During the period covered by this report we continued our research on the development and application of adaptive numerical methods for singularly perturbed initial-boundary value problems for partial differential equations. We continued our analysis of the stability of mesh moving schemes for one-dimensional parabolic problems. We also developed a moving mesh scheme with local refinement for two-dimensional hyperbolic systems and are considering a similar scheme for parabolic problems.

We are applying our methods to several interesting physical problems, such as, elastic-plastic solids, combustion, and a nonlinear Schrodinger equation which exhibits self-focusing.

John P. Thomas, Capt
INTERIM SCIENTIFIC REPORT

Air Force Office of Scientific Research Grant AFOSR-80-0192

Period: 1 June 1984 through 31 May 1985

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

Principal Investigator: Joseph E. Flaherty

Department of Computer Science
Rensselaer Polytechnic Institute
Troy, New York  12181

Approved for public release: distribution unlimited.
ABSTRACT

During the period covered by this report we continued our research on the development and application of adaptive numerical methods for singularly perturbed initial-boundary value problems for partial differential equations. We continued our analysis of the stability of mesh moving schemes and developed local refinement and moving mesh schemes for one-dimensional parabolic problems. We also developed a moving mesh scheme with local refinement for two-dimensional hyperbolic systems and are considering a similar scheme for parabolic problems.

We are applying our methods to several interesting physical problems, such as, elastic-plastic solids, combustion, and a nonlinear Schrödinger equation which exhibits self-focusing.

During the period covered by this report, we continued our research on the development and application of numerical methods for singularly perturbed ordinary and partial differential equations. We concentrated on partial differential equations; however, two of our papers [1,2] on numerical methods for singularly perturbed two-point boundary value problems appeared in the literature.

Professor Flaherty and several colleagues and graduate students have been continuing their research on adaptive finite difference and finite element methods for partial differential equations. Their analysis of the stability of several mesh moving schemes for hyperbolic and parabolic problems has been accepted for publication in the *Journal of Computational Physics* [8].

In this study we categorized the stability or instability of a large class of mesh equidistribution strategies. Among other things, this work explains why many popular techniques produce meshes that oscillate wildly from time-step-to-time step whenever the partial differential system is dissipative and suggests some stable mesh moving procedures.

Drew and Flaherty created a model for shear band instabilities that involves the rapid shearing of a slab of a visco-elastic material with small

---

1 See the list of publications and abstracts at the end of this report.
viscosity. They used our moving mesh procedures and an adaptive finite element code\textsuperscript{2} to solve their model and illustrated several possible mechanisms for shear band formations. Some of their preliminary findings appeared in the proceedings of the conference on \textit{Phase Transformations and Material Instabilities in Solids} \cite{3}. They are extending their model to include visco-plastic materials and a more accurate energy equation. In a somewhat related study, Slemrod and Flaherty considered appropriate finite difference schemes for phase transitions involving van der Waals fluids. They submitted their initial findings to \textit{Res Mechanica} \cite{7}, but are anxious to conduct further studies using their finite difference schemes in an adaptive setting.

Moving grid methods are effective at reducing dispersive errors in the vicinity of wave fronts; however, no method that uses a fixed number of computational cells can be used to compute a solution to a prescribed level of accuracy. For this reason, we have been studying and developing techniques that perform explicit error estimations which are used to add and delete elements as the temporal integration progresses. In this spirit, Adjerid and Flaherty \cite{10} developed a finite element method of lines where the mesh "lines" are adaptively moved to minimize artificial diffusion, but where elements are added and deleted during the integration. Piecewise linear finite elements are used to calculate the numerical solution and $p$-hierarchic quadratic

elements are used to estimate its error. Mesh motion is accomplished using one of the stable schemes studied in [8]. Ordinary differential equations are obtained for the finite element solution, the error estimate, and the mesh coordinates and these may be solved using existing software for stiff systems. We have applied this procedure to several problems, including some difficult combustion studies, and found some very encouraging results.

The elementary global refinement strategy that was used in [10] could be inefficient in many situations. Additionally, the mesh moving algorithm of [10] required users to specify a parameter that controlled relaxation times to an "ideal" mesh that equidistributes local error estimates. We have remedied both of these deficiencies and are now using an efficient local refinement strategy and an adaptive procedure for selecting the mesh relaxation parameter. The details of these algorithms and the results of several computational experiments have been incorporated into a manuscript that will be submitted for publication shortly [13]. We are also extending our procedures to two-dimensional problems and expect to have an experimental code available for testing shortly.

The approach of Adjerid and Flaherty [10,13] couples mesh motion to the solution. This produces a method with great numerical stability; however, there are many instances where this extra effort is not necessary. Thus, we are considering adaptive local refinement techniques that use rectangular and trapezoidal space-time elements. These methods discretize and solve a problem for one time step using a finite element-Galerkin procedure. At the end of
the time step, the discretization error is estimated, finer subgrids of space-time elements are added to regions of high error, and the problem is recursively solved again on these regions. The process terminates and the integration continues to the next time step when the estimated error on each grid is less than a prescribed tolerance. Preliminary work using uniform grids of rectangular elements was reported by Flaherty and Moore [4,6]. A third paper describing several aspects of local refinement methods and comparing our approach with a finite element method of lines due to Bieterman and Babuska [11] will appear in Accuracy Estimates and Adaptivity for Finite Elements. This work was performed in collaboration with Dr. M. B. Bieterman of Boeing Computer Services.

There is more to be done with our space-time local refinement codes. Flaherty and graduate student M. J. Coyle are concentrating on developing p-hierarchic error estimation techniques that are similar to those of Adjerid and Flaherty [10,13] for the method of lines. The essential difficulty here is the absence of any superconvergence in time. Flaherty and graduate student P. K. Moore side-stepped the error estimation question by using Richardson's extrapolation and have been concentrating on the appropriate initial and boundary conditions to apply at course-fine mesh interfaces. Coyle, Flaherty, and Newell have been trying to apply these local refinement methods to a focusing problem for the nonlinear Schrodinger equation [16]. Additionally, Jackson and Flaherty extended the finite element basis to include discontinuous trial functions. They used these in conjunction with a moving mesh scheme.
of Harten and Hyman\textsuperscript{3} to develop a method that is extremely well suited to the solution of hyperbolic systems with shocks. The method captures shocks and contact surfaces as true discontinuities without any artificial diffusion or oscillations. They are incorporating their findings into a paper that will be submitted for publication shortly [14].

We have developed an adaptive finite difference method for two-dimensional initial-boundary value problems. Preliminary work on a technique that used MacCormack's method to solve hyperbolic conservation laws on a moving grid of quadrilateral elements was reported by Arney and Flaherty [5]. This mesh moving technique used a clustering algorithm of Berger\textsuperscript{4} to locate and group regions of high error into rectangles that isolate spatially distinct phenomena. An algebraic mesh moving function was then used to move and align the mesh with the regions of high error. This procedure is very efficient and, unlike many other two-dimensional mesh moving techniques, it has no problem-dependent parameters. A second report on this method that contains numerous improvements and several applications has been submitted for publication in the \textit{Journal of Computational Physics} [12].


Major D. C. Arney is a U.S. Army officer who is on educational leave from the U.S. Military Academy and will complete his Ph.D. studies this summer under Flaherty's direction. He has combined the technique of [5,12] with a recursive local refinement strategy and used it to create an adaptive finite difference code for nonlinear two-dimensional hyperbolic systems. The code has been applied to several difficult compressible flow problems that contain shocks, contact surfaces, and expansions. It appears to be able to utilize the best features of mesh moving and refinement. Results of this investigation will be presented in Arney's Ph.D. dissertation [15].

There is quite a lot of interest in adaptive methods on the RPI campus. This past academic year, Flaherty gave a graduate course on the subject which was attended by students in Mathematics, Computer Science and Engineering.
2. **Interactions**

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


J. E. Flaherty visited Professor M. F. Wheeler at Rice University, Houston, 9-11 March 1985, and lectured on "Moving Finite Difference and Finite Element Methods with Local Refinement for Time Dependent Partial Differential Equations."

3. List of Publications and Manuscripts in Preparation

Publications:


In Press:

A MOVING MESH FINITE ELEMENT METHOD
WITH LOCAL REFINEMENT FOR PARABOLIC
PARTIAL DIFFERENTIAL EQUATIONS

Slimane Adjerid
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180 USA

Joseph E. Flaherty
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, New York 12180 USA

ABSTRACT

We discuss a moving mesh finite element method for solving
initial-boundary value problems for vector systems of partial differential
equations in one space dimension and time. The system is discretized using
piecewise linear finite element approximations in space and a backward
difference code for stiff ordinary differential systems in time. A spatial
error estimation is calculated using piecewise quadratic approximations that
use the superconvergence properties of parabolic systems to gain computational
efficiency. The spatial error estimate is used to move and locally refine the
finite element mesh in order to equidistribute a measure of the total spatial
error and to satisfy a prescribed error tolerance. Ordinary differential
equations for the spatial error estimate and the mesh motion are integrated in
time using the same backward difference software that is used to determine the
numerical solution of the partial differential system.

We present several details of an algorithm that may be used to develop a
general purpose finite element code for one-dimensional parabolic partial
differential systems. The algorithm combines mesh motion and local refinement
in a relatively efficient manner and attempts to eliminate problem-dependent
numerical parameters. A variety of examples that motivate our mesh moving
strategy and illustrate the performance of our algorithm are presented.

We discuss an adaptive mesh moving technique that can be used with a finite element difference or finite element scheme to solve initial-boundary value problems for vector systems of partial differential equations in two space dimensions and time. The mesh moving technique is based on an algebraic node movement function determined from the geometry and propagation of regions having significant discretization error indicators. Our procedure is designed to be flexible, so that it can be used with many existing finite difference and finite element methods. To test the mesh moving algorithm, we implemented it in a system code with an initial mesh generator and a MacCormack finite difference scheme on quadrilateral cells for hyperbolic vector systems of conservation laws. Results are presented for several computational examples. The moving mesh scheme reduces dispersive errors near shocks and wave fronts and thereby reduces the grid requirements necessary to compute accurate solutions while increasing computational efficiency.

ADAPTIVE REFINEMENT METHODS FOR NONLINEAR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

Michael Bieterman
Boeing Computer Services
Engineering Technology Applications
Tukwila, Washington 98118 USA

Joseph E. Flaherty
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, New York 12180 USA

and

Peter K. Moore
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180 USA

ABSTRACT

We consider two adaptive finite element techniques for parabolic partial differential equations (PDEs) that are based on using error estimates to control mesh refinement. One technique is a method of lines (MOL) approach that uses a Galerkin method to discretize the PDEs in space and implicit multi-step integration in time. Spatial elements are added and deleted in regions of high and low error and are all advanced with the same sequence of varying time steps. The second technique is a local refinement method (LRM) that uses Galerkin approximations in both space and time. Fine grids of space-time elements are added to coarser grids and the problem is recursively solved in regions of high error.

A MOVING FINITE ELEMENT METHOD WITH ERROR ESTIMATION AND REFINEMENT FOR
ONE-DIMENSIONAL TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

Slimane Adjerid
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180

Joseph E. Flaherty
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, New York 12180

Dedicated in memory of Richard C. DiPrima

Abstract

We discuss a moving finite element method for solving vector systems of
time dependent partial differential equations in one space dimension. The
mesh is moved so as to equidistribute the spatial component of the
discretization error in $H^1$. We present a method of estimating this error by
using $p$-hierarchic finite elements. The error estimate is also used in an
adaptive mesh refinement procedure to give an algorithm that combines mesh
movement and refinement.

We discretize the partial differential equations in space using a
Galerkin procedure with piecewise linear elements to approximate the solution
and quadratic elements to estimate the error. A system of ordinary
differential equations for mesh velocities are used to control element
motions. We use existing software for stiff ordinary differential equations
for the temporal integration of the solution, the error estimate, and the mesh
motion. Computational results using a code based on our method are presented
for several examples.

NUMERICAL STUDY OF QUENCHING OF INWARD PROPAGATING SPHERICAL FLAMES

J.E. Flaherty
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, New York 12180

M. L. Frankel, V. Roytburd
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180

and

G. I. Sivashinsky
Department of Mathematical Sciences
Tel-Aviv University
Tel-Aviv 69978, Israel

ABSTRACT

The phenomenon of quenching of cylindrical convergent flames is considered in the framework of constant density approximation. The parameters dependence of the effect is studied numerically using an adaptive finite element method. The numerical results are in a good agreement with predictions of theoretical analysis from (Frankel and Sivashinsky, 1984).

ON THE STABILITY OF MESH EQUIDISTRIBUTION STRATEGIES FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

J. Michael Coyle, Joseph E. Flaherty and Raymond Ludwig

Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180 USA

ABSTRACT

We study the stability of several mesh equidistribution schemes for time dependent partial differential equations in one space dimension. The schemes move a finite difference or finite element mesh so that a given quantity is uniform over the domain. We consider mesh moving methods that are based on solving a system of ordinary differential equations for the mesh velocities and show that many of these methods are unstable with respect to an equidistributing mesh when the partial differential system is dissipative. Using linear perturbation techniques, we are able to develop simple criteria for determining the stability of a particular method and show how to construct stable differential systems for the mesh velocities. Several examples illustrating stable and unstable mesh motions are presented.

NUMERICAL INTEGRATION OF A RIEMANN PROBLEM
FOR A VAN DER WAALS FLUID

by

M. Slemrod

and

J. E. Flaherty

Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180

ABSTRACT

In two recent papers, Slemrod has suggested that the well known
Lax-Friedrichs finite difference method may provide a natural method for the
numerical integration of initial value problems with an anomalous equation of
state, e.g., a van der Waals fluid. In this note we review these ideas and
present the results of a numerical experiment which attempts to simulate the
dynamics of a van der Waals like fluid.

ON LOCAL REFINEMENT FINITE ELEMENT METHODS FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

Joseph E. Flaherty
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, N.Y. 12180

and

U. S. Army Armament Research and Development Command
Large Caliber Weapon Systems Laboratory
Benet Weapons Laboratory
Watervliet, NY 12189

and

Peter K. Moore
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, NY 12180

ABSTRACT

We discuss an adaptive finite element method for solving initial-boundary value problems for vector systems of partial differential equations in one space dimension and time. The method uses piecewise bilinear rectangular space-time finite elements. For each time step, the grid is automatically refined in regions where the local discretization error is estimated as being larger than a prescribed tolerance. We discuss several aspects of our algorithm, including the tree structure that is used to represent the finite element solution and grids, an error estimation technique, and initial and boundary conditions at coarse-fine mesh interfaces. We also present the results of several computational examples and experiments.

A MESH MOVING TECHNIQUE
FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS
IN TWO SPACE DIMENSIONS

David C. Arney
Department of Mathematics
United States Military Academy
West Point, NY 10996
and
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, NY 12180
and
Joseph E. Flaherty
Applied Mathematics and Mechanics Section
Benet Weapons Laboratory
Watervliet, NY 12189
and
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, NY 12180

ABSTRACT

We discuss an adaptive mesh moving technique that is used with a finite difference or finite element scheme to solve initial-boundary value problems for vector systems of partial differential equations in two space dimensions and time. The mesh moving technique is based on an algebraic node movement function determined from the propagation of significant error regions. The algorithm is designed to be flexible, so that it can be used with many existing finite difference or finite element methods. To test the algorithm, we implemented the mesh mover in a system code along with an initial mesh generator and a MacCormack finite volume integrator to solve hyperbolic vector systems. Results are presented for several computational examples. The moving mesh reduces dispersion errors near shocks and wave fronts and thereby can reduce the grid requirements necessary to compute accurate solutions while increasing computational efficiency.

AN ADAPTIVE LOCAL REFINEMENT FINITE ELEMENT METHOD
FOR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

Joseph E. Flaherty and Peter K. Moore
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180

ABSTRACT

We discuss an adaptive finite element method for solving initial-boundary value problems for vector systems of partial differential equations in one space dimension and time. The method uses piecewise bilinear rectangular space-time finite elements. For each time step, the grid is automatically refined in regions where the local discretization error is estimated as being larger than a prescribed tolerance. We discuss several aspects of our algorithm, including the tree structure that is used to represent the finite element solution and grids, an error estimation technique, and initial and boundary conditions at coarse-fine mesh interfaces. We also present the results of several computational examples and experiments.

ADAPTIVE FINITE ELEMENT METHODS
AND THE NUMERICAL SOLUTION OF SHEAR BAND PROBLEMS

Donald A. Drew and Joseph E. Flaherty
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180

ABSTRACT

Shear bands are localized regions of very high shear strain which arise as a result of high rates of loading. They occur in metal forming and cutting processes and in impact and penetration problems. In this paper, we describe a model for the formation of shear bands in simple shear that involves the description of irreversible mechanical shear and the resulting heat release. The location of a shear band is unknown in advance, and the evolution results in large gradients of displacement, velocity, and temperature. Shear band formation, therefore, offers an interesting and physically important application of a code able to resolve small-scale transient structures.

In this paper, we use an adaptive finite element code to solve several problems involving shear band formation. The code automatically locates regions with large gradients and adaptively concentrates finite elements there in order to minimize approximately the development of shear bands under many circumstances and indicate some possible mechanisms for their formation.

NUMERICAL METHODS FOR STIFF SYSTEMS OF TWO-POINT BOUNDARY VALUE PROBLEMS

Joseph E. Flaherty

and

Robert E. O'Malley, Jr.
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180 USA

ABSTRACT

We develop numerical procedures for constructing asymptotic solutions of certain nonlinear singularly perturbed vector two-point boundary value problems having boundary layers at one or both endpoints. The asymptotic approximations are generated numerically and can either be used as is or to furnish a general purpose two-point boundary value code with an initial approximation and the nonuniform computational mesh needed for such problems. The procedures are applied to a model problem that has multiple solutions and to problems describing the deformation of a thin nonlinear elastic beam that is resting on an elastic foundation.

ON THE NUMERICAL SOLUTION OF SINGULARLY-PERTURBED VECTOR
BOUNDARY VALUE PROBLEMS
by
Robert E. O'Malley, Jr.
and
Joseph E. Flaherty
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180 USA

ABSTRACT
Numerical procedures are developed for constructing asymptotic solutions of certain nonlinear singularly-perturbed vector two-point boundary value problems having boundary layers at one or both end points. The asymptotic approximations are generated numerically and can either be used as is or to furnish a two-point boundary value code (e.g., COLSYS) with an initial approximation and a nonuniform computational mesh. The procedures are applied to a model problem that indicates the possibility of multiple solutions and problems involving the deformation of a thin nonlinear elastic beam resting on a nonlinear elastic foundation.


In Preparation:


A DISCONTINUOUS FINITE ELEMENT SCHEME FOR HYPERBOLIC SYSTEMS OF CONSERVATION LAWS

T. L. Jackson
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180

Joseph E. Flaherty
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, New York 12180

ABSTRACT

We develop an adaptive finite element method for solving hyperbolic systems of conservation laws in one space dimension and time. The method uses discontinuous piecewise linear trial functions and continuous piecewise cubic test functions on a moving mesh of triangular space-time elements. The mesh is moved by a technique that uses a weighted average of the local characteristic speeds to select nodal velocities. We show that discontinuous finite element approximations on a moving mesh have the potential of accurately resolving physical discontinuities in the solution. Several computational examples are presented to illustrate the performance of the method.

AN ADAPTIVE MESH ALGORITHM FOR
SOLVING SYSTEMS OF TIME DEPENDENT
PARTIAL DIFFERENTIAL EQUATIONS

David C. Arney
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York  12180

ABSTRACT

We discuss an adaptive mesh algorithm that can be used with a finite difference or finite element scheme to solve initial-boundary value problems for vector systems of time dependent partial differential equations in two space dimensions. Our algorithm combines the adaptive techniques of mesh moving, static rezoning, and local mesh refinement. The nodes of a coarse mesh of quadrilateral cells are moved by a simple algebraic node movement function, determined from the geometry and propagation of regions having statistically significant discretization error or mesh movement indicators. The local mesh refinement method recursively divides cells of a moving coarse mesh within clustered regions that contain nodes with large error until a user prescribed error tolerance is satisfied. These finer grids are properly nested within the moving coarse mesh to provide for simpler data structures and interface conditions between the finer and coarser meshes.

Our procedure is designed to be flexible, so that it can be used with many existing finite difference and finite element schemes and with different error estimation procedures. To test our adaptive mesh algorithm, we implemented it in a system code with an initial mesh generator, a MacCormack finite difference scheme for hyperbolic vector systems of conservation laws, and a Richardson extrapolation based error estimation. Results are presented for several computational examples.

The moving mesh technique reduces dispersive errors near shocks and wave fronts. Therefore, it reduces the grid requirements necessary to compute accurate solutions and thus increases computational efficiency. The local mesh refinement provides smaller mesh spacings and time steps in regions where the problem is difficult to solve, thus providing increased accuracy and enabling error tolerances to be achieved.

To be submitted to the faculty of Rensselaer Polytechnic Institute in partial fulfillment for the degree of Doctor of Philosophy in Mathematics.
FOCUSING PROBLEMS FOR A NONLINEAR SCHRODINGER EQUATION

J. M. Coyle

and

Joseph E. Flaherty
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12180 USA

and

Alan C. Newell
Program in Applied Mathematics
University of Arizona
Tucson, AZ 85721 USA

ABSTRACT

We consider a cylindrically symmetric Schrodinger equation with a cubic nonlinearity. It is known that this equation has solutions that self-focus if the initial data is strong enough. We study this problem numerically using a self-adaptive finite element code and seek to determine (i) the quantitative nature of the solution as it focuses and (ii) whether the solution will still focus in the presence of a small amount of dissipation.

In preparation for Physica D.
END

FILMED

11-85

DTIC