During the period covered by this grant, we conducted research on the development and application of adaptive numerical methods for singularly perturbed initial-boundary value problems for partial differential equations. We studied both local refinement methods and methods of lines techniques using properly nested and overlapping grids. The geometric modeling capabilities of our procedures were improved through the use of finite quadtree and octree encoding schemes; parallel versions of adaptive procedures on shared-memory computers were developed; and variable-order finite element methods to be used with adaptive p- and hp-refinement were created.
FINAL SCIENTIFIC REPORT

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Title of Research: Numerical Methods for Singularly Perturbed Differential Equations with Applications

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ABSTRACT

During the period covered by this grant, we conducted research on the development and application of adaptive numerical methods for singularly perturbed initial-boundary value problems for partial differential equations. We studied both local refinement methods and methods of lines techniques using properly nested and overlapping grids. The geometric modeling capabilities of our procedures were improved through the use of finite quadtree and octree encoding schemes; parallel versions of adaptive procedures on shared-memory computers were developed; and variable-order finite element methods to be used with adaptive p- and hp-refinement were created.

During the period covered by this grant, we conducted research on the development and analysis of finite difference and finite element methods for steady and transient partial differential systems in one, two, and three space dimensions. A list of publications is given in Section 3 and some of our key findings are highlighted below.

Using a local refinement finite difference or finite element method, error estimates of solutions generated on a coarse spatial grid for one time step are used to create finer space-time subgrids in regions where greater resolution is needed. The problem is recursively solved on these finer grids until prescribed accuracy criteria have been satisfied. The process continues in this manner proceeding from coarse time step to coarse time step. Flaherty et al. [2-4] reported on a two-dimensional local refinement procedure that uses uniform space-time grids with finer grids overlapping coarser ones. Solutions on overlapping grids at the same level of our tree data structure are obtained using the Schwarz alternation principle, which appears to be efficient and robust. We introduced the concept of a ‘‘megagrid’’ that contains all overlapping grids of the same and/or finer levels of the tree. The megagrids greatly simplify data management and searching problems associated with overlapping grid methods. The procedure used to solve linear systems on the various grids has been improved by using an incomplete orthogonalization procedure.\footnote{Y. Saad, “Practical Use of some Krylov Subspace Methods for Solving Indefinite and Nonsymmetric Linear Systems,” \textit{SIAM J. Sci. Stat. Comput.}, 5 (1984), pp. 203-228.}

This and additional improvements to the clustering algorithm that is used to define local grids have been reported in a paper [3] that appeared as part of the proceedings of the workshop on \textit{Adaptive Computational Methods for Partial Differential Equations} that was organized by J. E. Flaherty, M. S. Shephard, and J. D. Vasilakis and held at the Rensselaer Polytechnic Institute. A more detailed analysis of the method will appear shortly [4].

The success of high-order methods and adaptive hp-refinement techniques on elliptic
systems has led us to investigate analogous procedures for time-dependent problems. The transient situation is far more difficult than the steady one due to the need to balance spatial and temporal errors combined with the difficulty of obtaining reasonable estimates of the global temporal discretization error. Martin Berzins of Leeds University visited Rensselaer during the course of this grant. He is an expert on global temporal error estimation and high-order (spectral) approximation. In collaboration, we have been investigating the use of singly implicit Runge-Kutta (SIRK) methods and backward difference formulas (BDFs) with high-order restarting to achieve high temporal orders of accuracy. A report on a method for one-dimensional problems that combines h- and p-refinement will be submitted for publication shortly.

Local mesh refinement finite volume software for hyperbolic systems [1, 5, 6] has been combined with finite quadtree mesh generation procedures for the solution of two-dimensional problems, respectively. These studies combine motion of a coarse "base" mesh with local temporal and spatial mesh refinement. In contrast to the overlapping grid procedures, fine grids are properly nested within coarse mesh cells; thus, reducing interpolation difficulties at mesh interfaces. The quadtree mesh generation procedures are used to create the initial grids, respectively, on complicated domains. The mesh generation techniques are completely automatic and their tree data structure nicely matches the tree structure that we employ for local refinement. Two-dimensional codes have been written and are being used to solve transonic flow problems about airfoils, wings, and wing-body combinations. A three-dimensional version is under development. Parallel versions of the adaptive procedure have been implemented on shared-memory MIMD computers [7]. Several static and dynamic load-balancing strategies indicate the effectiveness of using adaptive methods in parallel computational environments. One static strategy utilizes a posteriori error estimates that are furnished as part of our adaptive mesh-refinement process to calculate approximations of the computational effort needed to reduce the error estimate to prescribed levels. These work estimates are then used to schedule processors...
to balance loading.

A parallel adaptive procedure for solving elliptic problems on shared-memory computers has also been developed [7, 8]. Our technique combines quadtree mesh generation with $h$- and $p$-refinement. A preconditioned conjugate gradient method with either an element-by-element (EBE) or a symmetric successive over-relaxation (SSOR) preconditioner is used to solve the linear systems that arise from the finite element discretization. “Coloring” of arbitrary finite element meshes in order to avoid critical sections is a complex operation. By exploiting the underlying quadtree grid structure, we have developed procedures to color quadrants of the tree with six or eight colors. Four is provably the minimum number of colors that are needed; however, the six- and eight-color schemes have linear time-complexity. The six-color scheme performs significantly better than the eight-color scheme. Edge coloring schemes are being developed for higher-order finite element approximations.

We are anxious to have our adaptive software used by scientists and engineers and, in order to make it easier for them to do so, we developed a symbolic interface to our software [2, 3]. Users of this interface can describe their problems in a relatively natural language. Appropriate solution techniques are suggested after some dialogue with the user about the peculiarities of the problem at hand and code for evaluating functions, Jacobians, boundary conditions, etc., is generated automatically from the symbolic input and is linked with the relevant adaptive procedures.
2. Interactions

Professor Flaherty lectured and/or visited the following conferences and organizations during the period covered by this report:

J. E. Flaherty held technical discussions with Dr. John Walter of the U. S. Army's Ballistics Research Laboratory at the Rensselaer Polytechnic Institute, March 13, 1989.


J. E. Flaherty held technical discussions with Dr. Alex Woo of the NASA Ames Research Center at the Rensselaer Polytechnic Institute, April 25, 1989.

J. E. Flaherty and B. K. Szymanski (of Rensselaer's Computer Science Department) hosted the Fifth Parallel Computing Circus, April 28, 29, 1989 at the Rensselaer Polytechnic Institute. Approximately seventy scientists attended this symposium and featured twenty-one talks by faculty and graduate students.

J. E. Flaherty attended the Fourth International Conference on Supercomputing at Santa Clara, May 1-5, 1989. He presented an invited lecture on "An Environment for the Parallel Solution of Parabolic Partial Differential Equations."

J. E. Flaherty and R. Biswas, a graduate student supported by this grant, attended the Seventh Army Conference on Applied Mathematics and Computing at West Point, June 6-9, 1989. He lectured on "Numerical Experiments in Adaptive Mesh Methods."

J. E. Flaherty held technical discussions with Dr. John Walter of the U. S. Army's Ballistics Research Laboratory at the Rensselaer Polytechnic Institute, September 25, 1989.

J. E. Flaherty and P. K. Moore, a Postdoctoral Fellow supported by this grant, attended the workshop on Reliability in Computational Mechanics in Austin, October 26-28, 1989. J. E. Flaherty presented an invited lecture on "Parallel Computations with Adaptive Methods for Partial Differential Equations."


J. E. Flaherty and M. Benantar, a graduate student supported by this grant, attended the Fourth SIAM Conference on Parallel Processing for Scientific Computing in Chicago, December 11-13, 1989. He lectured on "Parallel Element-by-Element Techniques for Elliptic Systems using Finite Quadtree Meshes."


J. E. Flaherty attended a DARPA Meeting on "The Direct Simulation of Turbulence" in San Diego on May 14, 1990.
3. List of Publications.


