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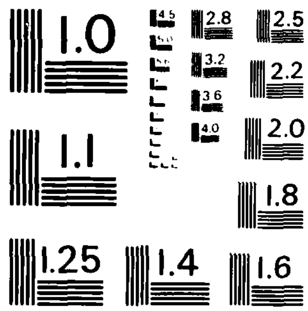
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This research was an effort to explore further the promise of the moving finite element method for the solution of difficult large-gradient PDE problems in 2-D. The results of this research indicate that: (i) the MFE method does extend logically and practically to 2-D, and (ii) extensive continuing research is needed in several task areas in order to advance further applications of the MFE method, per se, and to also pursue further advances which are essential to all adaptive PDE solution methods.

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MOVING FINITE ELEMENTS IN 2-D

FINAL REPORT

June 30, 1983

U.S. ARMY RESEARCH OFFICE

CONTRACT NUMBER DAAG29-81-C-0020

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1. FOREWORD

The moving finite element (MFE) method was discovered in the mid-1970's by Professor Keith Miller at U.C. Berkeley. By the late 1970's a small number of other researchers had successfully applied this novel numerical solution method for partial differential equations (PDE's) to several large-gradient test problems in 1-D. The early results were quite surprising and, in some cases, startling with regard to the apparent capacity of the MFE method to resolve highly disparate scales of physical dissipation processes in advection-diffusion problems. Such persistent computational dilemmas as Gibbs overshooting and undershooting, numerical diffusion, grid node tangling, small grid aspect ratios, and remap aliasing, which had historically hindered the resolution of many other numerical PDE solution methods, were essentially eliminated by the MFE method. In subsequent 1-D applications in gas dynamics, continuum mechanics, thermal hydraulics, and laser design problems, physical dissipation effects which occur over extremely small scales in shocks and other large-gradient travelling waves were resolved with very high levels of accuracy and grid node economies. But notwithstanding these promising results in 1-D, it was by no means certain that the MFE method could be extended effectively to 2-D.

Faced with considerable scientific risk, the presently reported research effort embarked in 1981 on an effort to explore further the promise of the MFE method for the solution of difficult large-gradient PDE problems in 2-D. The results of this research which are reported below indicate that: (i) the MFE method does extend logically and practically to 2-D, and (ii) extensive continuing research is needed in several task areas in order to advance further applications of the MFE method, per se, and to also pursue further advances which are essential to all adaptive PDE solution methods.

The investigators in this research effort acknowledge with special gratitude the support by the Army Research Office of this novel research at that critical early time when the scientific risks and uncertainties were so great.

2. TABLE OF CONTENTS

3. FINAL REPORT

A. Statement of the Problem

As discussed in the Foreword, the MFE method is a new PDE solution approach in which the grid co-ordinates themselves are dependent variables which are calculated continuously at each time step in order to minimize PDE residuals. It is now known that such a PDE approach with all of the distinctive features of the MFE method had never been investigated extensively and reported prior to the work of Miller[1,2] and of Gelinas, Doss and Miller.[3] Given the early developments of the MFE method in 1-D, the objectives of the present research effort were simple and clear: (i) to gain an improved understanding of the basic mathematical and numerical properties and needs of the MFE method in higher spatial dimensions, and (ii) to reduce the MFE method to practice for the solution of important classes of PDE's in 2-D.

B. Summary of the Most Important Results

This summary is presented in two segments. The first segment summarizes briefly the significant milestones which have already been reported in journal articles and in technical conference proceedings during this project; and the second segment discusses in somewhat greater detail those significant results, and especially future research needs, which have not yet been presented extensively in either journal submittals or at technical conferences.

1. Summary of Previously Reported Results

- The MFE method does reduce to practice in 2-D logically and practically for large classes of large-gradient travelling wave problems;

- The MFE method with simple regularization functions and simple grid triangularizations solves pure advection (planar square wave), advection-diffusion (Burger's and Navier-Stokes equations for planar shocks), and heat transfer problems in 2-D with high levels of accuracy, stability, and nodal efficiency.

- *Extremely large grid aspect ratios* ($O(10^3)$) *can be used effectively in* 2-D MFE computations;

- Direct matrix solution of the MFE equations by L-U decomposition is accurate and reliable for small grid meshes (10 x 10); but becomes storage-limited for large grid meshes. The MFE method and other potent PDE solvers contain highly skewed matrices which do not have diagonally dominant terms in the solution of many advection-diffusion problems on inhomogenous grid meshes. Advanced iterative matrix solvers have been developed in this work which provide significant advantages in such matrix problems vis à vis existing iterative solvers which have previously been used mostly for elliptic equations on relatively uniform grid meshes.

- Zero-Neumann and Dirichlet boundary conditions are used effectively on simple problem domains for planar and moderately skewed waveforms.

- The additional degrees of freedom which are available in 2-D for nodal motions have a beneficial effect on MFE integration properties and on MFE nodal economy, vis à vis comparable results of identical test problems on the more highly constrained grid meshes in 1-D.

- MFE code structures in 2-D are amenable to vectorization and to efficient use on envisioned *advanced computers*.

2. Summary of Previously Unreported Results

Having established the early milestones mentioned above, work currently in progress is focussed on a host of issues and research needs which are essential not only for the MFE method but also for any other advanced adaptive mesh PDE method which may be used in truly large-scale 2-D computations. As in the past, some of the emerging MFE results in 2-D may be *unique and/or contrary to some conventional wisdoms. In any case,* the emerging MFE results in 2-D suggest important lines of research which should be pursued more intensively in the future by both ourselves and others. The discussion in this section will draw heavily upon the work discussed in Reference 4 and will emphasize research needs and perspectives.

- MFE Node Movement Properties

The highly skewed Burger's problem with shock gradients of 10^3 on a 16 x 16 grid mesh in Reference 4 exhibits extensive nodal migrations and extensive shearing over nearly the entire problem domain. Consequently, the MFE method enjoys huge nodal savings (by factors of 10^4-10^6) relative to other fixed node or non-optimal adaptive PDE solution methods in this problem. It is important to note here that the Laplacian operator in Burger's model equations represents actual physical dissipation processes which cannot be legitimately eliminated or otherwise obscured or ignored by numerical PDE solution methods. Inviscid solvers are thus inappropriate in Burger's model problems because they not only neglect Laplacian operators in the PDE's under study but, in addition, generate shocks with gradient shapes and magnitudes that are governed exclusively by the selected grid spacing or by purely numerical dissipative processes in the inviscid method, per se. This critical discussion is not intended to denigrate the extensive research efforts on inviscid PDE solvers and/or fixed node PDE methods where they legitimately apply; but it does suggest that efforts to accommodate Laplacian operators of physical processes and efforts to investigate more optimal adaptive grid methods for use in many existing PDE methods which are applied to physical advection-diffusion problems should now assume greatly increased significance. In the meantime, the MFE method is proving to be a certain kind of research pacesetter, and it is providing various clues to some of the other significant areas where mathematics research can profitably be intensified, as will be discussed further below.

- ODE Solvers for PDE Methods

The current effort has shown that most existing ODE solvers are not well-suited for ready implementation in either the MFE method or numerous other advanced PDE methods. This critical comment is, again, not intended to denigrate the impressive advances in ODE research and development during the past decade; instead, it is intended to bring a strong new focus upon the needs of PDE solution methods, in general, and more specifically upon the pressing needs of adaptive grid PDE methods which use stiff ODE solvers to solve discretized PDE's on highly distorted grids. (Large, distorted grid meshes may, in turn, augur for iterative linear solvers which can solve poorly conditioned matrix equations, as will be discussed further below.)

A basic difficulty which has come to the fore in the present MFE research is that most ODE solver packages have been designed to accommodate many different types of classic ODE problems. By classic, one refers here to such problems as chemical kinetics systems in which the dependent variables (e.g. species concentrations) are all generically the same. The error and time step controlling policies in solvers designed for classic ODE problems are usually less than satisfactory for applications to PDE solution methods. In PDE systems, the spatial dependence of generically dissimilar variables comes into play. In fluid dynamics problems, for example, the overall array of PDE variables which have been discretized on N grid nodes $(x_1, x_2, \ldots, x_N)$ can be represented as $\{\rho_1, m_1, E_1; \rho_2, m_2, E_2; \ldots; \rho_N, m_N, E_N\}$, where $\rho_1 \equiv \rho(x_1)$, $\rho_2 \equiv \rho(x_2)$, etc. An ODE solver then operates on this array of discretized PDE variables as a single large vector $\{y_1, y_2, y_3, y_4, \ldots y_{3N-2}, y_{3N-1}, y_{3N}\}$, where $y_1 = \rho_1$, $y_2 = m_1$, $y_3 = E_1$, $y_4 = \rho_2$, etc. Because the error control policies in the Gear ODE package, for example, are based upon an L^2 norm of all normalized quantities $y_i/(y_i)_{max}$, unacceptably large errors can be admitted in some individual components of ρ, m, or E at arbitrary spatial locations. A much better measure for error control policies in PDE applications are maximum norms applied to each discretized PDE variable. The implementation of alternative norms is found to extend deeply into the logical structure of most ODE software packages, and alterations must usually be performed by someone who is intimately familiar with the ODE package.

Significant levels of effort have thus been devoted in our recent work to revisions of Gear's basic ODE method for MFE computations. This has involved wholesale alterations of the internal Gear code structure, extensive considerations of scaling of MFE problem variables, and inevitably, the development of entirely new ODE integration procedures which better serve PDE solution needs.

These extensive modifications of Gear's ODE solver have sufficed to solve moderately challenging PDE's with modest numbers of MFE grid nodes as can be seen in the References and in Section C below. But it is now clear, also, that completely new ODE code structures will be needed in pending large-scale MFE computations. We have, therefore, undertaken the development of a low-order Runge-Kutta integration package for MFE computations. This solver addresses several PDE needs: First, error control measures operate on flexibly ordered variable arrays using maximum norms on a (PDE) component-by-component basis. Second, PDE solutions have been found to require much more gradual time step advancement policies than have been built into most classic ODE solvers.* This distinction between classic ODE and PDE time step properties apparently stems from the fundamentally coupled space-time dependences in PDE systems, vis à vis classic ODE problems which have no direct or implied spatial dependences. Whereas it is computationally worth the effort to attempt very large incremental increases (sometimes by several orders of magnitude) in Δt in classic ODE applications -- even if such attempts may sometimes fail -- one finds that the computational penalties for unsuccessful large Δt increases in PDE applications are much more severe because space-time couplings augur intrinsically for more gradual Δt advancement policies. Third, time step control policies now include convergence criteria for the use of iterative linear systems solvers in the ODE package. Such iterative solvers should henceforth be used in large-scale MFE computations in order to minimize computer memory requirements. Fourth, low-order ODE methods are now used because high-order solvers provide no apparent advantages in MFE applications and because low-order methods simplify the numerical logic, improve the code reliability, and avert possible errors associated with changes of order which are sometimes present in classic ODE system solvers. Finally, constraints on allowable fractional changes in PDE dependent variables are incorporated in the overall time step control policy in the new ODE solver. This new ODE solver is presently being implemented for use in large-scale MFE computations. Detailed descriptions of this solver, in conjunction with MFE test applications, should appear in forthcoming journal submissions.

*These policies also extend deeply into the ODE code structure.

From these initial results it is clear that renewed ODE research efforts on PDE-related problems, from several possible conceptual bases, is now timely if not long overdue. Our own efforts have barely begun to uncover many of the most pressing needs, much less to perform the extensive detailed tasks of numerical analysis which should now be pursued. Certainly, current PDE research would benefit from expanded ODE efforts which deal with: (i) scaled and unscaled systems of incommensurate variables on arbitrarily connected grid meshes, (ii) linkage of certain Δt-sensitive convergence criteria into the general ODE integration control policy, and (iii) splitting of the solution of the grid node equations from the solution of the discretized equations for the physical variables.

- Linear Solvers for the MFE Method

Advection-diffusion equations have steadfastly resisted (if not defied) satisfactory numerical solution whenever they have been used to describe physical processes over highly disparate scales. The basic difficulty derives from the nature of the matrix equations which must be solved in numerical PDE methods that are applied to these problems. The matrix equations for discretized advection-diffusion PDE's are large, sparse linear systems in which the matrices are non-symmetric and are not dominated by terms on the diagonal. The skewness of these PDE matrices can become quite large for large Δt's and for highly distorted grid meshes, both of which are key factors in efficient solutions by any numerical method of these types of advection-diffusion equations.

Testing and analysis in this recent MFE work has revealed that most available linear solvers have relatively poor rates of convergence when such significant large elements can occur away from the diagonal in non-symmetric matrices. For example, such iterative matrix solution methods as conjugate gradient, multi-grid and numerous other modern linear systems solvers which work well for symmetric matrices in discretized elliptic equations and/or for uniform grid meshes do not converge satisfactorily in presently considered advection-diffusion problems. The source of difficulty for the existing linear solvers clearly derives from the highly skewed matrices and their off-diagonal dominance. We have also shown that the direct L-U decomposition method which has been used in the Gear method until recently becomes both noisy and computer-storage limited when large bandwidths arise in problems with more than a moderate number of MFE grid nodes. Again, we do not wish to denigrate the extensive ongoing work on linear systems solvers--but, rather, to call attention to these essential keys to further progress in PDE research.

In view of these findings, we have developed in collaboration with Professor Keith Miller one promising new approach to handling more effectively those imposing PDE requirements on linear systems solvers. This new matrix solution scheme has, so far, achieved good convergence rates for Δt's which may be 10 to 20 times greater than the large values of Δt called for by the ODE integrator. (It is generally hoped in PDE solutions that the time step size is determined by the truncation error of the ODE integrator and not by severely limited convergence properties of the linear solver.) This advanced linear solver has solved the Burger's equations discussed above with the same CPU cost as the direct L-U decomposition method in the Gear solver; but the iterative solver operates successfully with greatly reduced storage requirements. Implementation of this new linear solver for large-scale MFE computations is progressing well, and details of this new approach may appear in future journal submissions. Clearly, our initial efforts on a more adequate linear solver for advection-diffusion problems have only barely opened a new facet of research which now warrants much more intensive theoretical and practical analyses, both by ourselves and by many others.

- Regularization

Regularization techniques have rarely been used systematically, if at all, in PDE research in the past. There is thus presently great confusion and misunderstanding of the role of regularization techniques in PDE solution methods. On the one hand, many practitioners of conventional PDE methods suspect that regularization is an unfair trick by which one can force PDE solutions to come out in any desired manner and that such methods, therefore, cannot be trusted. On the other hand, regularization methods are proving to be valid and powerful mathematical tools which can now be applied to achieve effective grid movement criteria systematically and to ensure that high PDE solution accuracy is also achieved in the process.

Only the simplest, first-generation regularization functions have been used in 2-D MFE problems to date. These penalty functions act like springs and/or dashpots in their action on mesh triangle altitudes. The current MFE penalty functions in 2-D allow mesh triangles to distort more or less arbitrarily, so long as mesh altitudes remain positive and maintain some designated minimum length. This simple strategy has worked remarkably well in a broad range of 2-D problems, including all of the results discussed in this report. We are presently probing the limits of adequacy of this simple first-generation regularization method in such extended applications as Mach stems in gas dynamics and dynamic impact problems in continuum mechanics because in the long run there is no fundamental reason, or desire, for the MFE mesh to always be as highly skewed as physical flow lines in extremely sheared flows. (It is nevertheless encouraging at this stage of development that the mathematical potency of the MFE method is sufficiently great to handle such large grid aspect ratios effectively.) Alternative regularization criteria which would promote mesh homogeneity (e.g., by minimization of grid triangle aspect ratios) are presently under consideration for use in conjunction with the first-generation regularization functions. These new criteria are expected to improve numerical conditioning properties and thus lead to greater computational economy in MFE codes. Mesh homogeniety should also be a significant factor in applications which must resolve turbulent eddies and/or other rotating flows.

We have now barely opened a potentially vast area of investigation of regularization techniques for adaptive PDE meshes. This is certainly one of the key areas where we, and perhaps many others, can profitably expend greater efforts, particularly in view of the very attractive MFE properties which are emerging in: (i) alternative co-ordinate systems and (ii) the treatment of interface phenomena, both of which have a direct bearing on, and relationship to, alternative regularization methods. Here also the MFE method serves as a certain type of research forecaster in suggesting means of applying these new mathematical methods of regularizing PDE node motions in both new and conventional PDE methods so as to resolve such historically persistent dilemmas as singularities at origins of spherical and cylindrical coordinate systems, artificial smearing of interfaces, unduly constrained grid aspect ratios, numerical diffusion, severe time step constraints, and efficient grid node utilization.

- Alternative Co-ordinate Systems

Initial work is in progress on 2-D MFE calculations in cylindrical co-ordinates. These results also provide guidance for later developments in spherical co-ordinates. The major issue of present interest is the apparently natural elimination of singularities at the origin. Such singularities have historically plagued many conventional PDE methods. But now the MFE discretization is formulated in terms of well-defined inner products which eliminate such possible singularities. For example, the inner products of the term (y/r) with the MFE basis function α, taken over the interval Δr, is given by

$$\int_{\Delta r} (y/r) \cdot \alpha \cdot r dr = \int_{\Delta r} y \cdot \alpha dr \quad .$$

The integral of $\alpha \cdot y \, dr$ is essentially analytic and is readily evaluated everywhere on the problem domain. This attractive MFE property in cylindrical co-ordinates obviously holds in a similar manner in spherical co-ordinates. The properties of these r-weighted norms are naturally different than the MFE inner products which were used in the Cartesian co-ordinate systems considered in earlier MFE work. Analysis and testing of these properties associated with r-weighted norms and of node controlling penalty functions in cylindrical coordinates have been undertaken recently and extensive continuing work is needed in order to understand and exploit the benefits of this analytic MFE formulation of otherwise troublesome PDE operators in cylindrical and spherical co-ordinates.

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C. List of Publications and Technical Reports

1. Gelinas, R.J., S.K. Doss, and N.N. Carlson, "Moving Finite Element Research for Shock Hydrodynamics, Continuum Mechanics, and Combustion," Proceedings, First Army Conference on Applied Mathematics and Computing, Sponsored by the Army Mathematics Steering Committee, George Washington University, Washington, DC, May 9-11, 1983.

2. Gelinas, R.J., S.K. Doss, and N.N. Carlson, "Moving Finite Element Solutions of Shock Interaction Effects," Proceedings, Fluid Interface Instabilities and Front Tracking Workshop, Los Alamos National Laboratory, Los Alamos, NM, February 1-4, 1983.

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8. R.J. Gelinas and S.K. Doss, "DYLA - Moving Finite Element Code in 1-D: User Instruction Manual," Science Applications Report prepared for EG&G, Idaho Falls, ID, May 1981.

Manuscripts in Preparation

Seven manuscripts are in various stages of preparation for journal submission, as indicated below:

Title	Authors	Journal
1. Analytic Properties of the MFE Method	S.K. Doss, N.N. Carlson, R.J. Gelinas	SIAM
2. Applications of The Moving Finite Element Method in 2-D	R.J. Gelinas, S.K. Doss, K. Miller, N.N. Carlson	J.Comp.Phys.
3. Real Versus Non-Physical Dissipation Processes in Shock Calculations	R.J. Gelinas, S.K. Doss, N.N. Carlson	J.Applied Physics
4. An O.D.E. Solver for PDE Applications	K. Miller, N.N. Carlson, S.K. Doss	J.Comp.Phys.
5. Irregular Reflection of Planar Shocks in 2-D	R.J. Gelinas, S.K. Doss, N.N. Carlson	Physics of Fluids
6. Applications of the MFE Method in Continuum Mechanics	R.J. Gelinas, S.K. Doss, N.N. Carlson	J.Comp.Phys.
7. Analysis of Alternative Basis Functions in the MFE Method	S.K Doss, N.N. Carlson, R.J. Gelinas	J.Comp.Phys. or SIAM

D. Participating Personnel

The personnel associated with this research effort are:

Mr. Neil N. Carlson	(Neil is a full-time SAI employee with a B.S. degree in Mathematics. He will enroll as a graduate student in Mathematics at U.C. Berkeley in Fall, 1983. He will probably pursue his Ph.D. degree as a student of Prof. Keith Miller.)
Dr. M. Jahed Djomehri	(Student of Prof. Keith Miller; graduated with Ph.D., 1983.)
Dr. Said K. Doss	
Dr. Robert J. Gelinas	
Dr. J. Peter Vajk	
Programmers	(O. Ofiesh, S. Schell, and D. Robles)

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