and practical issues of numerical methods for systems of moment equations, which should make substantial improvements in the accuracy and performance. My former Ph.D. student, Kenneth Jarman, is working at Pacific Northwest National Laboratory, and funding is anticipated for continued collaboration. Efforts are actively underway to organize this with several investigators at Los Alamos National Laboratory.

Expository Papers. Over the years I have written several invited expository papers. My strong interest in the physics of flow in porous media began with background work for the SIAM volume [64]; that paper was also the first to draw the connection between cell-centered finite differences and mixed finite element methods. The 1989 survey for the petroleum industry's geophysics community [49] dealt with the computational requirements of the modules that comprise different types of reservoir models, and the implications for demand for supercomputing capabilities. In 1994, the organizer of a quadrennial review of research in hydrology asked me to write a critical review of recent work on multiphase multi-component transport [51]; from this I learned a great deal about the experimental literature as well as modeling. I believe that this is my only paper that has no equations. These papers demonstrate well the long-term interdisciplinary nature of my work and reputation.

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