MOVING FINITE ENVELOPES

M.J. Baines

Numerical Analysis Report 12/87

Keywords: Moving Finite Elements, Characteristics, Regularisation.

The work reported here forms part of the research programme of the Institute for Computational Fluid Dynamics at Oxford and Reading.

Abstract

A description is given of the Moving Finite Element Method and its relationship with the Method of Characteristics and with Optimisation. A key feature is the use of the envelope of the driving function. For hyperbolic equations the issue of parallelism is resolved. The concept of the envelope is then used to extend the range of the theory to include diffusion operators and to motivate regularisation for resolving the issue of parallelism in this case.

1. Introduction

The Moving Finite Element (MFE) method belongs to the class of adaptive grid methods in which the mesh evolves simultaneously with the solution. Both the evolution of the mesh and the solution are generated from the governing differential equation in the manner described below. The method was invented by K. Miller[1] of the University of California and has been used by many authors (Gelinas et al[2], Mosher[3], Mueller & Carey[4], Wathen and Baines[5], Hrymark[6] and others) to solve problems in which sharp features need to be resolved and tracked.

We describe here the derivation of MFE given by Mueller and Carey[4]. Consider the partial differential equation

$$\frac{\partial u}{\partial t} = \mathcal{L}u \tag{1.1}$$

where $u = u(x,t)$ and $\mathcal{L}$ is a spatial differential operator in the space variables x. Define a coordinate transformation between x,t and new independent variables ξ,τ by

$$x = \hat{x}(\xi,\tau) \quad , \quad t = \tau \quad ; \quad \hat{u}(\xi,\tau) = u(x,t) \tag{1.2}$$

for which the partial derivatives satisfy

$$\frac{\partial u}{\partial t} = \frac{\partial \hat{u}}{\partial \tau} + \frac{\partial \hat{u}}{\partial \xi}\frac{\partial \xi}{\partial t} = \frac{\partial \hat{u}}{\partial \tau} - \frac{\partial u}{\partial x}\frac{\partial \hat{x}}{\partial \tau} \tag{1.3}$$

Then (1.1) becomes

$$\frac{\partial \hat{u}}{\partial \tau} - \frac{\partial u}{\partial x}\frac{\partial \hat{x}}{\partial \tau} = \mathcal{L}u \tag{1.4}$$

or, using the notation

$$\dot{u} = \frac{\partial \hat{u}}{\partial \tau} \quad , \quad \dot{x} = \frac{\partial \hat{x}}{\partial \tau} \quad , \quad u_x = \frac{\partial u}{\partial x} \quad , \tag{1.5}$$

$$\dot{u} - u_x \dot{x} - \mathcal{L}u = 0 \quad . \tag{1.6}$$

Now define

$$R(\dot{u},\dot{x}) = \dot{u} - u_x \dot{x} - \mathcal{L}u \tag{1.7}$$

and let $\|R\|$ be the L_2 norm of R defined in a suitable way. Both R and $\|R\|$ are zero by virtue of (1.6). If however u and x are restricted to sets of admissible trial functions, R is a residual, no longer zero, and the problem may be cast as a least squares variational problem by minimising $\|R\|_2$ over $\dot{u}$ and $\dot{x}$. In this way we obtain the weak forms

$$\langle R,\psi\rangle = 0 \qquad \langle R,u_x\chi\rangle = 0 \tag{1.8}$$

for all admissible test functions $\psi(=\delta\dot{u})$ and $\chi(=\delta\dot{x})$.
Constraints, for example a lower bound on the Jacobian of the transformations, may easily be introduced through the use of penalty functions.

Introducing finite element approximations

$$u = \sum_j u_j(\tau)\alpha_j(\xi) \qquad x = \sum_j x_j(\tau)\alpha_j(\xi) \tag{1.9}$$

where the $\alpha_j(\xi)$ are basis functions for the approximation space, we find that

$$\dot{u} = \sum \dot{u}_j \alpha_j \qquad \dot{x} = \sum \dot{x}_j \alpha_j \tag{1.10}$$

and that (1.8) gives

$$\langle R,\ \alpha_i \rangle = 0 \qquad \langle R,\ u_x \alpha_i \rangle = 0 \quad \forall i \tag{1.11}$$

Substitution for R from (1.7) and using (1.10) yields a nonlinear system of ordinary differential equations of the form

$$A(\underline{y})\dot{\underline{y}} = \underline{g}(\underline{y}) \tag{1.12}$$

where $A(\underline{y})$ is an extended mass matrix and $\underline{y}$ is a vector of the nodal and coordinate unknowns U_j and X_j. The ODE system (1.12) may be integrated from specified initial data to obtain U_j and X_j at a later time. With piecewise linear elements this is identical to Miller's method[1].

It has been shown by Wathen & Baines[5] that for piecewise linear elements the mass matrix $A(\underline{y})$ has a special decomposition which leads to rapid inversion. However, most authors integrate (1.12) approximately by an implicit procedure using a Newton solver for the nonlinear system.

The matrix $A(\underline{y})$ of (1.12) becomes singular in the event of collinear nodes (for piecewise linear elements) and there are special

problems when nodes collide or overtake. For these reasons most authors use penalty functions as essential regularisers in the minimisation of $\|R\|$.

2. Relation with Characteristics

We present here an interpretation of the procedure described in §1 in the continuous case.

First let $\mathcal{L}u = F(x,u_x)$ so that (1.6) becomes

$$\dot{u} - u_x\dot{x} - F(x,u_x) = 0. \tag{2.1}$$

For each point P of initial data (see fig. 1a) we may evaluate u_x and $F(x,u_x)$ and plot them as a point L in u_x,F space (fig. 1b). Moreover (2.1) is the equation of a line L in $\dot{x},\dot{u}$ space (fig. 1c). As P varies along the initial data in fig. 1a the point L in fig. 1b traces out a curve and the line L in fig. 1c traces out a pencil of lines (envelope). Fig. 1b is the point-line dual of fig. 1c.

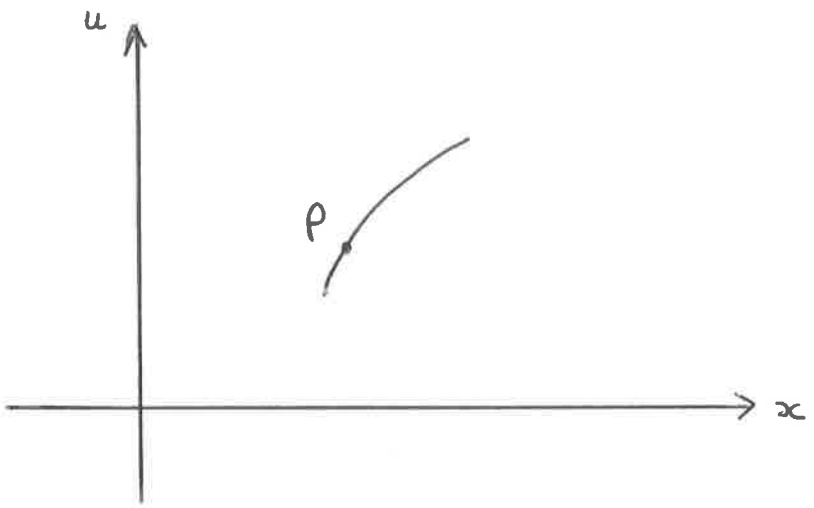

fig. 1a

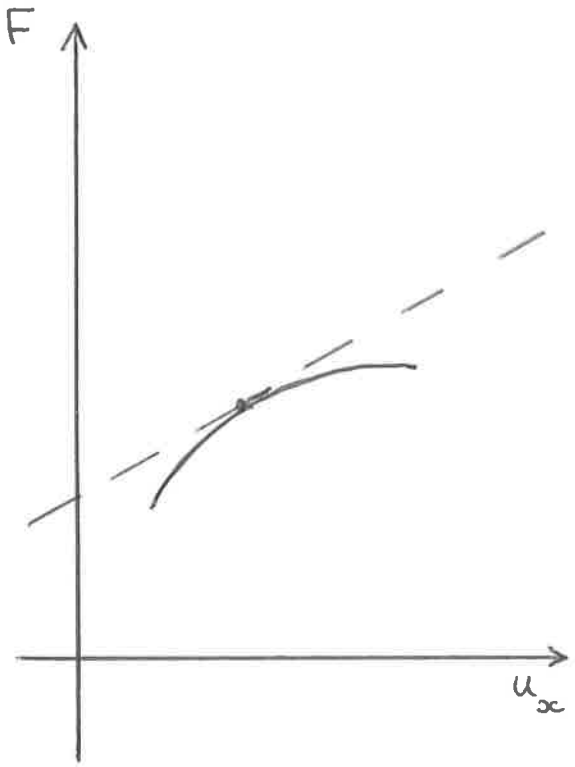

fig. 1b

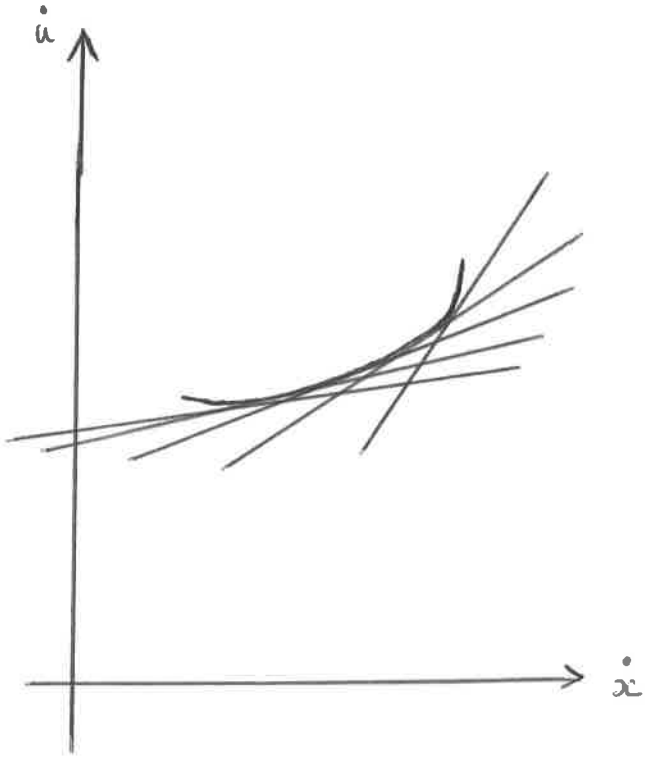

fig. 1c

Consider now a general point K with coordinates $\dot{x}_o, \dot{u}_o$ in fig. 1c. From (1.7) $R(\dot{u}_o, \dot{x}_o)$ is the perpendicular distance of K from the line L. The L_2 norm $\|R\|_2$ is an integral of R^2 taken over all points P of initial data and is a measure of the distance of a set of points {K} from the set of lines {L}. Minimisation of $\|R\|_2$ w.r.t. small variations in both $\dot{u}_o$ and $\dot{x}_o$ leads to the conclusion that {K} lies on the envelope of {L} as P varies. This is because small variations in P (and therefore u_x, regarded as a parameter) will lead to only small variations in the stationary values $\dot{x}_o$ and $\dot{u}_o$ of $\|R\|$.

Correspondingly, in the dual space (fig. 1b) the set of lines {K} are tangent to the curve traced out by L as P varies. Since the slope of the line K is $-\dot{x}_o$, we have at the minimum point

$$\dot{x} = -\frac{\partial F}{\partial u_x} \quad \Rightarrow \quad \dot{u} = F - u_x \frac{\partial F}{\partial u_x} \ . \tag{2.2}$$

Discrete approaches to minimising the norm of R of (1.7) (including MFE) are attempts to approximate these equations.

Equations (2.2) are a subset of the characteristic equations[7] for the problem (1.1) with $Lu = F(x,u_x)$. The others are

$$\dot{u}_x = \frac{\partial F}{\partial x} \ , \quad \dot{u}_t = 0. \tag{2.3}$$

For example, if $F(x,u_x) = u_x^2$ the equations (2.2), (2.3) give

$$\left.\begin{aligned} \dot{x} &= 2u_x, & \dot{u} &= -u_x^2 \\ \dot{u}_x &= 0, & \dot{u}_t &= 0 \end{aligned}\right\} \tag{2.4}$$

To generalise the argument to the case $\mathcal{L}u = F(x,u,u_x)$, suppose that the solution u is given implicitly by

$$g(t,x,u) = 0 \tag{2.5}$$

so that

$$g_t + g_u u_t = 0 \ , \quad g_x + g_u u_x = 0 \tag{2.6}$$

Then, on multiplying (1.1) by $-g_u$ we obtain

$$g_t = -g_u F(x,u,-\frac{g_x}{g_u}) = \mathcal{F}(x,u,g_x,g_u), \tag{2.7}$$

say, where

$$\mathcal{F}(x,u,g_x,g_u) = -g_u F(x,u,-\frac{g_x}{g_u}). \tag{2.8}$$

Following the same argument as before we obtain

$$\dot{x} = \frac{\partial \mathcal{F}}{\partial g_x}\ ,\ \dot{u} = \frac{\partial \mathcal{F}}{\partial g_u}\ ,\ \dot{g} = \mathcal{F} - g_x \frac{\partial \mathcal{F}}{\partial g_x} - g_u \frac{\partial \mathcal{F}}{\partial g_u} \tag{2.9}$$

which, using (2.8), gives

$$\dot{x} = \frac{\partial F}{\partial u_x}\ ,\ \dot{u} = F - u_x \frac{\partial F}{\partial u_x}\ ,\ \dot{g} = 0 \tag{2.10}$$

(c.f.(2.2)). Moreover the other characteristic equations are

$$\dot{g}_x = \frac{\partial \mathcal{F}}{\partial x},\ \dot{g}_u = \frac{\partial \mathcal{F}}{\partial u}\ ,\ \dot{g}_t = 0 \tag{2.11}$$

(since $\mathcal{F}$ does not contain g) which give, using (2.6),

$$\dot{u}_x = \frac{\partial F}{\partial x} + u_x \frac{\partial F}{\partial u}\ ,\quad \dot{u}_t = F \frac{\partial F}{\partial u} \tag{2.12}$$

c.f. (2.3). (This may be achieved also by using x as the envelope parameter.) For example if $F(x,u,u_x) = -a(u)u_x$, as for a scalar hyperbolic conservation law (with wave speed a(u)), we obtain the equations

$$\dot{x} = a(u),\quad \dot{u} = 0,\quad \dot{u}_x = -a'(u)u_x^2,\quad \dot{u}_t = a(u)a'(u)u^2. \tag{2.13}$$

In higher dimensions, for the equation

$$u_t = F(x,y,u_x,u_y) \tag{2.14}$$

the equations are as for (2.7), namely

$$\dot{x} = \frac{-\partial F}{\partial u_x} \ , \ \dot{y} = \frac{-\partial F}{\partial u_y} \quad , \quad \dot{u} = F - u_x \frac{\partial F}{\partial u_x} - u_y \frac{\partial F}{\partial u_y} \tag{2.15}$$

$$\dot{u}_x = \frac{\partial F}{\partial x} \quad , \quad \dot{u}_y = \frac{\partial F}{\partial y}$$

while for

$$u_t = F(x,y,u,u_x,u_y) \tag{2.16}$$

an extension of the procedure (2.25) to $g(t,x,y,u) = 0$ yields equations corresponding to (2.15) together with $\dot{g} = 0$.

Instead of (2.2) we may set

$$\dot{x} = -F/u_x \tag{2.17}$$

immediately so that from (2.1)

$$\dot{u} = 0 \tag{2.18}$$

automatically, see [12]. To obtain $\dot{u}_x$ in this case note that

$$u_{xt} = F_x = \frac{\partial F}{\partial x} + \frac{\partial F}{\partial u}u_x + \frac{\partial F}{\partial u_x}u_{xx}$$

and that

$$\dot{u}_x = u_{xt} + \dot{x}u_{xx}$$

giving

$$\dot{u}_x = \frac{\partial F}{\partial x} + \frac{\partial F}{\partial u}u_x + \frac{\partial F}{\partial u_x}u_{xx} - \frac{u_{xx}}{u_x}F \quad . \tag{2.19}$$

In the case $F = -a(u)u_x$ we find that

$$\dot{x} = a(u), \quad \dot{u} = 0, \qquad \dot{u}_x = -a'(u)u_x^2 \tag{2.20}$$

as in (2.10), (2.13), so that the two strategies (2.2), (2.17) are indistinguishable in this case.

One feature of the connection with characteristics is that, because of the local nature of the solution, errors will tend to be propagated as if associated with ODEs. Thus, if an optimal grid is chosen on which to represent the solution initially such a grid will adapt in such a way that the representation remains optimal. This accords with the result of Morton[8] that the MFE grid carries the best L_2 fit to the solution.

3. Relation with Optimisation

Returning to the case $\mathfrak{L}u = F(x,u_x)$, so that (1.1) becomes

$$\frac{\partial u}{\partial t} - F(x,u_x) = 0, \tag{3.1}$$

let $F(x,u_x)$ define a Legendre Transformation with u_x and $\dot{x}$ as dual active variables, where

$$\frac{\partial F}{\partial u_x} = \dot{x}. \tag{3.2}$$

The dual of $F(x,u_x)$ is $G(x,\dot{x})$, which has the values of

$$G(x,\dot{x}) = u_x\dot{x} - F(x,u_x) \tag{3.3}$$

and derivatives

$$\frac{\partial G}{\partial \dot{x}} = u_x \quad , \quad \frac{\partial G}{\partial x} = \frac{\partial F}{\partial x} \quad , \quad \frac{\partial G}{\partial t} = -\frac{\partial F}{\partial t} \tag{3.4}$$

Then it may be shown[9] that the extremal of the functional

$$\phi(\phi) = \int_o^t G(\phi(\sigma),\phi(\sigma))d\sigma \tag{3.5}$$

which satisfies $\phi(t) = x(t)$ and a given condition at $t = 0$ is $\phi(\sigma) = x(\phi)$. Moreover, if we regard x,t as (independent) variables, it may further be shown that the extreme value of the function ϕ considered as a function of x and t is

$$\underset{\phi}{\text{ext.}} \int_o^t G(\phi(\sigma),\phi(\sigma)d\sigma = \int_o^t G(x(\sigma),\dot{x}(\sigma))d\sigma$$

$$= u(x,t) - u(x,0). \tag{3.6}$$

Again, writing the first of (3.4) as an imbedding,

$$\operatorname*{ext.}_{\dot{\phi}}(u_t + \dot{\phi}u_x - G(x,\dot{\phi})) = 0, \tag{3.7}$$

or

$$\operatorname*{ext.}_{\dot{\phi}}[\dot{u} - G(x,\dot{\phi})] = 0 \tag{3.8}$$

we find that

$$u(x,t) = \operatorname*{ext.}_{\dot{\phi}}\left[u(x+\dot{\phi}\Delta t, t+\Delta t) - \int_t^{t+\Delta t} G(x,\dot{\phi})d\sigma\right] + O(\Delta t) \tag{3.9}$$

$$= \operatorname*{ext.}_{\phi}\left[u(\phi(\sigma+\Delta t), t+\Delta t) - \int_t^{t+\Delta t} G(x,\dot{\phi})d\sigma\right] + (\Delta t) \tag{3.10}$$

which is the principle of optimality in dynamic programming applied to (3.6).

There are straightforward extensions in the case $\mathfrak{L}u = \mathfrak{F}(x,u,u_x)$ and to many variables.

4. Diffusion Operators

In generalising to $\mathfrak{L}u = F(x,u_x,u_{xx})$ we can make no further use of characteristics. But we may return to the envelope argument earlier and formally seek the envelope of (1.6) by taking its first variation in the form

$$-\delta u_x \dot{x} - \delta F = 0 \tag{4.1}$$

If we regard u_{xx} as depending on u_x then for smooth F and u this equation leads to

$$-u_{xx}\dot{x} - \frac{\partial F}{\partial u_x} u_{xx} - \frac{\partial F}{\partial u_{xx}} \frac{du_{xx}}{du_x} = 0. \tag{4.2}$$

For sufficiently smooth u we may approximate the last term to obtain

$$\dot{x} = - \frac{\partial F}{\partial u_x} - \frac{u_{xxx}}{u_{xx}} \frac{\partial F}{\partial u_{xx}}. \tag{4.3}$$

It is clear from (4.3) that this procedure for obtaining $\dot{x}$ breaks down when $u_{xx} = 0$ (zero curvature) and in that case there is no solution for $\dot{x}$ when minimising $\|R\|$ in the manner of §1. Moreover, provided that F varies slowly with x, large values of $\dot{x}$ are associated with small values of u_{xx} and vice versa. Large distortions are therefore associated with small curvature and small distortions with large curvature.

To make this point more precise consider the graph of the term

$$- \frac{u_{xxx}}{u_{xx}} \tag{4.4}$$

occurring in (4.3). This term is zero at zeros of u_{xxx} and there are vertical asymptotes at the zeros of u_{xx}, the two sets of zeros alternating with one another in general. Moreover, the x-derivative of (4.4) is

$$\left[\frac{u_{xxx}}{u_{xx}}\right]^2 - \frac{u_{xxxx}}{u_{xx}} \qquad (4.5)$$

which is positive sufficiently close to a zero of u_{xx} in general. Thus we obtain the qualitative picture of the graph of (4.4) shown in fig. 2.

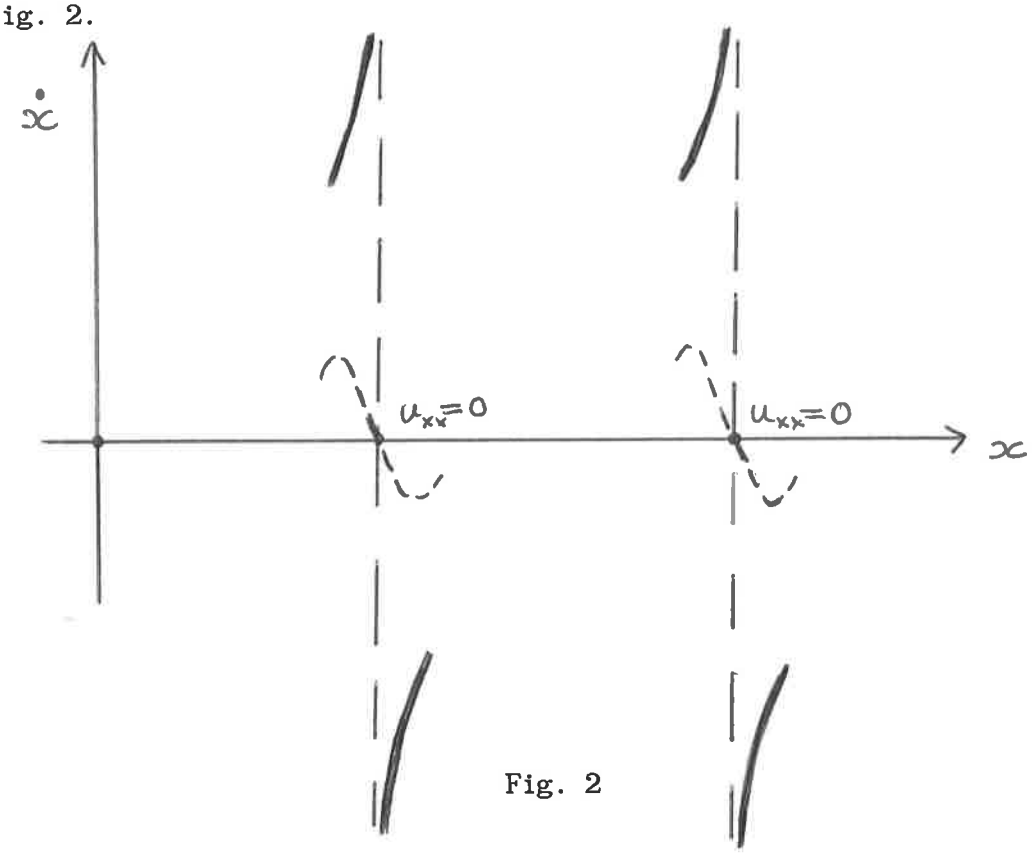

Fig. 2

It follows that the corresponding $\dot{x}$ is large and positive to the left of an asymptote and large and negative to the right of the same asymptote, indicating a deformation in x having the zeros of u_{xx} as cluster points, i.e. points move towards regions of zero curvature. The result is unaltered by the presence of the $\frac{\partial F}{\partial u_x}$ and $\frac{\partial F}{\partial u_{xx}}$ terms as in (4.3).

[In general, any numerical implementation will lead to impractically large and oscillatory speeds near to the zeros of u_{xx}, i.e. near zero

curvature. But see §7 below for the result of implementing the MFE method.]

A more satisfactory $\dot{x}$ from the point of view of associating low $\dot{x}$ with regions of high u_{xx}, and moving trajectories apart when u_{xx} is small (and avoiding singularities) is $\dot{x} \propto \epsilon u_{xx} u_{xxx}$ which is graphed in fig. 2.

5. The MFE Method

The discretisation (1.9) used directly in the orthogonality relations (1.8) yields the system (1.12). The matrix $A(\underline{y})$ in (1.12) consists of blocks of inner products of basis functions of the form

$$\int \alpha_i \alpha_j \, \omega \, dx \quad , \quad \int \alpha_i \alpha_j \, U_x \, \omega \, dx \quad , \tag{5.1}$$

where $\omega(x)$ is the weight function used in the definitions of the L_2 norm. In Miller's original method[1] ω was taken to be 1 but in more recent work Miller[8] uses a gradient weighting $\omega = (1 + U_x^2)^{-\frac{1}{2}}$, producing the Gradient Weighted MFE method (GWMFE).

With piecewise linear basis functions α_j any ω depending only on U_x is piecewise constant and may be taken through the integral sign in (5.1). In particular, the decomposition of $A(\underline{y})$ demonstrated by Wathen & Baines[5],

$$A(\underline{y}) = M^T C M, \tag{5.2}$$

remains valid. Here C is a square block diagonal matrix, each block being the corresponding elementwise mass matrix, and M is an assembly

matrix, also block diagonal (and square in one dimension) depending only on the constants U_x.

As a result of (5.2) the method is a local method in the sense that $\dot{U}_j, \dot{X}_j$ depends only on values of U_j, X_j at neighbouring nodes, as shown by Baines[11]. This is consistent with the connection with the method of characteristics in §2.

In solving

$$M^T C M \dot{\underline{y}} = \underline{g}(\underline{y}) \tag{5.3}$$

Baines and Wathen[10] write the method as a two step scheme

$$C\,\underline{w} = \underline{b} \tag{5.4}$$

$$M\,\dot{\underline{y}} = \underline{w} \tag{5.5}$$

with $M^T \underline{b} = \underline{g}(\underline{y})$, the first step being a local elementwise projection and the second step being a transfer of element information to the nodes.

In higher dimensions and in certain approaches to systems[13,14] the local character of the approximations is preserved if the procedure

$$\min_{\dot{\underline{y}}} \| C^{\frac{1}{2}} (M\dot{\underline{y}} - \underline{w}) \| \tag{5.6}$$

which produces (5.3) is replaced by

$$\min_{\dot{\underline{y}}} \| C_D^{\frac{1}{2}} (M\dot{\underline{y}} - \underline{w}) \| \tag{5.7}$$

where C_D is the diagonal of C. Then (5.3) is replaced by

$$M^T C_D M\dot{\underline{y}} = M^T C_D \underline{w} = M^T C_D C^{-1} \underline{b} \tag{5.8}$$

which is again local. The latter procedure may be shown[12] to be equivalent to a Petrov-Galerkin approach or simply to the use of a different norm for R (see §1). We shall refer to (5.3) as the global method and to (5.8) as the local method, although they are indistinguishable for one-dimensional scalar problems.

For systems of equations using a single moving grid a constraint may be imposed on the procedure (5.6) or (5.7) which enforces the various different grid speeds for each component to be identical[14,15]. Another use of constraints is to deal with the formation of shocks in one dimension. When node j overtakes node j+1 a simple constraint[5,11,12,16]

$$\dot{x}_j = \dot{x}_{j+1} = \text{shock speed} \tag{5.9}$$

may be imposed on the minimisation (5.6) or (5.7). These equality constraints are easy to impose without destroying the algebraic structure.

If nodes are collinear or coplanar in the initial data (or subsequently) the matrix $A(\underline{y})$ is singular as a result of M becoming singular. In that case $A(\underline{y})$ is not invertible (unless the rank of $\underline{g}(\underline{y})$ is reduced correspondingly). The situation parallels the vanishing of u_{xx} in §2. In the hyperbolic case $\delta\mathfrak{L}u$ vanishes simultaneously and there is a finite solution but in the parabolic case there is a singularity, unavoidable in general. Wathen & Baines[5]

suggest a modification to MFE in which the velocity of the offending node is overwritten with an averaged velocity over neighbouring nodes, but other authors combat the situation with penalty terms in the minimisation of $\|R\|$.

Similarly, if nodes overtake (perhaps as the result of inaccurate time integration) the matrix C of (5.4) becomes singular. For problems involving diffusion Johnson, Wathen & Baines[5,16] (who use explicit time integration) consciously limit the time step so as to avoid node overtaking, but other authors again rely on regularisation procedures.

Time integration of (1.12) is usually carried out with finite differences, typically forward or backward Euler or a stiff solver. Johnson, Wathen & Baines[5,12,16] use explicit Euler which fits in well with controlling node overtaking, but other authors[1-4,6] use implicit methods in association with regularisation of the underlying minimisation. The former approach is faster per time step whereas the latter is more robust: in practice the time step is generally restricted by either node overtaking or convergence criteria.

6. Regularisations

The original MFE papers of Miller[1] contained regularisation penalty terms aimed at combatting the singularities mentioned above. Other authors, notably Mueller and Carey[4], have used the same approach and various strategies have been used to construct such penalty terms[17]. Generally the minimisation of $\|R\|$ (see §1) is replaced by minimising

$$\|R\|^2 + \epsilon_o^2\|P\|^2, \tag{6.1}$$

where P is the penalty and ϵ_o a suitable constant (chosen by Miller

to be of the order of the truncation error). The link with the method of characteristics in §2 is lost when this tactic is used, but the technique is very effective in practice.[17]

We have already discussed the need for a special procedure when the diffusion operator u_{xx} is present, in §2. It is clear from there (and also the corresponding discrete forms[11,12,15,18]) that regularisation is needed for either the $\dot{x}$ velocity or the tangential velocity. Thus some form of one or other of these velocities must appear in P together with any additional terms required to enforce other desirable features, for example node separation or reflection at boundaries.

It is possible[18] to introduce regularising terms to overcome the singularity discussed in §2 while still retaining the algebraic structure of §3. The resulting form of (1.12) then becomes

$$\{A(\underline{y}) + \epsilon_o^2 B(\underline{y})\}\dot{\underline{y}} = \underline{g}(\underline{y}) + \epsilon_o^2 \underline{h}(\underline{y}) \tag{6.2}$$

where
$$A(\underline{y}) = M^T C M \quad \text{or} \quad M^T C_D M \tag{6.3}$$

and
$$B(\underline{y}) = W^T C W \quad \text{or} \quad W^T C_D W \tag{6.4}$$

where W is a matrix which is in some sense orthogonal to the matrix M (c.f (3.3),(3.8)): $\underline{h}(\underline{y})$ may be prescribed. Both global and local regularised MFE methods may be constructed in this way.

7. Discussion

We now investigate the relation between the MFE method and the characteristic method of §2 which it imitates. In doing so we shall determine guidelines for discrete procedures to overcome the

singularities in MFE.

It has been shown[11,12] that the intermediate vector $\underline{w}$ appearing in (5.4) plays a key role in the MFE equations. This vector is a collection of element vectors which are the projections of $\mathcal{L}u$ into each element subspace. If the basis functions in a one-dimensional problem are as shown in fig. 3a,

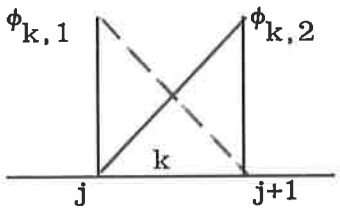

fig. 3a

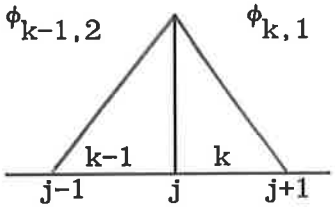

fig. 3b

then the projection of $\mathcal{L}u$ may be written

$$(\mathcal{P}u)_k = w_{k,1}\phi_{k,1} + w_{k,2}\phi_{k,2} \tag{7.1}$$

and then it may be shown[11,12] that

$$(\dot{U}_x)_k = \frac{w_{k,2} - w_{k,1}}{x_{j+1} - x_j}, \qquad \dot{X}_j = \frac{-(w_{k,1} - w_{k-1,2}).}{((U_x)_k - (U_x)_{k-1})} \tag{7.2}$$

See fig. 3b. These equations are discrete representations of equations in (2.10) and (2.12) where the $w_{k,i}$ are now playing the role of $\mathcal{L}u = F(x,u,u_x)$, approximately.

(i) Hyperbolic case

If $(U_x)_k - (U_x)_{k-1}$ is very small the second of (7.2) has a very small denominator, but according to (2.10) for hyperbolic equations it

should be approximating a derivative. Thus we expect $w_{k,1} - w_{k-1,2}$ to also be very small. The ratio of two very small numbers is however hard to compute and may lead to considerable error. Moreover $w_{k,1} - w_{k-1,2}$ will not necessarily tend to zero as $(U_x)_k - (U_x)_{k-1}$ tends to zero because of the dependence of w on x and u. Therefore, in order to avoid the potential parallelism singularity we should, for $(U_x)_k - (U_x)_{k-1}$ less than a certain tolerance, evaluate $\dot{X}_j$ as $-\frac{\partial F}{\partial u_x}$ with x,U taken as their values at the point j. This ensures cancellation. A similar argument applies to the first of (7.2). Again the recommendation is that, for $x_{j+1} - x_j$ (Δx, say) smaller than a certain tolerance, we should evaluate $(\dot{U}_x)_k$ as $\frac{\partial F}{\partial x}$ with x,U,U_x taken as their values at $\frac{1}{2}(x_{j+1} + x_j)$. This resolves the parallelism singularity.

(ii) Diffusion case

In the case of the diffusion operator $\mathfrak{L}u = u_{xx}$ we have already seen in §4 (around equation (4.4)) that singularity is unavoidable without some modification to the method, and the second of (7.2) exhibits a discrete form of the same difficulty. The singularity manifests itself as a very large $\dot{X}_j$ with no useful significance and leads to spuriously small time steps.

According to §4 nodes will move towards points of zero curvature leaving high curvature regions poorly resolved. This is completely contrary to the notion that nodes are transported into regions where they are most needed. Fortunately for MFE the calculated speeds in the case of piecewise linear elements are governed by the truncation error which (at least in one dimension) reverses the sign of $\dot{X}_j$, so that

nodes are forced towards high curvature regions, albeit with spuriously large velocities.

For $\mathcal{L}u = u_{xx}$ we can readily solve on a fixed grid (implicitly) and ignore the difficulty. However, for convection-diffusion problems there is a need for a moving grid method and the diffusion term must be treated properly since otherwise non-physical shocks may occur. The classical case is $\mathcal{L}u = -uu_x + \sigma u_{xx}$ which gives

$$\dot{x} = u - \frac{\sigma u_{xxx}}{u_{xx}} = \frac{uu_{xx} - \sigma u_{xxx}}{u_{xx}}. \tag{7.3}$$

As we saw in §2 this speed arises from the envelope construction on the equation

$$\dot{u} - u_x\dot{x} + uu_x - \sigma u_{xx} = 0 \tag{7.4}$$

which is equivalent in the limit to the minimisation of

$$\|R\|_2^2 = \|u - u_{xx} + uu_x - \sigma u_{xx}\|_2^2 \tag{7.5}$$

over $\dot{u}$ and $\dot{x}$. To avoid the occurrence of the potentially singular denominator u_{xx} in (7.3) we may add a regularisation to (7.5) which prevents $\dot{x}$ becoming large (c.f. (6.1)). Then $\|R\|_2^2$ becomes[18]

$$\|R\|_2^2 + \epsilon_o^2 \|P\|_2^2 \tag{7.6}$$

where $P = \dot{x}^2$ and ϵ_o is a (small) constant, leading to the discrete equations

$$\begin{bmatrix} \Delta x_k+\Delta x_{k-1} & -(U_x)_k\Delta x_k-(U_x)_{k-1}\Delta x_{k-1} \\ -(U_x)_k\Delta x_k-(U_x)_{k-1}\Delta x_{k-1} & (U_x)_k^2\Delta x_k+(U_x)_{k-1}^2\Delta x_{k-1}+\epsilon_o(\Delta x_k+\Delta x_{k-1}) \end{bmatrix} \begin{bmatrix} \dot{U}_j \\ \dot{x}_j \end{bmatrix}$$

$$= \begin{bmatrix} \Delta x_k W_{k,1} + \Delta x_{k-1} W_{k-1,2} \\ (-U_x)_k \Delta x_k W_{k,1} - (U_x)_{k-1}\Delta x_{k-1} W_{k-1,2} \end{bmatrix} \qquad (7.7)$$

(c.f. fig. 3b) Note that when $\epsilon_0 = 0$ the solution of (4.12) for $\dot{X}_j$ is the second of (7.2). If $\epsilon_0 \neq 0$ however, we move away from the equivalence with the envelope construction and find [18] that

$$\dot{x}_j = \frac{-(W_{k,1}-W_{k-1,2})((U_x)_k-(U_x)_{k-1})\Delta x_k \Delta x_{k-1}}{[(U_x)_k-(U_x)_{k-1}]^2 \Delta x_k \Delta x_{k-1} + \epsilon_o(\Delta x_k + \Delta x_{k-1})^2} \qquad (7.8)$$

$$= \frac{-(W_{k,1} - W_{k-1,2})}{(U_x)_k-(U_x)_{k-1} + \frac{\epsilon_o}{(U_x)_k-(U_x)_{k-1}} (\Delta x_k+\Delta x_{k-1})(\frac{1}{\Delta x_k} + \frac{1}{\Delta x_{k-1}})} \qquad (7.9)$$

which approximates

$$\dot{x} = \frac{uu_{xx} - \sigma u_{xxx}}{u_{xx} + \frac{\epsilon(x)}{u_{xx}}} \qquad (7.10)$$

for some $\epsilon(x)$. Here $\Delta x_k = x_k - x_{k-1}$ (see fig. 3a). The factor ϵ_o

has dimensions of U_x^2 and, if chosen proportional to a suitable combination of $(U_x)_k$ and $(U_x)_{k-1}$, the speed $\dot{X}_j \to 0$ under any of the three conditions (i) $(U_x)_k, (U_x)_{k-1} \to \infty$, (ii) $(U_x)_k - (U_x)_{k-1} \to 0$, (iii) one of $(\Delta x)_k, (\Delta x)_{k-1} \to 0$. The qualitative form of $\dot{x}$ is shown as the dotted line in fig. 2 for a general $\mathfrak{L}u$. Note that asymptotically the directions of the node velocities are unaltered but they are forced to zero near the asymptotes (zero curvature).

Similarly the discrete form (first of (7.2)) is singular when $\Delta x_k \to 0$. It may however be similarly regularised to give

$$(\dot{U}x)_k = \frac{W_{k,2} - W_{k,1}}{\Delta x_k + \frac{\epsilon_o'}{\Delta x_k}} \tag{7.11}$$

where ϵ_o' is a small constant, which prevents the potential singularity as $\Delta x_k \to 0$.

In all the above cases the ultimate accuracy of the method is left to the Galerkin equation for $\dot{U}_j$ obtained from (7.7) as

$$(\Delta x_k + \Delta x_{k-1})\dot{U}_j = w_{k,1}\Delta x_k + w_{k-1,2}\Delta x_{k-1} + [(U_x)_k \Delta x_k + (U_x)_{k-1}\Delta x_{k-1}]\dot{X}_j \tag{7.12}$$

Donnelly [19] has used equations (7.2) in tandem directly. He solves discrete MFE forms of the two equations (2.10) (i) and (2.12) (i), which in the case of the diffusion equation mimic the equations

$$\dot{x} = -\frac{2u_{xxx}}{u_{xx}} \quad , \quad \dot{u}_x = 3u_{xxx}. \tag{7.13}$$

The second of these is solved for u_x, then the first can be solved for x. Note that the solution u_x satisfies the usual maximum principle. This is preserved by Donnelly in his discrete version by using a fully implicit scheme.

8. The Mobile Element Method

We saw in §2, equation (2.17) et. seq., that if $\dot{x}$ is chosen so as to make $\dot{u} = 0$, we obtain the same continuous limit in the case $F = -a(u)u_x$ (the scalar conservation law). However, with this approach the discrete form differs from MFE, even in this special case.

Equations (1.11) are now replaced by

$$\langle R, \alpha_i \rangle = 0 \qquad \langle -u_x \dot{x} - \mathfrak{L}u, u_x \alpha_i \rangle = 0 \qquad \forall i \tag{8.1}$$

(corresponding in the second case to the minimisation over $\dot{x}$ of

$$\| -u_x \dot{x} - \mathfrak{L}u \|^2) \tag{8.2}$$

and (1.12) can be written in the blocked form

$$\begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} \dot{\underline{U}} \\ \dot{\underline{x}} \end{bmatrix} = \begin{bmatrix} g_1(\underline{y}) \\ g_2(\underline{y}) \end{bmatrix} \tag{8.3}$$

Although we do not have the decomposition (5.2) overall we do have in the case of linear elements the decompositions

$$A_{11} = L^T C L \qquad A_{12} = L^T C L' \qquad A_{22} = L'^T C L' \tag{8.4}$$

where L, L' are constant rectangular assembly matrices, depending in the case of L' on the constants U_x. It is then easy to construct a local method using the ideas of (5.8) with

$$A_{11} = L^T C_D L \qquad A_{12} = L^T C_D L' \qquad A_{22} = L'^T C_D L' \tag{8.5}$$

and appropriate changes to the right hand side of (8.3).

One form of the resulting equations is given by

$$\dot{x}_j = - \frac{(W_{k,1}(U_x)_k + W_{k-1,2}(U_x)_{k-1})}{(U_x)_k^2 + (U_x)_{k-1}^2} \tag{8.6}$$

with $\dot{U}_j$ given by (7.13), although there are similar forms of (8.6) with different weights. The parallelism singularity is avoided except when $(U_x)_k = (U_x)_{k-1} = 0$, when recourse to the differential form $\dot{x} = \frac{\partial F}{\partial u_x}$ is possible. This is the Mobile Element Method of Edwards [20,21] and Edwards & Baines [14].

The significance of this method is that $\dot{u} = 0$ is imposed, enforcing the TVD (Total Variational Decreasing) property of hyperbolic conservation laws[22].

Both the MFE method and the Mobile Element Method may be extended to systems of equations with a single moving grid using an averaging process for the grid velocity. The Mobile Element Method minimises some norm of the vector of variables $\underset{\sim}{u}$ and, as argued by Edwards[20,21], in

this way has a natural stability not possessed by the same approach using MFE.

9. Conclusion

The connection between the Moving Finite Element Method and the Method of Characteristics has been brought out using the idea of envelopes. As well as providing understanding as to what the MFE method is trying to approximate, the connection may be used to give a consistent treatment of parallelism. In the case of operators involving diffusion the envelope may be used to study the directions of the nodal motion and to motivate a regularisation which avoids the parallelism singularity. It is also clear that any regularisation destroys the analogy with envelopes and/or characteristics.

10. Acknowledgements

I am indebted to David Porter for helpful discussion on §2 and §3 and to Mike Edwards, Simon Chynoweth and Andrew Priestley for useful suggestions.

11. References

1. Miller K. & Miller R.N. 1981 Moving Finite Elements Part I. SIAM J. Numer. Anal. 18, 1019-1032: Miller K. Moving Finite Elements Part II. SIAM J. Numer. Anal. 18 1033-1057.

2. Gelinas R., Doss S.K. and Miller K. 1981 The Moving Finite Element Method: Applications to General Partial Differential Equations with Multiple Large Gradients. J. Comput. Phys 40,202-249.

3. Mosher M.C. 1985 A Variable Node Finite Element Method. J. Comput. Phys 57,157-187.

4. Mueller A.C. & Carey G.F. 1985 Continuously Deforming Finite Elements for Transport Problems. Int J. Num. Meths. Eng. 21,2099.

5. Wathen A.J. & Baines M.J. 1985 On the Structure of the Moving Finite Element Equations. IMA J. Num. An. 5,161.

6. Hrymark A.H., McRae G.J. & Westerberg A.W. 1986 An Implementation of a Moving Finite Element Method. J. Comput. Phys. 163,168-190.

7. John F. 1975 Partial Differential Equations, Springer.

8. Morton K.W. 1983 Private Communication.

9. Gelfand I.M. and Fomin S.V. 1963 Galculus of Variations. Prentice Hall.

10. Miller K. 1983 Alternate Modes to Control the Nodes in the Moving Finite Element Method. Adaptive Computational Methods for Partial Differential Equations. Ed. Babuska I, Univ. of Maryland. p. 165-182. Miller K. 1984 Recent Results on Finite Element Methods with Moving Nodes. Proceedings of ARFEC Conference, Lisbon (Wiley). Carlson N. & Miller K. 1986 The Gradient Weighted Moving Finite Element Method in 2-D. Center for Pure & Applied Math. Report PAM-347, University of California, Berkeley.

11. Baines M.J. 1986 Locally Adaptive Moving Finite Elements. In Numerical Methods for Fluid Dynamics II ed. Morton & Baines. Oxford University Press.

12. Baines M.J. & Wathen A.J. Moving Finite Element Methods for Evolutionary Problems 1I : Theory. J. Comput. Phys. (to appear).

13. Baines M.J. & Wathen A.J. 1986 Moving Finite Element Modelling of Compressible Flow. Applied Numerical Mathematics 2, 495-514.

14. Edwards M.G. & Baines M.J. The Mobile Element Method. Submitted to J. Comput. Phys.

15. Baines M.J. 1986 Projections & Constraints II. Numerical Analysis Report 2/86, Dept. of Maths., Univ. of Reading, UK.

16. Johnson I.W., Wathen A.J. & Baines M.J. Moving Finite Element Methods for Evolutionary Problems II : Applications. J. Comput. Phys. (to appear).

17. Juarez-Romero D., Sargent R.H.W. & Jones W.P. 1987 The Behaviour of the Moving Finite Element Method in 1-D problems: Error Analysis & Control. Dept. of Chemical Engineering & Chemical Technology, Imperial College, London.

18. Baines M.J. 1986 Moving Finite Elements : Regularisation Techniques. Numerical Analysis Report 19/86, Dept. of Maths., Univ. of Reading, UK.

19. Donnelly, J.D.P. 1986 A Version of Moving Finite Elements for 1-D Parabolic Equations. Oxford University Computing Laboratory Numerical Analysis Report, UK.

20. Edwards M.G. 1985 The Mobile Element Method. Numerical Analysis Report 20/85, Dept.of Maths., University of Reading, UK.

21. Edwards M.G., 1987 Moving Element Methods with Emphasis on the Euler Equations, Ph.D. Thesis, University of Reading, U.K.

22. Harten A. 1983 High Resolution Schemes for Hyperbolic Conservation Laws. J. Comput. Phys. 49, 357.