Coupled Systems Nonlinear PDE's, Operator Splitting, Adaptive Gridding

Complex physical phenomena involving transport of heat or fluids are often modeled by coupled systems of nonlinear, time-dependent partial differential equations. Research has addressed each phase of the modeling process, utilizing physical, mathematical, numerical, and computational concepts. Techniques for treating systems of transport equations via modified method of characteristics, front tracking and mixed finite-element spatial discretizations have been developed. Adaptive grid refinement methods are capable of resolving important dynamic local phenomena. Stability of the partial differential equations (OVER)
and their numerical counterparts have been studied. Computational procedures involving efficient data structures, preconditioning, domain decomposition, and vectorization and parallelization have been developed.
NUMERICAL AND ANALYTICAL METHODS IN NONLINEAR
PARTIAL DIFFERENTIAL EQUATIONS

FINAL TECHNICAL REPORT

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I. STATEMENT OF THE PROBLEMS STUDIED

Complex physical phenomena involving chemically reacting systems or the transport of heat or fluids are often modeled by coupled systems of time-dependent, nonlinear partial differential equations. The difficulties in understanding the stability of the differential equation systems and in designing efficient, accurate numerical methods for their solution are widely recognized and were the focus of this research. We have worked on four general aspects of the analysis and numerical approximation of systems of partial differential equations. These areas of research are: (1) modeling aspects and stability analysis for nonlinear time-dependent partial differential equations; (2) use and analysis of finite element or finite difference methods to discretize coupled systems of nonlinear differential equations; (3) development of adaptive or local grid refinement capabilities to resolve local phenomena in large-scale applications; and (4) development of data structures, preconditioners, and efficient solution algorithms for large-scale problems on new computer architectures. Emphasis has been placed upon multiphase or multicomponent, transport-dominated flow processes with dynamic local phenomena. The research also involved a mix of analysis, algorithm development, and large-scale computation using newer computer architectures.
II. SUMMARY OF KEY RESULTS

The advent of orders-of-magnitude better computing capabilities has allowed the modeling of more complicated physical phenomena. The incorporation of more detailed physics in our models has necessitated the use of more sophisticated mathematics and numerics in the modeling process. In this way, a broader range of mathematics is needed for applications. The mathematical techniques which are used to model the transport of multicomponent or multiphase flows are representative of those needed for many other applications, such as chemically reacting or thermally driven flows, and have been studied as typical models to develop our understanding and capabilities. The equations which have been considered are strongly convection-dominated equations that have transport aspects of hyperbolic partial differential equations but which have thin moving regions with viscous effects where the modeling of diffusion is critical.

In order to treat the transport-dominated aspect of convection-diffusion type equations, we have developed [2,6,29,30,31,37] a "modified method of characteristics" temporal technique which can be combined with either finite difference or finite element spatial discretization. The computational aspects of this technique are much simpler than a true method of characteristics and can be extended to higher space dimensions with relative ease. In [30,37], we extended these ideas to transport problems with nonlinear and nonconvex flux functions. There are strong correlations with these and front tracking methods, but these techniques can incorporate the important diffusion phenomena much more readily. Ideas derived from characteristics-based methods have also been studied [35] to stabilize the transport-dominated problems, replacing the standard upstream weighting techniques which can cause serious problems for coupled nonlinear systems [2,3].

Ewing and co-workers have been successful in applying finite element tech-
niques to fluid flow simulation problems. Mixed finite element methods for accurate fluid velocities are described in [1,2,5-7,11,13,18,24,25,29,31,42]. Asymptotic error estimates for these procedures are described in [6,14,39-43]. Petrov-Galerkin variational methods and operator-splitting techniques have also been analyzed in [30,37] to treat the transport-dominated model problems. Applications to various engineering applications are described in [3,16,18,21,24,29,35]. Codes have been developed by Ewing, Russell, and graduate student Joe Koebbe, and with coworkers in Norway [35,37].

A major effort has also been concentrated upon adaptive and local grid refinement techniques for resolution of local behavior. References [4,8,10,12,17,18,20,22,23,34,35] survey various aspects of local and adaptive grid refinement. A truly local refinement requiring a complex data structure for efficient implementation is described in [4,8,12,17,22]. Work is under way to implement these algorithms on a new Alliant parallel architecture computer recently acquired by Ewing's research group at the University of Wyoming using, in part, a DoD equipment grant. Patch types of local refinement which can be done more easily incorporated in large existing codes are described in [10,28,30,34,36-38]. Codes for implementing these concepts are being developed by graduate student Paul Jacobs and are almost complete.

Codes for modeling applications require the input of physical parameters that often cannot be measured directly. Various new methods for parameter determination are presented in [15,32,33,34]. Graduate students James Sochacki and Tao Lin have worked with Ewing on this analysis and corresponding code development.

Efficiency of computation is critical for the large-scale modeling applications. Applications of preconditioned conjugate-gradient methods were described in [26]. A variety of preconditioners and conjugate-gradient-like methods have
been coded and are currently being vectorized by graduate student Mark Oliver. Research is beginning on parallelization of these algorithms. Other preconditioners which allow a type of local refinement via domain decomposition are described in [28,30]. We are working on incorporation of these methods in large existing codes. Graduate students Joe Koebbe and Peng Lu and postdoc Uma Prasad [38] have been working on multiphase, multicomponent fluid flow codes with Ewing.

Finally, we have been looking at stability analyses for certain nonlinear, time-dependent partial differential equations [9,27,C1,C2]. Professor Brian Straughan from the University of Glasgow visited the University with partial support from this grant and to work with Professors Ewing and George on these problems. A joint paper [27] numerically considered a form of Burger's equation with various powers of the nonlinearity to understand the effect of initial conditions on these nonlinearities. Professor Straughan has extended this work to other convection-diffusion applications in [C1,C2].
III. LIST OF PUBLICATIONS

A. EWING'S PUBLICATIONS


36. Adaptive grid-refinement techniques for treating singularities, heterogenei-


40. Numerical method for a model for the incompressible nuclear waste-disposal contamination in porous media (with Yirang Yuan and Gang Li), (in preparation).

41. The finite element method with moving mesh for local interpolation for in-
compressible miscible displacement (with Yirang Yuan and Gang Li), (in preparation).

42. A time-discretization procedure for a mixed finite element approximation of the incompressible nuclear waste-disposal contamination in porous media (with Yirang Yuan and Gang Li), (in preparation).

43. Finite difference methods for a model for compressible flow for the nuclear waste-disposal contamination in porous media (with Yirang Yuan and Gang Li), (in preparation).

44. Hyperbolic perturbation methods for parameter estimation of the numerical model for distributed systems (with Tao Lin), (in preparation).

B. Ewing’s Books


C. Other Supported Publications

1. Stability criteria for convection with large viscosity variations (B. Straugh-

2. Finite amplitude instability thresholds in penetrative convection (B. Straug-
IV. INVITED PRESENTATIONS

A. INVITED ADDRESSES


24. “Mathematical modeling in the energy and environmental sciences.” (Series of 10 invited lectures) Principal Lecturer at NSF-CBMS Conference, Morgantown, West Virginia, June 2-6, 1986.


B. INVITED COLLOQUIA AND SPECIAL SEMINARS

21. National University of Mexico, Mexico City, Mexico, September 29, 1986.
22. Tulsa University, Tulsa, Oklahoma, October 29, 1986.
33. Chalmers University of Technology and The University of Göteborg, Göteborg, Sweden, April 1, 1987.
V. PARTICIPATING SCIENTIFIC PERSONNEL

A. STUDENTS

1. James S. Sochacki – Ph.D., 1985
2. Upal R.B. Obeysekare – M.S., 1985
3. Joseph V. Koebbe
4. D. Lowell Smylie
5. Paul Jacobs
6. Mark Oliver
7. Tao Lin
8. Peng Lu

B. FACULTY

1. Brian Straughan
2. John H. George
3. Robert Sharples
4. Uma Prasad
END
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