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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)
The moving finite element (MFE) method is a new PDE solution method which has shown significant promise in 1-D for the numerical solution of some of the most difficult problems under study with extremely large, but finite, gradients. The overall objective of the present research is to explore further the promise of the continuous node moving properties of the MFE method in 2-D. For this, both the logical structure of the MFE method and its reduction to practice in 2-D are under investigation in this project. This initial (CONTINUED)

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research in 2-D focuses upon such simple conservation equations as heat, travelling wave, and Burger's equations. Work in this initial reporting period has resulted in significant computational economies for both unvectorized versions of the MFE method as it currently exists and for vectorized versions which may emerge in later efforts. A working test code which is needed for essential scientific exploration and further enhancement of the MFE method in higher dimensions has been brought to nearly an operational stage of execution during this period.

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MOVING FINITE ELEMENTS IN 2-D

First Research Progress & Forecast Report

Reporting Period: June 8, 1981 to December 8, 1981

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MATTHEW J. KERPER

Chief, Technical Information Division

I. MATHEMATICAL INTRODUCTION

In order to discuss concisely the progress of research during this reporting period, the basic formulation of the MFE method in 2-D is presented immediately below.

Consider a general system of PDE's, $\dot{U} = L(U)$, or

$$\begin{aligned}\dot{u}_1 &= L_1(U) \\ \dot{u}_N &= L_N(U)\end{aligned}\quad (1)$$

Using piecewise linear approximants of $u_k = \sum_j a_{kj}(t) \cdot \alpha_k^j(x, y)$ on a hexagonally connected triangular mesh (see Figure 1), application of the chain rule to the differentiation of u_k gives

$$\dot{u}_k = \sum_j \dot{a}_{kj} \alpha_k^j + \dot{x}_j \beta_k^j + \dot{y}_j \gamma_k^j, \text{ where} \quad (2)$$

$$\alpha_k^j = \frac{\partial u_k}{\partial a_{kj}}, \quad \beta_k^j = \frac{\partial u_k}{\partial x_j}, \quad \gamma_k^j = \frac{\partial u_k}{\partial y_j}. \quad (3)$$

The functions α_k^j , β_k^j , and γ_k^j are basis functions at each node, j , corresponding to the effect on the piecewise linear functions u_k by the $N + 2$ parameters a_{kj} , x_j , and y_j . It can be shown readily by taking tiny increments in a_{kj} , or x_j , or y_j that all three basis functions α , β and γ are piecewise linear functions having their support in the hexagon of six triangles surrounding the j^{th} node. It turns out that α_k^j is independent of k ; it is continuous and takes on the value 1 at the center of the hexagon and 0 at the other nodes. The functions β_k and γ_k are discontinuous at the center and on the inner edges of the hexagon; they vanish identically on the outer edges of the hexagon.

Ordinary differential equations (ODE's) are derived for the parameters of the MFE method by requiring that the parameter derivatives $\{\dot{a}_{1j}, \dots, \dot{a}_{Nj}, \dot{x}_j, \dot{y}_j\}$ are evaluated at each instant so as to formally minimize the L^2 norm of the PDE residuals, $\dot{U} - L(U)$, plus regularization terms. The variational equations for this minimization yield the following system of ODE's:

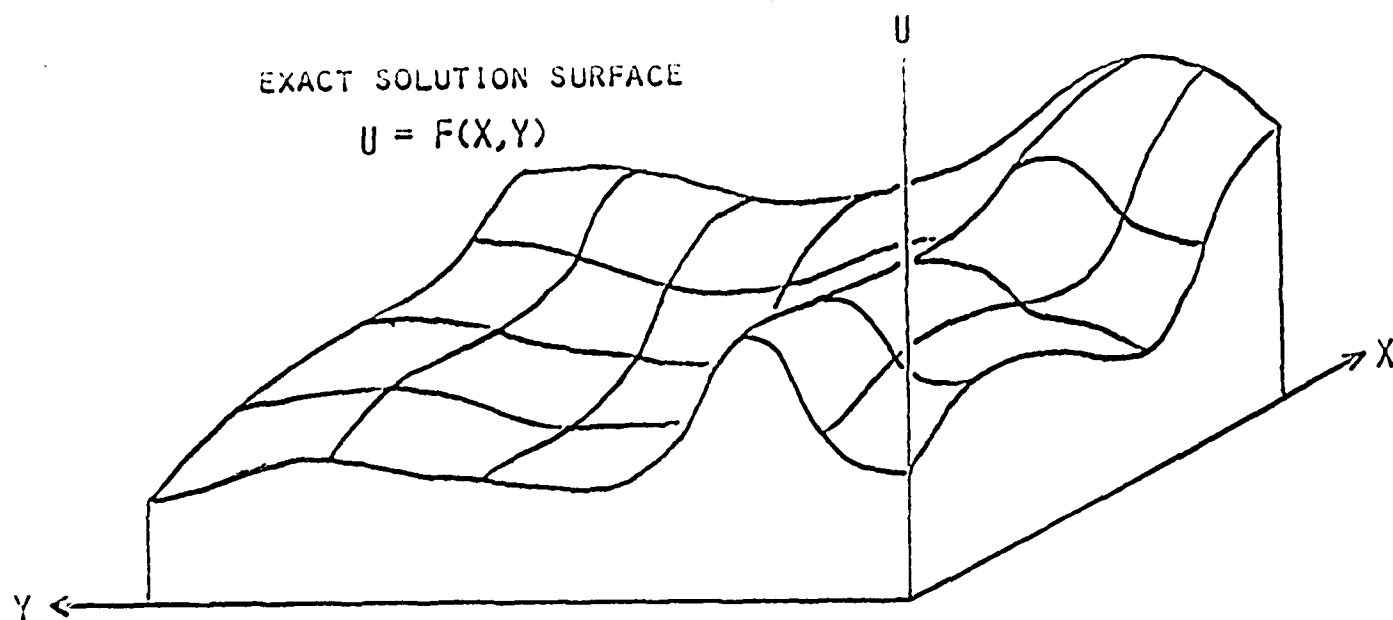


FIGURE 1-A. EXACT SOLUTION SURFACE, WITH LINES OF
 CONSTANT X AND CONSTANT Y .

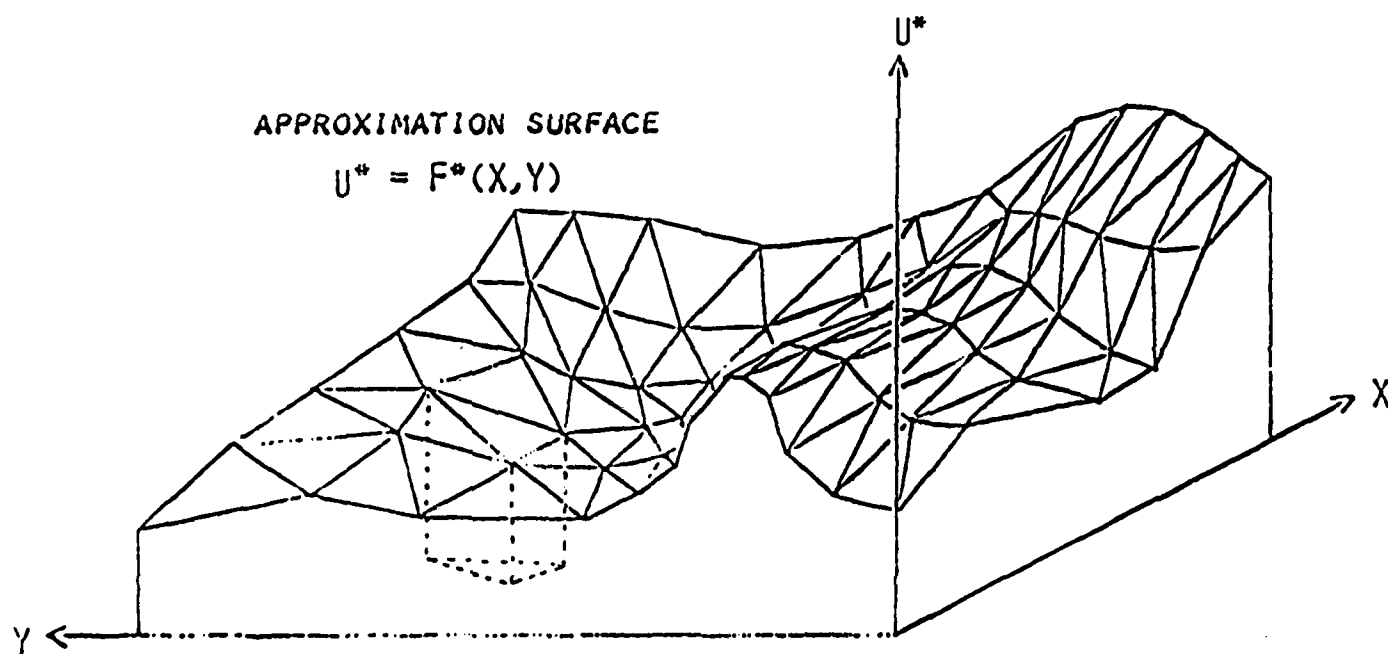


FIGURE 1-B. APPROXIMATE SOLUTION REPRESENTED BY
 PIECEWISE LINEAR FUNCTIONS MAKING UP
 HEXAGONALLY CONNECTED TRIANGULAR FACETS.
 IFE UNKNOWNNS ARE $\{a1_j, \dots, aN_j, x_j, y_j\}$

$$\sum_j (\alpha^j, \alpha^i) \dot{\alpha} k_j + (\beta k^j, \alpha^i) \dot{x}_j + (\gamma k^j, \alpha^i) \dot{y}_j = (L_k(U), \alpha^i) \text{ for } k = 1, \dots, N, \quad (4a)$$

$$\begin{aligned} \sum_{k=1}^N \sum_j (\alpha^j, \beta k^i) \dot{\alpha} k_j + (\beta k^j, \beta k^i) \dot{x}_j + (\gamma k^j, \beta k^i) \dot{y}_j \\ = \sum_{k=1}^N (L_k(U), \beta k^i) + (\text{regularization terms}) \end{aligned} \quad (4b)$$

$$\begin{aligned} \sum_{k=1}^N \sum_j (\alpha^j, \gamma k^i) \dot{\alpha} k_j + (\beta k^j, \gamma k^i) \dot{x}_j + (\gamma k^j, \gamma k^i) \dot{y}_j \\ = \sum_{k=1}^N (L_k(U), \gamma k^i) + (\text{regularization terms}) \end{aligned} \quad (4c)$$

The sums on j in Eqns. (4) run over the seven neighboring nodes of i (including the i^{th} node itself) in the hexagonal grid. Equations (4) thus provide the basic working equations of the MFE method in 2-D. This system of ODE's is written for purposes of numerical solution in the form

$$C(y)\dot{y} - g(y) = 0, \quad (5)$$

where $y(t) = (a_1, \dots, x_1, y_1; a_2, \dots, x_2, y_2; \dots)$ is the vector of unknown parameters, and the "mass matrix" $C(y)$ is symmetric and positive definite. This system of ODE's can be extremely stiff, and such stiff ODE solvers as the Gear method and an implicit Runge-Kutta method are used for the numerical solutions of Equations (4) and (5).

Obviously, the evaluation of the numerous inner product terms in Eqns. (4) is tedious, and the overall organization of an efficient code structure for the general solution of Eqns. (4) and (5) in 2-D is quite exacting. These are the major tasks which have been performed during this reporting period and which will be summarized and discussed further below.

RESEARCH PROGRESS

The overall objective of this research is to explore the promise of the continuous node moving properties in 2-D of the MFE method (a new numerical PDE solution method) for the effective solution of problems with extremely large, but finite, gradients. Such problems arise in numerous scientific and engineering applications which are of interest to the U.S. Air Force. Accordingly, this research necessarily involves both fundamental analysis of the numerical method, itself, and reduction to practice of the MFE method in order to carry out the essential scientific testing and advancement of the basic method in higher dimensions.

Problems which can be written in conservation form as

$$u_t = -c_1 \cdot f_x - c_2 \cdot g_y + c_3 \cdot (u_{xx} + u_{yy}) \quad (6)$$

are being investigated in the current stages of research. The immediate objective of this first year's research is to develop a working MFE code in 2-D which can solve such simple equations as the heat equation, a single travelling wave, and Burger's equations, in order to study at an early date the basic node moving properties of the MFE method in 2-D. (All of these simple equations are obtained by appropriate choices of coefficients c_1 , c_2 , and c_3 and functions f_x and g_y in Eqn. (6).) The first working code version is nearly operational at this time. Table 1 presents a brief summary of the status of essential tasks conducted in this research.

DISCUSSION AND ADDITIONAL INFORMATION

The work during this reporting period has been heavily devoted to code development and analysis of the logical structure of the MFE method in two dimensions. As a result of these efforts, significant computational economies have been realized for both unvectorized versions of the method as it currently exists and, more importantly, for vectorized versions which will undoubtedly emerge in later efforts.

TABLE 1 - SUMMARY OF PROGRESS

Basis Functions

MILESTONE: Using piecewise linear basis functions, develop inner products of the operators in Eqn. (6) by numerical integration.

STATUS: Completed. Some operators in gas dynamics equations have also been evaluated, coded, and tested. Both simple and composite Simpson's (Newton-Cotes) methods are used on triangle edge (line) integrations. Both simple and composite midpoint rules are used for integrations on triangle areas.

Regularization

MILESTONE: Develop penalty functions which prevent grid mesh tangling for the MFE nodes.

STATUS: Completed.

Grid Mesh Generation

MILESTONE: Assess automatic grid mesh generators for compatibility with the data structures in the MFE method.

STATUS: Scoping completed.

Matrix Solution

MILESTONES:

- (a) Apply existing direct factorization methods.
- (b) L-U decomposition of banded matrix.
- (c) Point and line relaxation methods.
- (d) Alternating Direction Implicit (ADI).

STATUS: Completed.

STATUS: Completed.

STATUS: Completed.

STATUS: Two-directional ADI completed. Dynamic ADI in three directions warrants additional research, as do efficient iterative matrix solution methods.

Boundary Conditions

MILESTONES:

- (a) Stationary Dirichlet and zero-Neumann conditions.
- (b) Time-dependent Dirichlet conditions.
- (c) Non-zero Neumann and mixed boundary conditions.

STATUS: Completed.

STATUS: Completed.

STATUS: Barely started.

The nature of these economies are illustrated, for example, by the structure of equations (4) above which are written on a node-by-node basis (via the summations over j on nodes). Although compact for purposes of theoretical derivations and expositions, this node-by-node ordering of operations turns out not to provide the most efficient architecture for MFE computations of those PDE operators which appear in Eqn. (6). Alternatively, the structure of the MFE method and the topology of hexagonally connected triangular basis functions lend themselves to both logical and practical computational economies when the method is executed on a triangle-by-triangle basis. This alternative course is the one which is being implemented in the present work.

In scoping studies of grid mesh generation methods, it has become evident that hexagonally connected triangular mesh generation methods are basically compatible with the MFE method. The logical structure and mode of PDE solution execution by the MFE method again contributes to this conclusion. So long as the MFE method continues to exhibit robustness in its continuous node movement properties, the use of grid mesh generation routines would be required only for problem initializations. All solution regridding subsequent to initialization is continuously performed, in effect, by the MFE method itself based upon its own stringent minimization criteria. It is, in fact, preferable to not introduce a generically different mesh generation method on an in-line basis into the transient MFE solutions. This anticipated restriction to problem initializations reduces greatly the role and the demands upon other mesh generation methods which would be used in conjunction with the MFE method. In those problems which may require some infrequent remapping of MFE solutions in order to reach final solutions, one would undoubtedly choose to interrupt the MFE solution, regrid the numerical PDE solution data at that stage, and then proceed again with the MFE solution as a new initial-value problem. For this type of procedure, the MFE method would be viewed as the dynamic mesh generation procedure and the alternative mesh generation method would be viewed as the static initialization procedure. It thus appears that if any revisions at all are required, it would be only minor alterations of mesh indexing and of triangle orientations which may be needed in some of the available triangular mesh generation packages in order to serve effectively as an initialization method for MFE solutions. Further work in this area of mesh generation for initialization will be taken up again in later stages of research when more complex applications are considered.

Matrix solution methods for the large, banded, stiff system of MFE equations have been tested extensively during this reporting period. The results of this testing indicate that L - U decomposition of the banded matrix of the MFE method is a reasonable choice for this early stage of research where immediacy, reliability, and ease of implementation outweigh computational efficiency in small test problem applications. (In later stages of research it will be necessary to implement more efficient matrix solution methods for larger and/or more complex PDE systems, as will be indicated in the discussion below.) Point and line relaxation methods have also been tested during this reporting period and found to converge too slowly to be useful in current MFE research. Two-directional ADI methods were similarly tested and were found to be well-suited for implementation with the MFE method on a quadrilateral grid. For the hexagonally connected triangular mesh which is used in the present effort, three-directional (in contrast to two-directional) ADI methods will be required. Although a large amount of additional research is needed before three-directional ADI can be used effectively with the MFE method, dynamic ADI methods are sufficiently promising that such further research certainly appears to be warranted for large-scale MFE applications in the future. Indeed, dynamic ADI and perhaps other splitting methods presently appear to be mandatory in order to achieve desired economies when large-scale applications are considered. In anticipation of these later matrix solution needs, the investigation of more efficient iterative solution methods has also been started. At this time, partial block Gauss elimination and incomplete orthogonalization of a conjugate gradient solution method are in the early scoping stages and are showing some signs of promise.

No major deviations from the planned course of research have been made during this reporting period and none are anticipated during the next reporting period. So far as maintaining an alert for potential problems which may arise, the adequacy of numerical Jacobians is under constant surveillance. Testing during the present period indicates that essential levels of computational accuracy in Jacobian evaluations are likely to be maintained by the numerical discretization methods which are used in current code versions. Constant monitoring of this portion of MFE calculations is warranted because such a large and tedious coding effort of analytic Jacobian expressions would be required in the event that numerical Jacobian evaluations were found to be inadequate.

The following professional personnel participated in the research conducted during this reporting period:

Dr. M. Jahed Djomehri (student of Prof. Keith Miller, U.C. Berkeley)
Dr. Said K. Doss
Dr. Robert J. Gelinas
Dr. J. Peter Vajk

No significant changes are anticipated in the commitments of key personnel during the next reporting period.

Papers were presented at:

IMACS International Symposium, Lehigh University; 6/30-7/2/81; "The Moving Finite Element Method: A Semi-Automatic Solver for Diverse PDE Applications," by R. J. Gelinas and S. K. Doss.

LASL Adaptive Mesh Workshop, Los Alamos, NM; August 5-7, 1981; "The Moving Finite Element Method: Implementation of a 2-D Code," by J. P. Vajk, S. K. Doss, R. J. Gelinas, and K. Miller.

SIAM Meeting, October 26-28, 1981, Cincinnati, OH; "Solution of the Gas Dynamics Equations in 1-D by the Moving Finite Element Method," by S. K. Doss.

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