M A T H E M A T I C S D E P A R T M E N T

MOVING FINITE ELEMENTS AND APPROXIMATE LEGENDRE TRANSFORMATIONS

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Numerical Analysis Report 5/89

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U N I V E R S I T Y O F R E A D I N G

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Abstract

The Moving Finite Element method is reviewed and broken down into a number of steps. The central step is a semi-discrete procedure which is exact for class of one-dimensional scalar nonlinear PDE's, the resulting ODE system approximating the equations of characteristics. For more general PDE's the procedure is preceded by a projection step which is element-by-element; for higher dimensions it is followed by a projection step which is node-by-node .

The semi-discrete procedure is shown to be a Legendre transformation from the data to the nodal velocities, which has a useful geometrical interpretation based on an envelope construction. With projection included it becomes an approximate Legendre transformation of general applicability. The tranformation may also be used to construct a dual PDE which may be easier to solve numerically.

The structure is used to analyse nodal movement and to give new recipes for time-stepping and the avoidance of singularities.

Contents

1. Introduction

In recent years there has been much interest in the quality of the computational grids needed to resolve the numerical solution of differential equations . Many workers are now using irregular grids and the construction (and reconstruction) of these grids together with the quality of the solutions obtained on them has become a major consideration. Whilst the original motivation for irregular grids was economy of gridpoints, particularly in the regions where the solutions are smooth, it is now clear that for some problems sufficient resolution may be unobtainable practically in any other way in regions where the solution varies rapidly . At the same time considerable care is required in the design of grid variations to ensure that the solution is enhanced and not degraded by the character of the grid.

The Moving Finite Element (MFE) method of Miller ([22]-[25],[7]) belongs to the class of adaptive grid methods in which the mesh is evolved simultaneously with the solution. In the MFE method the evolution of the mesh and the solution are generated from the governing differential equation in the manner described below. The method has been used by many authors [22]-[25],[23],[16],[27],[28],[33],[4], [15], [19] to solve problems in which sharp features need to be resolved and tracked.

In this report we discuss the connection between the MFE approach and the Method of Characteristics. The moving grid framework provides a setting which the Legendre transformation may be used to good effect. The associated envelope construction also yields a nice geometrical characterisation of the MFE approximation.

The form of the report is as follows. In the latter part of this introduction we summarize the MFE approach. In section 2 we discuss an

idea originally developed in [1] for finding semi-discrete exact moving finite element solutions in one dimension. This is used as a framework in which to study projections of general operators in sections 3 and 5. Section 4 is devoted to the Legendre transformation and the different descriptions of the PDE and its discretisation. The framework is used in section 6 to discuss PDE's in higher dimensions. The advantage of the transformed variable is brought out and this is also exploited in section 7 on time-stepping strategies. In section 8 we discuss how general Legendre transformations can be approximated in this way and in section 9 draw some conclusions. This section also contains some practical points on dealing with singularities.

We recall the Lagrangian framework and approach to the derivation of MFE given by Mueller and Carey in ref. [28]. 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 an operator containing all derivatives in the space variable x. Define a coordinate transformation (assumed non-singular) between x,t and new independent variables ξ,τ by

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

for which the partial derivatives satisfy

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

Then (1.1) becomes, in a Lagrangian frame,

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

which, using the notation[1]

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

may be written as

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

To determine both $\dot{u}$ and $\dot{x}$ from (1.6) requires a further equation.

If $\hat{u}$ and $\hat{x}$ are restricted to functions $\hat{U}$ and $\hat{X}$, belonging to sets of admissible trial functions, (1.6) becomes a residual,

$$\frac{\partial \hat{U}}{\partial \tau} - \frac{\partial U}{\partial x}\frac{\partial \hat{X}}{\partial \tau} - \mathcal{L}\hat{U} = R\left[\frac{\partial \hat{U}}{\partial \tau}, \frac{\partial \hat{X}}{\partial \tau}\right] \tag{1.7}$$

say, no longer zero in general. There are however special situations where R will be zero and these are considered in detail in the next section. It turns out that there is enough generality in these cases to provide a useful framework for comparison with more general situations.

When $R \neq 0$ the problem of determining the time derivatives of $\hat{U}$ and $\hat{X}$ may be cast as a least squares variational problem by minimising

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[1]Here and in what follows u_x is a notation for $\hat{u}_\xi / x_\xi$ (see (1.3)).

the L_2 norm of R over $\frac{\partial \hat{U}}{\partial \tau}$ and $\frac{\partial \hat{X}}{\partial \tau}$. This gives the weak forms

$$< R,\psi > = 0 \qquad < R,u_x\chi > = 0 \tag{1.8}$$

for all admissible test functions $\psi(= \delta\dot{u})$ and $\chi(= \delta\dot{x})$,

where $$< R,S > = \int_{\xi_1}^{\xi_2} R\, S\, w\, d\xi \tag{1.9}$$

(w being a weight function)

and $$||R||_2^2 = < R,R > \tag{1.10}$$

is the L_2 norm of R with weight w defined over a suitable range (ξ_1,ξ_2) of ξ. Thus (1.8) gives two equations to determine $\dot{U}$ and $\dot{X}$.

Introducing finite element basis functions $\hat{\alpha}_j(\xi)$ in the ξ space (see fig 1.1) we can write $\hat{U}$ and $\hat{X}$ in the forms

$$\hat{U} = \sum_j \hat{U}_j(\tau)\hat{\alpha}_j(\xi) \qquad \hat{X} = \sum_j \hat{X}_j(\tau)\hat{\alpha}_j(\xi) \tag{1.11}$$

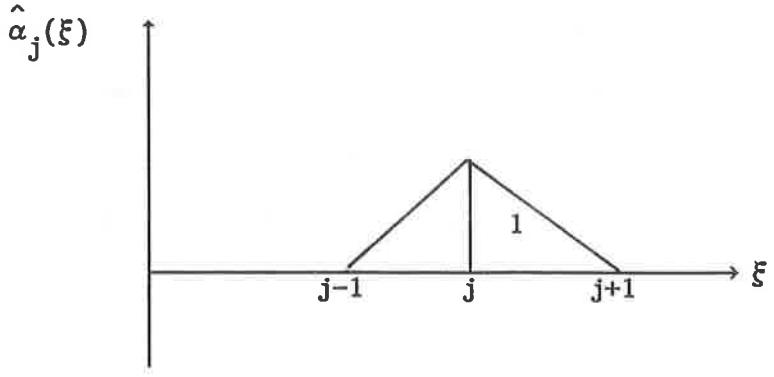


Fig. 1.1

where the $\hat{U}_j(\tau)$ are time-dependent coefficients, and the τ time derivatives are

$$\dot{U} = \sum_j \dot{U}_j \hat{\alpha}_j \qquad \dot{X} = \sum_j \dot{X}_j \hat{\alpha}_j \tag{1.12}$$

where $$\dot{U} = \frac{\partial \hat{U}}{\partial \tau} \,, \quad \dot{X} = \frac{\partial \hat{X}}{\partial \tau} \,, \quad \dot{U}_j = \frac{\partial \hat{U}_j}{\partial \tau} \,, \quad \dot{X}_j = \frac{\partial \hat{X}_j}{\partial \tau} \tag{1.13}$$

Then with $\psi = \chi = \hat{\alpha}_i$ the weak forms (1.8) become

$$\left.\begin{aligned} \langle R, \hat{\alpha}_i \rangle &= \langle \dot{U} - U_x \dot{X} - \mathcal{L}U, \hat{\alpha}_i \rangle = 0 \\ \langle R, U_x \hat{\alpha}_i \rangle &= \langle \dot{U} - U_x \dot{X} - \mathcal{L}U, U_x \hat{\alpha}_i \rangle = 0 \end{aligned}\right\} \ \forall i \tag{1.14}$$

which can be seen to be equivalent to minimising

$$||\dot{U} - U_x \dot{X} - \mathcal{L}U||_2 \tag{1.15}$$

over $\dot{U}_i$ and $\dot{X}_i$, i.e. Miller's method [22],[23]. Constraints, for example a lower bound on the Jacobian of the transformation or upper bounds on the relative nodal velocities, may be introduced through the use of penalty functions (see [22],[23],[28],[17],[20]).

Substitution of (1.11), (1.12) into (1.14) yields a nonlinear system of ordinary differential equations of the form

$$A(\underline{y})\dot{\underline{y}} = \underline{g}(\underline{y}) \tag{1.16}$$

where $A(\underline{y})$ is an extended mass matrix and $\underline{y}$ is a vector of the nodal

and coordinate unknowns $\hat{U}_j$ and $\hat{X}_j$. The ODE system (1.16) may be integrated from specified initial data to obtain $\hat{U}_j$ and $\hat{X}_j$ at a later time. This is a method of lines [15] and, with piecewise linear elements, is identical to Miller's method [22],[23].

The matrix $A(\underline{y})$ in (1.16) consists of blocks of inner products of basis functions of the form

$$\int \alpha_i \alpha_j \, w \, dx \quad , \quad \int \alpha_i \alpha_j \, U_x \, w \, dx \quad , \tag{1.17}$$

where w is the weight function used in the definitions of the L_2 norm. In Miller's original method [22],[23] w was taken to be 1 but in more recent work Miller [25], [7] uses a gradient weighting $w = (1+U_x^2)^{-\frac{1}{2}}$, producing the Gradient Weighted MFE method (GWMFE).

With piecewise linear basis functions α_j, any w depending only on U_x is piecewise constant and may be taken through the integral sign in (1.17). In particular, the decomposition of $A(\underline{y})$ demonstrated by Wathen & Baines [34],[3],

$$A(\underline{y}) = M^T C M \quad , \tag{1.18}$$

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 (1.18) 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 [2]. This is consistent with the connection with the

method of characteristics (see §2). However the result is also true, less naturally, for diffusion operators.

In solving

$$M^T C M\dot{\underline{y}} = \underline{g}(\underline{y}) \tag{1.19}$$

Baines and Wathen [3] write the method as a two step scheme

$$C\underline{W} = \underline{b} \tag{1.20}$$

$$M\dot{\underline{y}} = \underline{W} \tag{1.21}$$

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 [3],[4],[12],[13] the local character of the approximations is preserved if the procedure

$$\min_{\dot{\underline{y}}} ||C^{1/2}(M\dot{\underline{y}}-\underline{W})|| \tag{1.22}$$

which produces (1.19) is replaced by

$$\min_{\dot{\underline{y}}} ||C_D^{1/2}(M\dot{\underline{y}}-\underline{W})|| \tag{1.23}$$

where C_D is the diagonal of C . Then (1.19) is replaced by

$$M^T C_D M\dot{\underline{y}} = M^T C_D \underline{W} = M^T C_D C^{-1}\underline{b} \tag{1.24}$$

which is again local. The latter procedure may be shown [3] to be equivalent to a Petrov-Galerkin approach or, as shown by K. Miller, simply to the use of a different norm for R (see ref. [26]). We shall refer to (1.19) as the global method and to (1.24) as the local method, although (if penalty functions are absent) they are indistinguishable for one-dimensional scalar problems.

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 (1.16) is not solvable (unless the rank of $\underline{g}(\underline{y})$ is reduced correspondingly). Wathen & Baines [33] suggest a modification to MFE in which the velocity of the offending node is overwritten with a velocity averaged 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 (1.20) becomes singular. For problems involving diffusion, Johnson, Wathen & Baines [19] (who use explicit time integration) consciously limit the time step so as to avoid node overtaking, but other authors again rely on regularistion procedures.

Time integration of (1.16) is usually carried out with finite differences, typically forward or backward Euler or a stiff solver. Johnson, Wathen & Baines [19] use explicit Euler which fits in well with controlling node overtaking, but other authors,e.g. [22]-[25],[7],[16], [17],[27],[28],[15] 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.

The original MFE papers of Miller [22],[23] contained regularisation penalty terms aimed at combatting the singularities mentioned above. Other authors, notably Mueller and Carey [28], have used the same approach and various strategies have been used to construct such penalty terms [5],[20]. Generally the minimisation of $||R||$ (see (1.15)) is replaced by minimising

$$||R||^2 + \epsilon^2||P||^2 , \tag{1.25}$$

where P is the penalty and ϵ a suitable constant (chosen by Miller to be of the order of the truncation error). The link with the method of characteristics in section 2 is lost when this tactic is used, but the technique is very effective in practice.

In this report we discuss the connection between the MFE approach to solving PDEs and the Method of Characteristics. We also show that by using the Legendre transformation and an envelope construction we can clarify the structure of the approximation.

2. Semidiscrete Exact Solutions in One Dimension

Writing (1.7) in the form

$$\dot{U} - U_x\dot{X} - \mathcal{L}U = R \tag{2.1}$$

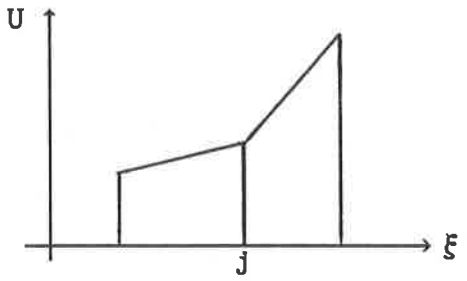
we first investigate those forms of $\mathcal{L}U$ for which there exist $\dot{U},\dot{X}$, belonging to the space S_h of piecewise linear continuous functions, for which R vanishes identically.

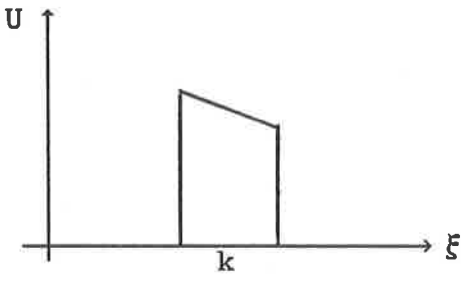
Since U_x is piecewise constant $(= U_\xi / X_\xi)$ the Lagrangian derivative $\dot{U} - U_x \dot{X}$ lies in the space of piecewise linear discontinuous functions, D_h say. Thus, from (2.1), if $\mathcal{L}U \in D_h$ we can find $\dot{U}, \dot{X} \in S_h$ such that R vanishes. We shall first demonstrate how this may be done for the equation

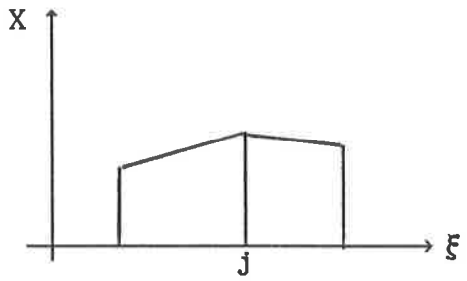
$$u_t + H(u_x) \equiv \dot{u} - u_x \dot{x} + H(u_x) = 0 \tag{2.2}$$

in which case (2.1) with $R = 0$ becomes

$$\dot{U} - U_x \dot{X} + H(U_x) = 0 \tag{2.3}$$







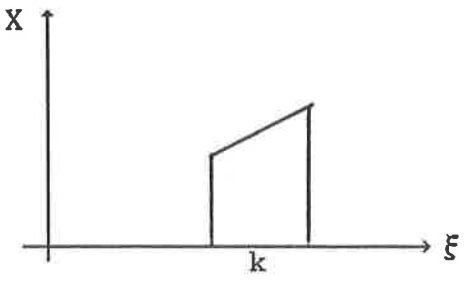


Fig. 2.1.

Fig. 2.2.

In (2.3) the first term $\in S_h$ and the other terms $\in D_h$. To extract the nodal values $\dot{X}_j, \dot{U}_j$ consider the jumps in each term across

a node j (see Fig. 2.1.). Using the square bracket notation $[]_j$ for such jumps we have from (2.3)

$$0 - [U_x]_j \dot{X}_j + [H]_j = 0 \tag{2.4}$$

since $\dot{U}$ and $\dot{X}$ are continuous at each node. Provided that $[U_x]_j \neq 0$ we find that

$$\dot{X}_j = [H]_j/[U_x]_j \tag{2.5}$$

Dividing (2.3) by U_x and considering the jumps in each term of the resulting equation across node j gives

$$[U_x]_j^{-1} \dot{U}_j - 0 + [U_x^{-1} H]_j = 0 \tag{2.6}$$

from which

$$\dot{U}_j = -[U_x^{-1} H]_j/[U_x^{-1}] \tag{2.7}$$

Now, considering jumps in U_x, U and X across an element k (see Fig. 2.2), using the bracket notation $\{ \}_k$ for such jumps, we have using (2.3)

$$(\dot{U}_x)_k = \frac{\partial}{\partial \tau}\left[\{U\}_k/\ \{X\}_k\right] = \left[\{\dot{U}\}_k - U_x\{\dot{X}\}_k\right]/\{X\}_k \tag{2.8}$$

$$= - \{H\}_k/\{X\}_k = 0 \tag{2.9}$$

since $H(U_x)$ is constant across an element.

Taking the limit of (2.5) as $[U_x]_j \to 0$ with X_j fixed, and the limit of (2.9) as $\{X\}_k \to 0$ with $(U_x)_k$ fixed, leads to the equations

$$\dot{x} = \frac{\partial H}{\partial u_x} = \frac{dH}{du_x} \qquad \dot{u}_x = -\frac{\partial H}{\partial x} = 0 \ . \tag{2.10}$$

Similarly, the limit of equation (2.7) as $[U_x]_j \to 0$ with X_j fixed is

$$\dot{u} = \frac{-\partial}{\partial u_x^{-1}} (u_x^{-1} H) = -H + u_x \frac{dH}{du_x} \ . \tag{2.11}$$

Equations (2.10)-(2.11) are the characteristic ODE's for the PDE (2.2) (see [10]).

Now consider the equation

$$u_t + H(x,u_x) \equiv \dot{u} - u_x \dot{x} + H(x,u_x) = 0 \tag{2.12}$$

with H <u>linear</u> in x . Equation (2.3) becomes

$$\dot{U} - U_x \dot{X} + H(X,U_x) = 0 \tag{2.13}$$

and since $H(X,U_x)$ is linear in X there is an exact solution for $\dot{U}$, $\dot{X}$ in S_h .

By the same argument as before

$$\dot{X}_j = [H]_j / [U_x]_j, \quad \dot{U}_x = -\{H\}_k / \{X\}_k \tag{2.14}$$

and $$\dot{U}_j = -[U_x^{-1}H]_j/[U_x^{-1}]_j \tag{2.15}$$

with limits as $[U]_j \to 0$, $\{X\}_k \to 0$

$$\dot{x} = \frac{\partial H}{\partial u_x} \qquad \dot{u}_x = -\frac{\partial H}{\partial x} \tag{2.16}$$

and

$$\dot{u} = -H + u_x \frac{\partial H}{\partial u_x} \tag{2.17}$$

Equations (2.16)-(2.17) are the characteristic ODE's for the PDE (2.12) and equations (2.14)-(2.15) are approximations to these equations.

Similarly for the equation

$$u_t + H(x,u,u_x) \equiv \dot{u} - u_x\dot{x} + H(x,u,u_x) = 0 \tag{2.18}$$

with $H(X,U,U_x)$ <u>linear</u> in X and/or U (but not bilinear), equation (2.14) and (2.15) still hold, but the limits are

$$\dot{x} = \frac{\partial H}{\partial u_x} \qquad \dot{u}_x = -\frac{\partial H}{\partial x} - \frac{\partial H}{\partial u} u_x \tag{2.19}$$

$$\dot{u} = -H + u_x \frac{\partial H}{\partial u_x} \tag{2.20}$$

which are the characteristic ODE's for (2.18).

The solutions of (2.14)-(2.15) therefore approximate the properties of the solution of (2.2), (2.12) or (2.18) by characteristics [10],[13], although the domain of dependence is spread either side of the

characteristic.

In classical PDE theory [10], if u is absent from $H(x,u,u_x)$ in (2.12), equations (2.16) form a Hamiltonian system, decoupled from (2.17), for the independent calculation of x and u_x : the function u may ultimately be calculated from (2.17). Similarly, in the discrete case (2.13), with $\dot{U},\dot{X} \in S_h$, $\dot{U}_x \in D_h$, the functions $\dot{X}$ and $\dot{U}_x$ can be calculated independently and the function $\dot{U}$ may ultimately be constructed from (2.8).

These results hold for semidiscrete solutions of equation (2.12) (or (2.18)) with H linear in x (and/or u).

Some examples are

(i) $$u_t - u_x^2 = 0 \tag{2.21}$$

for which

$$\dot{X}_j = - (U_x)_L - (U_x)_R \qquad (\dot{U}_x)_k = 0 \tag{2.22}$$

$$\dot{U}_j = - (U_x)_L \, (U_x)_R \tag{2.23}$$

where L,R refer to elements to the left and to the right of node j .

(ii) $$u_t + uu_x = 0 \tag{2.24}$$

for which

$$\dot{X}_j = - U_j \qquad (\dot{U}_x)_k = - U_x^2 \tag{2.25}$$

$$\dot{U}_j = 0 \tag{2.26}$$

An example which is not of the given form is

$$\text{(iii)} \qquad u_t + f(u)_x = 0 \tag{2.27}$$

the standard conservation law. By solving instead

$$w_t + f(w_x) = 0 \tag{2.28}$$

(which is of the given form) for w and putting $u = w_x$ we can obtain the solution of (2.24) indirectly. For this equation the $\dot{X}, \dot{U}$ and $\dot{U}_x$ are given by (2.5), (2.7) and (2.9) with u, H replaced by w, f. Hence

$$\dot{X}_j = [f]_j/[U]_j \qquad \dot{U}_k = 0 \tag{2.29}$$

in line with (2.22), (2.23) when $f(u) = \frac{1}{2} u^2$ (although U here is piecewise constant).

Note that the jump condition at a shock for the conservation law (2.24) is the first of (2.29) with $\dot{X}_j$ interpreted as the shock speed. Shocks may be modelled by enforcing a simple discontinuity in $u(= w_x)$, corresponding to constraining $(\dot{U}_x)_k = 0$ when a segment of the solution becomes vertical (and allowing $\dot{U}_k$ to go free) (ref. [2]). Moreover, the link with characteristics ensures that a geometrical entropy condition is approximately respected [29].

3. Local Projections

If $\mathcal{L} U \notin D_h$ the above results are not valid since (2.13) can no

longer be satisfied with $\dot{U}, \dot{X} \in S_h$. However we may project $\mathcal{L}U$ into D_h and then proceed as before. Since D_h is the space of piecewise linear discontinuous functions the projection may be carried out in each element separately.

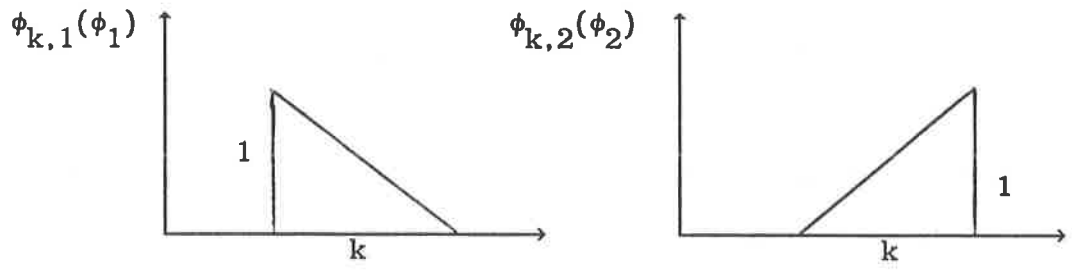


Fig. 3.1

For example, in the L_2 case the normal equations are

$$< W_1\phi_1 + W_2\phi_2 - \mathcal{L}U \ , \ \phi > = 0 \tag{3.1}$$

where ϕ is one of two possible linear basis functions in a single element (Fig. 3.1) and the W's are coefficients which already appeared in (1.20). By combining the ϕ's to form $\hat{\alpha}_i$ and $- U_x\hat{\alpha}_i$ (c.f. Figures (1.1),(3.1)) and using (1.21), we see that (3.1) is equivalent to minimising

$$||R||_2 = ||\dot{U} - U_x\dot{X} - \mathcal{L}U||_2 \tag{3.2}$$

over $\dot{U}_i$ and $\dot{X}_i$, i.e. Miller's method [22],[23]. However we emphasize that (3.1) is a local elementwise projection involving only the solution of a 2 x 2 system (see ref. [3]).

Consider now the equation

$$u_t + H(x,u,u_x) \equiv \dot{u} - u_x\dot{x} + H(x,u,u_x) = 0 \tag{3.3}$$

where H is a general function. Let the result of a set of local projections of $H(X,U(X),U_x)$ into D_h be $\tilde{H}(X,U_x)$ where $\tilde{H}$ is linear in X in each element. (Note that $\tilde{H}$ will not contain the function U within the element in question although it will contain values of U (and X) at the end points of the element). Then, by the argument in section 2, for the projected function $\tilde{H}$

$$\dot{X}_j = [\tilde{H}]_j/[U_x]_j \qquad (\dot{U}_x)_k = - \{\tilde{H}\}_k/\{X\}_k \tag{3.4}$$

$$\dot{U}_j = -[U_x^{-1}\ \tilde{H}]_j/[U_x^{-1}]_j \tag{3.5}$$

as in section 2. We recall that if u is absent from (3.3), equations (3.4) form a decoupled Hamiltonian-type system.

For example, for the conservation law

$$u_t + f(u)_x = 0 \tag{3.6}$$

we take the local projection of $f(u)_x$ which in the L_2 case is given by, say

$$f(U)_x = - W_1\phi_1 - W_2\ \phi_2 \tag{3.7}$$

where ϕ_1,ϕ_2 are local elementwise basis functions (see fig. 3.1) and W_1,W_2 are coefficients satisfying

$$C\begin{bmatrix} W_1 \\ W_2 \end{bmatrix} = -\int_1^2 f(U)_x \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} dx \tag{3.8}$$

over each element, where $C = \{C_{k\ell}\}$: $C_{k\ell} = \langle \phi_k, \phi_\ell \rangle$. The eigenvectors of C are $(1 \quad 1)^T$ and $(-1 \quad 1)^T$ with eigenvalues $\frac{1}{2}\{X\}$ and $\frac{1}{6}\{X\}$ respectively. So

$$\frac{1}{2}\{X\}(W_1+W_2) = -\int_1^2 f(U)_x \, dx = -\{f(U)\} \tag{3.9}$$

and

$$\frac{1}{6}\{X\}\{W\} = -\int_1^2 f(U)_x \{\phi\} \, dx = -\left[f(U)_2 + f(U)_1 - \frac{2}{\{X\}}\int_1^2 f(U) \, dx\right] \tag{3.10}$$

from which, in particular

$$\dot{U}_x = -\{f(U)\}/\{X\} = \{W\}/\{X\} \tag{3.11}$$

$$= \frac{-6}{\{X\}^2}[f(U)_2 + f(U)_1 - \frac{2}{\{X\}}\int_1^2 f(U) \, dx] \, . \tag{3.12}$$

Now consider the set of local elementwise projections of $H(X,U(X), U_x)$ into T_h , the set of piecewise constant functions on the mesh. Denote this weaker projection by $\bar{H}(U_x)$. Then by the argument in section 2, for the weaker projected function $\bar{H}$

$$\dot{X}_j = [\bar{H}]_j/[U_x]_j \qquad (\dot{U}_x)_k = 0 \tag{3.13}$$

$$\dot{U}_j = -[U_x^{-1} \bar{H}]_j/[U_x^{-1}]_j \, . \tag{3.14}$$

For this weaker projection, therefore, the slopes U_x do not alter with τ . (The projection is of Petrov-Galerkin type (see ref. [3].)

In the above example, take (3.7) with $W_1 = W_2 = W$. From (3.9), (3.13),

$$W = - \{f(U)\}/\{X\} \tag{3.15}$$

$$\dot{X}_j = - \frac{[\{f(U)\}/\{X\}]_j}{[U_x]_j} \tag{3.16}$$

The use of penalty functions in the projection will generally destroy its local character. Other constraints, such as demanding that the nodes be fixed, will do the same.

4. Legendre Transformations and the Envelope Construction

We now introduce the Legendre transformation which plays a central role in describing the structure and its approximation.

It is well known that the relationship between a function u and its slope m ,

$$m = \frac{du}{dx} \tag{4.1}$$

generates a Legendre transformation between x and m (ref.[30]). Inversion of (4.1) determines another function $v(m)$ such that

$$x = \frac{dv}{dm} \tag{4.2}$$

where v takes the values of

$$mx - u \ . \tag{4.3}$$

Here u and v are Legendre dual functions satisfying

$$u - mx + v = 0 \ . \tag{4.4}$$

The symmetry implies that x is the slope of the v(m) function.

Note that if u(x) is a straight line, v(m) is constant, while if u(x) is only piecewise linear in x , each piece generates a point value of v(m).

Similarly the relationship (first of (2.10))

$$\dot{x} = \frac{dH}{du_x} \tag{4.5}$$

from the theory of characteristics for the PDE (2.3) generates a Legendre transformation between u_x and $\dot{x}$ which has the inversion

$$u_x = \frac{dG}{d\dot{x}} \tag{4.6}$$

where $G(\dot{x})$ is the Legendre dual function $H(u_x)$ satisfying

$$H - u_x\dot{x} + G = 0 \ . \tag{4.7}$$

From (2.2) we identify G as $\dot{u}(\dot{x})$. In dynamics G and H are the Lagrangian and Hamiltonian functions.

When H contains x as well as u_x, as in (2.12), (4.5) is replaced by the first of (2.16) and x acts as a passive variable in the theory. The same is true if H contains x, u_x and u, as in (2.18), when both x and u act as passive variables.

In what follows the notation m will be used for u_x and M for U_x.

It is useful to obtain the equation corresponding to (2.2), (2.12) or (2.18) in terms of v, using (4.4). Differentiating (4.4) with respect to τ we have

$$\dot{u} - \dot{m}x - m\dot{x} + \dot{v} = 0 \tag{4.8}$$

from which, using (4.1) and (4.2), equations (2.2), (2.12) or (2.18) become

$$\dot{v} - v_m\dot{m} - H = 0 \ . \tag{4.9}$$

From the second of (2.16) or (2.19) there exists a Legendre transformation between m and x (see (4.2)) which has the inversion

$$v_m = -\frac{\partial E}{\partial \dot{m}} \tag{4.10}$$

The dual function E satisfies

$$H + v_m\dot{m} + E = 0 \tag{4.11}$$

where, from (4.9), we deduce that

$$E = -\dot{v} \tag{4.12}$$

The Legendre transformation has an envelope construction which will be useful in characterising approximations ([30],[31]). We describe this construction in relation to equation (4.5). For each point P of initial data (see Fig. 4.1) we may evaluate u_x and $H(u_x)$ and plot them as a point L in u_x,H space (Fig. 4.2). Moreover, for each value of u_x,H , (2.2) is the equation of a line, denoted by ℓ , in $\dot{x},\dot{u}$ space (Fig. 4.3). As P varies along the curve of inital data in Fig.4.1, the point L in Fig.4.2 traces out a curve and the line ℓ in Fig.4.3 traces out a pencil of lines (envelope). Fig.4.2 is the point-line dual of Fig.4.3 (ref. [30]). The construction exhibits the Legendre Transformation between the dual functions $H(u_x)$ and $\dot{u}(\dot{x})$ geometrically.

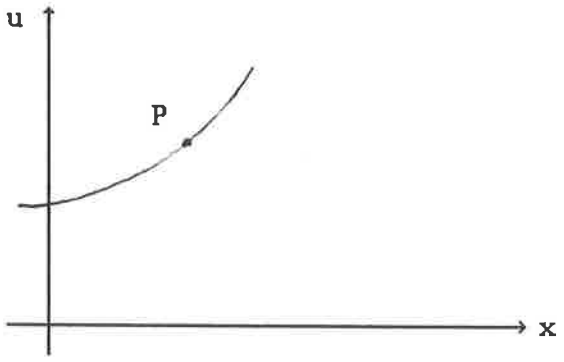


Fig.4.1

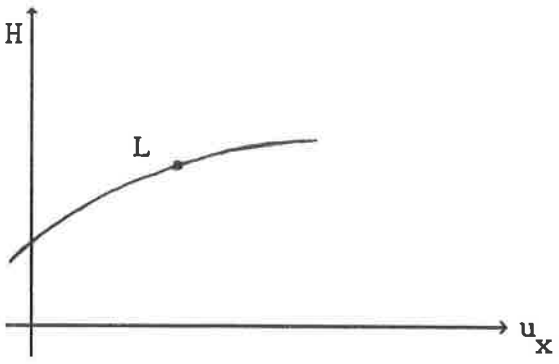


Fig. 4.2

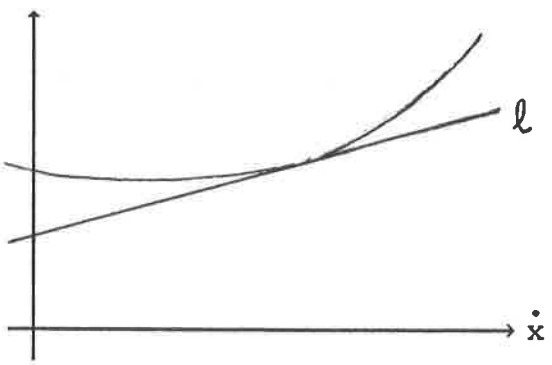


Fig. 4.3

In the discrete case discussed in section 2, $U_x = M$ is piecewise constant and therefore takes only discrete values, one for each cell, as does $H(M)$ (see Fig. 4.4). The data is therefore represented in m, H space as a series of points L_k, each of which determines a line ℓ_k in the dual $\dot{x},\dot{u}$ space (fig. 4.5). (If the discrete points in m, H space are simply sampled values taken from the continuous data curve $H(m)$, then they are the vertices of a chordal polygon connecting points on the data curve.)

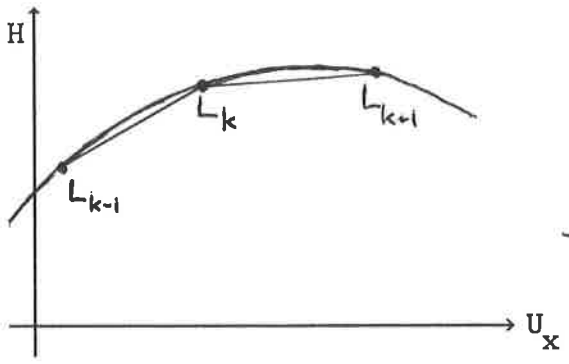


Fig. 4.4

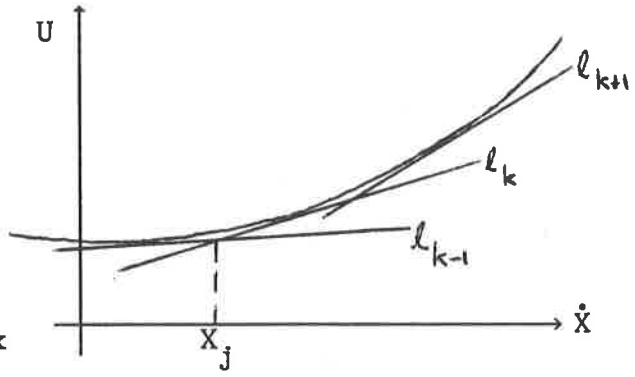


Fig. 4.5

From equation (2.5) the velocity $\dot{X}_j$ of node j is given by the slope of the line joining two of the points, L_k and L_{k-1} say, on the $H(m)$ curve. By the duality of the Legendre transformation it follows that $\dot{X}_j$ is at the point of intersection of the two corresponding tangents ℓ_k and ℓ_{k-1} to the envelope in $\dot{x}$, $\dot{u}$ space (see Figs 4.1, 4.2). Moreover $\dot{U}_j$ must also be at this intersection since it satisfies (2.3).

Since $\dot{X}$ and $\dot{U}$ are linear in ξ (and therefore in each other)

within each element, they are given by intermediate points along each tangent, corresponding in the dual diagram (Fig. 4.4) to sets of lines through each discrete point on the $H(m)$ curve.

In generalising to $H(X,U,M)$ with H linear in X and/or U the same construction holds with X and/or U as passive variables, the relationship (2.14)-(2.15) still holding. For more general H the projection of section 3 is needed to produce $\tilde{H}$ in the right space to enforce the properties $\dot{X}$, $\dot{U} \in S_h$, $M \in T_h$.

Finally, in this section we return to equation (4.9) for the variable v dual to u . Let $H(x,m)$ be linear in x of the form

$$H(x,m) = H_o(m) + xH_1(m) \ . \tag{4.13}$$

Then (4.9) becomes

$$\dot{v} - x\dot{m} - H_o(m) - xH_1(m) = 0 \ . \tag{4.14}$$

There is an exact solution for the discrete approximations $V,M \in T_h$, $X \in S_h$ with

$$\dot{M}_k = - H_1(M_k) \qquad \dot{V}_k = H_o(M_k) \ . \tag{4.15}$$

The first of these reproduces the second of (2.14) and is a set of decoupled ODE's for the M_k . Once these have been calculated the second of (4.15) enables V_k to be found.

The inversion of the Legendre transformation, from M, V to X, U, is effected by applying the same argument used in section 2 to the

discrete form of (4.4)

$$U - MX + V = 0 \tag{4.16}$$

yielding (c.f. (2.14) and (2.15))

$$X_j = [V]_j/[M]_j \qquad U_j = -[M^{-1}\ V]_j/[M^{-1}]_j \ . \tag{4.17}$$

This is an example of a Legendre transformation with distributed and accumulated singularities (ref. [31], p.112).

In the case of more general H the projection of section 3 onto $\tilde{H}$ must be done first, converting (4.15) to

$$\dot{M}_k = -\tilde{H}_1(M_k) \qquad \dot{V}_k = \tilde{H}_o(M_k) \ . \tag{4.18}$$

Note that $\tilde{H}_o$ and $\tilde{H}_1$ depend on the current configuration of the elements.

We return to this aspect in section 7 on time-stepping.

5. Second Order Equations in 1-D

For piecewise linear approximation the second order operator u_{xx} exists only in the sense of delta functions but L_2 projection into the space D_h is possible. For example if we write

$$\mathfrak{L}\tilde{U} = W_{k,1}\ \phi_{k,1} + W_{k,2}\ \phi_{k,2} \tag{5.1}$$

(c.f. (3.7)) for the L_2 projection of $\mathfrak{L}u$ into D_h, then using Miller's mollification procedure [23] or the Hermite cubic recovery

method [19] in (1.20), the $W_{k,1}$, $W_{k,2}$ of (5.1) are

$$\left.\begin{aligned} W_{k,1} &= \frac{1}{h_k}(-M_{k+1} + 3M_k - 2M_{k-1}) \\ W_{k,2} &= \frac{1}{h_k}(2M_{k+1} - 3M_k + M_{k-1}) \end{aligned}\right\} \tag{5.2}$$

where M_k denotes U_x in element k and $h_k = \{X\}_k = X_k - X_{k-1}$ is the length of the element.

This gives from (3.4)

$$-(M_k - M_{k-1})\,\dot{X}_j = \frac{1}{h_k}(-M_{k+1}+3M_k - 2M_{k-1}) - \frac{1}{h_{k-1}}(2M_k - 3M_{k-1} + M_{k-2}) \tag{5.3}$$

and

$$h_k^2\dot{M}_k = 3(M_{k+1} - 2M_k + M_{k-1}) \ . \tag{5.4}$$

The latter is evidently the difference form of a linear heat equation, although we should note that h_k varies with τ . The former is a difference form of

$$-h_j m'_j \dot{X}_j = m'_{j+\frac{1}{2}} - m'_{j-\frac{1}{2}} \tag{5.5}$$

where $m' = \frac{dm}{dx}$ and $h_j = \frac{1}{2}(h_k + h_{k-1})$, taking upwind forms of the derivatives on the right hand side.

Clearly from (5.3) there is no finite solution for $\dot{X}_j$ when $M_k = M_{k-1}$. Moreover in this case $\dot{X}_{j+1}$ satisfies

$$-(M_{k+1} - M_k)\,\dot{X}_{j+1} = \frac{1}{h_{k+1}}(-M_{k+2}+3M_{k+1} - 2M_k) - \frac{2}{h_k}(2M_{k+1} - M_k) \tag{5.6}$$

so that, if $M_k \neq M_{k+1}$

$$\dot{X}_{j+1} = \frac{2}{h_k} - \frac{1}{h_{k+1}} \frac{(-M_{k+2}+3M_{k+1}-2M_k)}{M_{k+1}-M_k} . \tag{5.7}$$

Adding a multiple of $M_k - M_{k-1}$ gives

$$\dot{X}_{j+1} = \frac{2}{h_k} - \frac{1}{h_{k+1}} \frac{(-M_{k+2}+3M_{k+1}-3M_k+M_{k-1})}{M_{k+1}-M_k} . \tag{5.8}$$

$$= \frac{2}{h_k} - h_{k+1} \frac{m'''(\theta)}{m'(\phi)} \tag{5.9}$$

by the Mean Value Theorem, where $\theta, \phi \in (X_k, X_{k+1})$. It follows that if

$$h_k h_{k+1} < 2 \min_{\phi} |m'(\phi)| / \max_{\theta} |m'''(\theta)| \tag{5.10}$$

then $\dot{X}_{j+1} > 0$ and node $j+1$ moves away from the singular point j . By a similar argument node $j-1$ also moves away from node j , which therefore has the character of an anti-cluster singular point.

It is interesting to note that the leading term in the Taylor expansion of the right hand side of (5.3) is

$$- 2h_j m'' \tag{5.11}$$

whereas that of (5.5) is

$$h_j m'' \tag{5.12}$$

the difference arising from the subtraction of the approximations to m' on the right hand side of (5.3). The implication is that if m' were better approximated (perhaps by higher order finite elements) then the sign of $\dot{X}_j$ would be reversed and a singular node j for which $M_k = M_{k-1}$ (near zero curvature) would become a cluster point, completely at variance with how nodes might be expected to move. This is not so surprising since, in order to approximate $\dot{u}_x = 0$ (see (2.10)) (which is evidently unnatural in a diffusion process), nodes would have to move immediately to points of maximum slope where the curvature is zero. In practice, linear finite element approximation fortuitously reverses this tendency, leaving however a question mark over higher order approximations.

A consequence of the anti-cluster property of the singular points, as pointed out by A.Wathen [36], is that nodes do not pass through zero curvature points and are confined to regions between then.

Now suppose generally that one of the slopes, say M_k, becomes very large. Then from (5.3), we have approximately

$$\left.\begin{aligned} -M_k\dot{X}_j &= \frac{3M_k}{h_k} - \frac{2M_k}{h_{k-1}} \\ M_k\dot{X}_{j+1} &= \frac{2M_k}{h_{k+1}} - \frac{3M_k}{h_k} \end{aligned}\right\} . \qquad (5.13)$$

Moreover, if the large slope is associated with small h_k (when nodes become very close but function values stay apart) we have the approximations

$$\dot{X}_j = -\frac{3}{h_k} \qquad \dot{X}_{j+1} = \frac{3}{h_k} \qquad (5.14)$$

indicating from the signs a natural springing effect, first noticed by P. Jimack [18].

We end this section by looking at the form of $\dot{V}_k$ in (4.15). Splitting the $\mathfrak{U}$ of (5.1), the negative of $\tilde{H}$, into its constant and linear parts gives

$$\tilde{H} = \tilde{H}_o + \tilde{H}_1 x = -(W_{k,1} + W_{k,2}) - (W_{k,2} - W_{k,1})x \tag{5.15}$$

which leads via (5.2), consistently with (4.15), to (5.4). The corresponding equation for $\dot{V}_k$ is

$$\dot{V}_k = -(W_{k,1} + W_{k,2}) = \frac{1}{h_k}(M_{k+1} - M_{k-1}) \ . \tag{5.16}$$

Once M_k is found from (5.4), V_k can be found from (5.16). Then (4.17) may be used to recover X_j and U_j.

We observe that the right hand side of (5.16) is the projection of u_{xx} into the space T_h.

6. Higher Dimensions

The argument in this section is given for two dimensions only but generalises to any number of dimensions.

The PDE corresponding to (2.2) in two dimensions, using an extension of the argument in section 1, is

$$u_t + H(u_x,u_y) \equiv \dot{u} - u_x\dot{x} - u_y\dot{y} + H(u_x,u_y) = 0 \tag{6.1}$$

and, corresponding to (2.1), (2.3) we have

$$R = \dot{U} - U_x\dot{X} - U_y\dot{Y} + H(U_x,U_y) \tag{6.2}$$

where $\dot{U},\dot{X},\dot{Y} \in S_h$, $H(U_x,U_y) \in T_h$, these spaces being respectively the space of piecewise linear continuous functions and piecewise linear constant functions on a triangular partition of the (ξ,η) plane (where η is the second reference variable).

In one dimension it was possible to find $\dot{U},\dot{X}$ such that $R \equiv 0$ but in higher dimensions this is no longer true. The reason is that $\dot{U} - U_x\dot{X} - U_y\dot{Y}$ belongs to a particular subset E_h of D_h, the space of piecewise linear discontinuous functions on the triangulation. The subset E_h, which depends on U_x,U_y, does not necessarily contain $H(U_x,U_y)$, which $\in T_h$. Moreover, if H is $H(x,y,u_x,u_y)$ where H is linear in x and y, then $H(X,Y,U_x,U_y) \in D_h$ but again $H \in E_h$ in general, so that we cannot find $\dot{U},\dot{X},\dot{Y}$ such that $R \equiv 0$.

The difficulty can be resolved by a projection of H into E_h, reminiscent of the projections $H \to \tilde{H}$ and $H \to \overline{H}$ discussed earlier. The projection into E_h is however a minor projection in comparison with the earlier ones, which were from infinite spaces to finite ones. (see ref. [3]).

Thus in the case of a general H we would first project $H \to \tilde{H}$ locally in each element, obtaining $\tilde{H} \in D_h$. Then a second projection of $\tilde{H}$ from D_h to E_h would be carried out, enabling $\dot{U},\dot{X},\dot{Y}$ to be chosen such that $R \equiv 0$.

To make the necessity for this second projection clearer consider a node j and let the suffix k range over its surrounding elements. After the projection $H \to \tilde{H}(X,Y,U_x,U_y)$ in which $\tilde{H}$ is a linear function of X and Y, for R to be zero we require

$$\dot{U}_j - (U_x)_k \dot{X}_j - (U_y)_k \dot{Y}_j + \tilde{H}(X_j,Y_j,(U_x)_k,(U_y)_k) = 0 \qquad (6.3)$$

for all k. In a standard triangulation k runs from 1 to 6, but there are only three unknowns $\dot{U}_j, \dot{X}_j$ and $\dot{Y}_j$. Hence the need for a further projection. If we use L_2 projection with area weighting we have the least squares equations

$$\left.\begin{aligned}
(\Sigma A_k)\dot{U}_j - (\Sigma M_k A_k)\dot{X}_j - (\Sigma N_k A_k)\dot{Y}_j + \Sigma A_k \tilde{H}_k &= 0 \\
-(\Sigma M_k A_k)\dot{U}_j - (\Sigma M_k^2 A_k)\dot{X}_j + (\Sigma M_k N_k A_k)\dot{Y}_j - \Sigma M_k A_k \tilde{H}_k &= 0 \\
-(\Sigma N_k A_k)\dot{U}_j + (\Sigma M_k N_k A_k)\dot{X}_j + (\Sigma N_k^2 A_k)\dot{Y}_j - \Sigma N_k A_k \tilde{H}_k &= 0
\end{aligned}\right\} \qquad (6.4)$$

where $\dot{U}_j, \dot{X}_j, \dot{Y}_j$ are now averaged values, A_k is the area of an adjacent triangular element and we have used the notation M_k, N_k for $(U_x)_k$, $(U_y)_k$. This reproduces (1.23) and (1.24). The same projection with a different weighting (the square root of the element mass matrix - see (1.22)), leads to the standard MFE method. The two projections $H \to \tilde{H}$ and the finite L_2 projection above are combined into a single L_2 projection into the space E_h.

A notable exception to the necessity for projection is the equation

$$u_t + auu_x + buu_y \equiv \dot{u} - u_x\dot{x} - u_y\dot{y} + auu_x + buu_y = 0 \qquad (6.5)$$

where a,b are constants, for which

$$R = \dot{U} - U_x\dot{X} - U_y\dot{Y} + aUU_x + bUU_y \qquad (6.6)$$

vanishes identically with

$$\dot{U}_j = 0\,, \quad \dot{X}_j = aU_j, \qquad \dot{Y} = bU_j\,. \qquad (6.7)$$

On the other hand the same example with au, bu replaced by nonlinear functions a(u), b(u) certainly requires projection.

Rather than consider other examples at this stage we prefer to invoke the procedure of section 4 using a Legendre transformation. In two dimensions we have

$$m = \frac{\partial u}{\partial x} \qquad n = \frac{\partial u}{\partial y} \tag{6.8}$$

inverted to give

$$x = \frac{\partial v}{\partial m} \qquad y = \frac{\partial v}{\partial n} \tag{6.9}$$

where

$$u - mx - ny + v = 0 \ . \tag{6.10}$$

Since

$$\dot{u} - m\dot{x} - n\dot{y} = - (\dot{v} - x\dot{m} - y\dot{n}) \tag{6.11}$$

(6.1) becomes

$$\dot{v} - x\dot{m} - y\dot{n} - H(m,n) = 0 \tag{6.12}$$

and correspondingly

$$R = \dot{V} - X\dot{M} - Y\dot{N} - H(M,N) \ . \tag{6.13}$$

This time, since $\dot{V},\dot{M},\dot{N},H \in T_k$ there is no difficulty in writing down

solutions for $\dot{V},\dot{M},\dot{N}$, which make $R \equiv 0$; in fact

$$\dot{V}_k = H(M_k,N_k) \ , \quad \dot{M}_k = 0 \ , \quad \dot{N}_k = 0 \ . \tag{6.14}$$

Generalising to $H(x,y,m,n)$ with H a linear function of x and y , so that

$$H(X,Y,M,N) = H_o(M,N) + X\, H_1(M,N) + Y\, H_2(M,N) \tag{6.15}$$

we have in a similar manner

$$\dot{V}_k = H_o(M_k,N_k), \quad \dot{M}_k = - H_1(M_k,N_k) \ , \quad \dot{N}_k = -H_2(M_k,N_k) \ . \tag{6.16}$$

As in the case of (4.15), M_k and N_k can be found by solving the second and third of (6.16) simultaneously: when this is done the first of (6.16) can be solved for V_k . Having found values of M_k and N_k and V_k for each element - effectively the gradient and negative intercept (on the U axis) of each plane - it remains to convert this information back into nodal positions and values. The mechanism for this is contained in (6.10) but in the discrete case

$$R = U - MX - NY + V \tag{6.17}$$

there is now no guarantee that functions $U,X,Y \in S_h$ can be extracted. The situation is exactly the same as for (6.2) where $\dot{U},\dot{X},\dot{Y}$ were to be recovered from $R \equiv 0$.

To obtain $\dot{U},\dot{X},\dot{Y}$ we therefore need to project, for example as for

(6.2) yielding (6.4) without the dots and with $\tilde{H}_k$ replaced by V_k. In the notation of section 1 ((1.16)-(1.24)), this is identical with

$$M^T C_D M \underline{y} = - M^T C_D \overline{\underline{V}} \tag{6.18}$$

where $\overline{\underline{V}}$ is a vector containing the V_k (repeated twice for each element). Alternatively, we many replace C_D in (6.18) by the element mass matrix C obtaining the standard MFE matrix (1.18).

Geometrically the effect of the projection required to make $R = 0$ in (6.2) or (6.17) is to convert the trace on the (ξ,η) plane of the intersections of a set of planes into a triangulation. The projection is needed to complete the cycle of "triangulation - projection into D_h - solution for M,N,V - projection into E_h - new triangulation" sequence. It therefore modifies the tangent plane construction, the two-dimensional equivalent of Fig. (4.5).

Since equations (6.16) are pointwise ODE's the strategy of the method of characteristics in converting the PDE into a set of ODE's has been carried out, and so (6.16) have within them approximately the same information possessed by characteristic equations.

In the case of the second order operator

$$\mathfrak{L}u = \nabla^2 u \tag{6.19}$$

the projection into the space D_h can be carried out using mollification or recovery with the result that equations (6.16) become of the form

$$\dot{V}_k = H_o(M_k, N_k, M_\ell, N_\ell) \tag{6.20}$$

$$\left.\begin{aligned} \dot{M}_k &= - H_1(M_k, N_k, M_\ell, N_\ell) \\ \dot{N}_k &= - H_2(M_k, N_k, M_\ell, N_\ell) \end{aligned}\right\} \tag{6.21}$$

where ℓ ranges over the elements with a side common to the element k . Quantities depending on the configuration are also present and the solution for V,M,N is more difficult to obtain. The principle of obtaining M,N, then V and finally U,X,Y is still illuminating however.

7. Time-Stepping

As with many time dependent finite element algorithms time-stepping in the standard MFE method is carried out by finite differences. Having generated the coupled system of nonlinear ODE's (1.16) (or an extended version of the same form) most authors then apply an implicit stiff solver to the system on the grounds that it is expected to be stiff due to the abundance of degrees of freedom. Only one approach [3],[19] uses an explicit solver (the simplest Euler one step method) with however sufficient success as to cast doubt on the need for an expensive stiff solver. (In view of the relationship of the ODE's with Hamilton's equations it is clear that time-stepping for symplectic systems may also have an important part to play [14].)

Within the present framework we can in one dimension use the decoupled equations (4.18) to do the time-stepping. Consider (2.12) with $H(X,U_x)$ of the form

$$H(X,M) = H_o(M) + X\, H_1(M) \tag{7.1}$$

in each element k . For this function the time derivatives in the transformed variables are given by (4.15). The first of these

$$\dot{M}_k = - H_1(M_k) \tag{7.2}$$

may be time-stepped independently for each k using any standard ODE solver for a single equation. The second,

$$\dot{V}_k = H_o(M_k) \tag{7.3}$$

gives then a simple integration for V_k using quadrature. Inversion of the transformed variables is accomplished by (4.17).

For equations of the form (3.3) we first perform a projection into the space D_h giving

$$\tilde{H}_o(M) + X\,\tilde{H}_1(M) \tag{7.4}$$

in each element k . The procedure above may still be followed for the ODE's involving M_k and V_k (with tildas on H_o, H_1) , but it should be realised that the projected functions depend on values of U,X at end nodes of the element k and these must be frozen in the integration if iteration is to be avoided.

Now consider the example (2.24) for which

$$\dot{M}_k = - M_k^2 \tag{7.5}$$

This has the exact solution (dropping the suffix k)

$$M = \frac{M(0)}{1+M(0)\,t} \tag{7.6}$$

where $M = M(0)$ at $t = 0$. Clearly M decreases with t, leading to steepening negative gradients and the formation of a shock. The discrete form of (7.5) which yields the approximate solution of (7.5) closest to (7.6) is

$$\frac{M^{n+1}-M^n}{\Delta t} = - M^n M^{n+1} \tag{7.7}$$

giving

$$M^{n+1} = \frac{M^n}{1+M^n \Delta t} \tag{7.8}$$

where Δt is the time step and n, $n+1$ refer to time levels t and $t + \Delta t$.

Defining

$$\mu = M^{-1} \tag{7.9}$$

equation (7.5) and its exact solution become

$$\dot{\mu} = 1 \qquad \mu = \mu(0) + t \tag{7.10}$$

and here Euler explicit time-stepping on μ is obviously sufficient.

The equation for V is the second of (4.15) which, using (3.9), is

$$\dot{V}_k = M_k(U_{k,1} + U_{k,2}) \tag{7.11}$$

A possible time-stepping for V is

$$V^{n+1} = V^n + \frac{\Delta t}{2} (M^n + M^{n+1}) (U_1^n + U_2^n) \qquad (7.12)$$

using explicit values for U_1, U_2. With M^{n+1}, V^{n+1} known U^{n+1}, X^{n+1} can be constructed. [Of course in this example $\dot{U}_j = 0$ which in practice circumvents the use of the V equation.]

For the general scalar conservation law it can be shown from (3.9) and (3.12) that

$$\dot{U}_x = \frac{f''(U_\theta)}{\{X\}} \qquad \dot{V} = 2\,\frac{\{f(U)\}}{\{X\}} \qquad (7.13)$$

where U_θ lies in the interval (U_1, U_2). Time-stepping along the lines suggested above (Euler explicit for μ and trapezium integration for V) can still be done with end values of U and X frozen. Then U^{n+1}, X^{n+1} can be recovered as before. The general idea behind this approach is that it works exactly for H's of the form (7.1) and is an approximation only to the extent that H departs from (7.1).

For the second order operator u_{xx} we have seen that the corresponding equations for M and V are

$$\dot{M}_k = \frac{3}{h_k^2}\,\delta^2 M_k \qquad \dot{V}_k = \frac{1}{h_k}(M_{k+1} - M_{k-1}) \qquad (7.14)$$

(see (5.4) and (5.16)). As remarked earlier, the first of these resembles a semi-discrete approximation of the linear heat equation

for m (see refs. [3],[11]) . The ideal time-stepping for this equation is the one step fully implicit algorithm, since this maintains the inherent maximum principle contained in the equation (even with h_k^2 variable). Once M_k is known at the new time level V_k may be found by the trapezium rule. With M,V found we can recover X,U .

Similarly, in two dimensions, with

$$H(X,Y,M,N) = H_o(M,N) + X\,H_1(M,N) + Y\,H_2(M,N)$$

the ODE's for M,N and V are the semi-discrete equations (6.16). The procedure of solving for M,N (now coupled) and subsequently for V can again be followed. For more general H, projection into D_h is needed first. Time-stepping of the M,N system is more delicate here, since the system could be stiff, but at least it is only 2×2 . As in section 6, a further projection is needed to recover X,Y and U .

The two-dimensional examples

$$u_t + u_x^2 + u_y^2 \equiv \dot{u} - u_x\dot{x} - u_y\dot{y} + u_x^2 + u_y^2 = 0 \qquad (7.15)$$

$$u_t + axu_x + byu_y \equiv \dot{u} - u_x\dot{x} - u_y\dot{y} + axu_x + byu_y = 0 \qquad (7.16)$$

which become in their discrete M,N,V forms

$$R = \dot{V} - X\dot{M} - Y\dot{N} - M^2 - N^2 = 0 \qquad (7.17)$$

$$R = \dot{V} - X\dot{M} - Y\dot{N} - aXM - bYN = 0 \qquad (7.18)$$

giving respectively

$$\dot{M}_k = 0 \qquad \dot{N}_k = 0 \qquad \dot{V}_k = M^2+N^2 \tag{7.19}$$

$$\dot{M}_k = -\,aM_k \qquad \dot{N}_k = -\,bN_k \qquad \dot{V}_k = 0 \tag{7.20}$$

are exceptional in that M,N do not interact: more general equations will always involve this interaction (see (6.16)). Time-stepping in these examples is rather obvious.

The two dimensional analogue of (7.14), corresponding to the operator $\nabla^2 u$, yields ODE's for M and N that are rather complicated, but the equation for V is simply

$$\dot{V} = \sum_s (M\,\lambda_s + N\,\upsilon_s)\ell \tag{7.21}$$

where s runs over the sides of the element k and λ_s, υ_s are direction cosines of the outward normal to side s. Time-stepping in this case is therefore concentrated on how to solve the $\dot{M},\dot{N}$ equations for M and N.

Note that, compared with time-stepping strategies used hitherto, the use of the ODE's for M,N,V ensures the greatest compactness of the stencil and enables implicitness to be introduced in a selective and well-understood way.

8. Approximation of the Legendre Transformation

In some applications of numerical methods it is necessary to be able to construct an approximate Legendre transformation (see e.g. ref.

[9]). The reason is exactly the same as for the method described in this report, namely, that the evolution of the transformed variable is much easier to follow than that of the original variables. In the work of Chynoweth et.al. [9] there is the added advantage of being able to characterise the evolution of meteorological fronts in the transformed variable more easily than in the original variable. The same may be true for nonlinear first order PDEs in the formation of shocks.

The basic construction involves numerical approximation of (4.1)-(4.4) or (6.8)-(6.10). We have already described a method of carrying out this transformation approximately when U,X or $U,X,Y \in S_h$ and V,M or $V,M,N \in T_h$. This transformation is unsymmetrical in the sense that the two sets of functions belong to different spaces, of piecewise linear continuous and piecewise constant functions, respectively, but this seems not unnatural in view of the point/line duality of the transformation (see [30],[8]).

We illustrate the approximate Legendre transformation in a neutral notation [30],[6]. Let X,Y be functions of single variables x,y, respectively, and let the exact Legendre transformation be described by the equations

$$x = \frac{dY}{dy} \qquad y = \frac{dX}{dx} \qquad X + Y - xy = 0 \qquad (8.1)$$

Suppose now that $X,\ x \in S_h$ and $Y,\ y \in T_h$ and that in terms of piecewise linear basis functions $\hat{\alpha}_j$

$$x = \sum x_j \hat{\alpha}_j \qquad X = \sum X_j \hat{\alpha}_j \qquad (8.2)$$

(c.f. (1.11)). Then in one dimension we have from (2.5) that the approximate transformation is given by

$$x_j = [Y]_j/[y]_j \qquad X_j = -[y^{-1}Y]_j/[y^{-1}]_j \qquad (8.3)$$

together with the third of (8.1). This corresponds to the tangent construction described in section 4.

In higher dimensions let X,Y be functions of $\underline{x},\underline{y}$, respectively, where $\underline{x} = \{x_i\}$, $\underline{y} = \{y_i\}$, $(i = 1,2, \ldots d)$, d is the number of dimensions, and let the exact transformation be given by

$$x_i = \frac{\partial Y}{\partial y_i} \qquad y_i = \frac{\partial X}{\partial x_i} \qquad X + Y - \underline{x}.\underline{y} = 0 \qquad (8.4)$$

Using the corresponding spaces S_h, T_h and basis functions $\hat{\alpha}_j$ we cannot now satisfy the third of (8.4) everywhere, except in an averaged sense (see section 6). Choosing an L_2 average with area (A_k) weighting in adjacent elements k gives equations corresponding to (6.4), namely

$$\begin{bmatrix} \Sigma A_k & -\Sigma A_k \underline{y}_k^T \\ -\Sigma A_k \underline{y}_k & \Sigma A_k \underline{y}_k \underline{y}_k^T \end{bmatrix} \begin{bmatrix} \tilde{X}_j \\ \tilde{\underline{x}}_j \end{bmatrix} = \begin{bmatrix} -\Sigma A_k Y_k \\ \Sigma A_k \underline{y}_k Y_k \end{bmatrix} \qquad (8.5)$$

$\tilde{X}_j$, $\tilde{\underline{x}}_j$ being the averaged values of X_j, $\underline{x}_j$. Equation (8.5) is of the form (1.24) and gives the solution in S_h closest in the L_2 norm to the tangent construction of section 4.

In [952the approximations to the dual variables are a little different, being polygonal intersections of planes (in two dimensions)

in one of the variables and point values in the other. However, the only difference between the procedure described there and that described here is in the projection used above, which converts the polygonal approximation into a triangulation. Although there is an additional degree of approximation involved, computations carried out on the piecewise linear representation on triangles are much easier.

9 Conclusion

In this report we have sought first of all to bring out the correspondence between the Moving Finite Element method and the method of characteristics for first order PDE's by stressing the similarities as strongly as possible. This has meant relying on a model equation,

$$u_t + \tilde{H}(x,u,u_x) = 0 \qquad (9.1)$$

with $\tilde{H}$ linear in x and/or u, in one dimension and showing that the MFE equations closely resemble the characteristic equations in this instance. The connection is traced to the commonality of a Legendre transformation between the data and the characteristics/nodal trajectories when the approximating spaces are S_h and T_h. For more general equations a finite element type projection may be used to carry H into the $\tilde{H}$ of (9.1).

The benefits of this approach are that the discretised forms of the characteristic equations are separated from the projection details, that the goals of the MFE procedure are clarified, and that the distinct aspects of the procedure may be analysed separately for the purposes of predicting nodal speeds, time-stepping and, it is anticipated, error

analysis. This approach is thought to be more fruitful than a combined approach in which these various aspects are studied together.

For example, an important feature of the MFE method has always been how to cope with the so-called "parallelism" singularity which occurs when the matrix A of (1.18) becomes singular as a result of the matrix M losing rank. This corresponds to collinear nodes or some degree of local 'flatness' of the solution U . It has motivated both the introduction of pragmatic penalty functions and other procedures which recognise the impossibility of solving the MFE equations in this event. However, once we know that the goal of the method is the calculation of $\dot{x}$ given by the first of (2.16), the remedy is straightforward, as follows.

If $[U_x]_j$ is very small the first of (3.4) has a very small denominator, but according to (2.16) the right hand side should be approximating the derivative $\partial H/\partial u_x$. Thus we expect $[\tilde{H}]_j$ to also be very small. The ratio of two very small numbers is hard to compute and usually leads to considerable error. Moreover $[\tilde{H}]_j$ will not necessarily tend to zero as $[U_x]_j$ tends to zero in practice because of the approximate nature of $\tilde{H}$ depending on the approximation of x and u . Therefore, for $(U_x)_k - (U_x)_{k-1}$ less than a certain tolerance, we should, in order to avoid the parallelism "singularity", evaluate $\dot{X}_j$ as $\partial H/\partial u_x$ with the values of X,U taken at the point j . A similar argument applies to the second of (3.4) . Again the recommendation is that, for $[X]_k$ smaller than a certain tolerance, we should evaluate $(\dot{U}_x)_k$ as $-\partial H/\partial u_x$ with x,u,u_x taken as their values at, say, $\frac{1}{2}(x_{j+1} + x_j)$. This resolves the parallelism singularity.

An alternative numerical approach can also be suggested for the calculation of $\dot{X}_j$. By taking a weak form of the first of equations (2.16) directly, namely,

$$< \hat{\alpha}_i, \dot{x} - \frac{\partial H}{\partial u_x} > = 0 \ , \tag{9.2}$$

we may replace the second of equations (1.14) and avoid the singularity of the system (1.16) altogether. Even more directly the strong form of the first of (2.16) may be used.

Similar arguments hold for the second of (3.4) when $\{X\} = 0$ and in two-dimensions when the system of (6.4) becomes singular.

The same problem of "parallelism" arises in the treatment of the second order operator u_{xx} but this time it is not solved so easily. In line with the approach of this report we observe that the parallelism singularity is a feature only of the mapping of elementwise information on to the nodal velocities. It is not present in the local projection of section 3, nor does it appear in the time-stepping. It arises in the calculation of the $\dot{U},\dot{X}$ variables from U_x and H , or, in the transformed variables, <u>after</u> the time-stepping in the inverse transformation to calculate U and X from V and M .

In the former case we may add a penalty P to the minimisations (1.22) or (1.23). For example, if $P = \dot{x}^2$ this leads in the case of (1.23) to the discrete equation (c.f. [32])

$$\begin{bmatrix} h_k + h_{k-1} & -M_k h_k - M_{k-1} h_{k-1} \\ -M_k h_k - M_{k-1} h_{k-1} & M_k^2 h_k + M_{k-1}^2 h_{k-1}^2 + \epsilon\,(h_k + h_{k-1}) \end{bmatrix} \begin{bmatrix} \dot{U}_j \\ \dot{X}_j \end{bmatrix}$$

$$= \begin{bmatrix} h_k W_{k,1} + h_{k-1} W_{k-1,2} \\ -M_k h_k W_{k,1} \quad -M_k h_{k-1} W_{k-1,2} \end{bmatrix} \tag{9.3}$$

This equation is local about a node but in the case of (1.22) the equations are global.

Note that when $\epsilon = 0$ the solution of (9.3) for $\dot{X}_j$ is consistent with (5.3). If $\epsilon \neq 0$ however, we find that

$$\dot{X}_j = - \frac{(W_{k,1}-W_{k-1,2})(M_k-M_{k-1})h_k h_{k-1}}{(M_k - M_{k-1})^2 h_k h_{k-1} + \epsilon(h_k+h_{k-1})^2} \tag{9.4}$$

$$= - \frac{(W_{k,1}-W_{k-1,2})}{M_k-M_{k-1} + \epsilon(h_k+h_{k-1})(\frac{1}{h_k}+\frac{1}{h_{k-1}})/(M_k-M_{k-1})} \tag{9.5}$$

which approximates

$$\dot{x} = - \frac{m''}{m' + \frac{\epsilon}{m'}} . \tag{9.6}$$

(c.f. (5.5)). The factor ϵ has the dimensions of M^2 and, from (9.5), we see that the speed $\dot{X}_j \to 0$ under any of the three conditions (i) $M_k, M_{k-1} \to \infty$, (ii) $M_k - M_{k-1} \to 0$, (iii) one of $h_k, h_{k-1} \to 0$. Asymptotically the directions of the node velocities are unaltered but they are prevented from becoming infinite near the points of zero curvature. The approximate form (9.5) retains the properties of nodal speed direction and nodal springing described in section 5.

Similarly there is a discrete form for $\dot{M}_k$ which is singular when $h_k \to 0$. It may however be similarly regularised to give

$$\dot{M}_k = \frac{W_{k,2} - W_{k,1}}{h_k + \frac{\epsilon'}{h_k}} \simeq \frac{m''}{1 + \frac{\epsilon'}{h_k^2}} \tag{9.7}$$

where ϵ' is a small constant, which can be used to prevent the potential singularity as $h_k \to 0$.

In all the above cases the ultimate accuracy of the method is left to the appropriate Galerkin equation for $\dot{U}_j$. In the case of (1.23) this is obtainable from (9.3) as

$$(h_k + h_{k-1})\dot{U}_j = W_{k,1}\, h_k + W_{k-1,2}\, h_{k-1} + [M_k h_k + M_{k-1}\, h_{k-1}]\dot{X}_j \quad (9.8)$$

which directly approximates (2.11).

Moving on to other aspects of this report, we have observed that the mapping from the data to the nodal speeds in the case of equation (9.1) is an example of a Legendre transformation. Where additional projections are incorporated, as for example in the case of more general functions H and in the case of higher dimensions to map the speeds into S_h , the mapping is an approximate Legendre transformation. In the latter case we extracted the procedure to present a general approximate Legendre transformation between dual functions in spaces S_h and T_h (section 8).

The Legendre transformation may also be used to convert the PDE to be solved into another which may be solved more easily. From a numerical point of view this converts a problem to be solved in a piecewise linear space to one posed in a piecewise constant space (or pointwise). In effect the linearity of the representation is temporarily put aside and finite difference methods take over. This may be particularly useful in designing a time-stepping scheme. Of course the transformation has to be inverted, either ultimately or after each time step, and we can do this using the approximate Legendre

transformation referred to above.

The accuracy of semi-discrete Galerkin methods is well-known. It is the time-stepping which destroys this accuracy on fixed grids but in the present method we expect to preserve this accuracy by the integration along characteristic trajectories. Also on the subject of accuracy it is anticipated that the structure presented here will stimulate the development of error analysis for this method. It has already been shown [21],[33] that, for nodes moved along characteristics, much higher accuracy is achieved than for fixed nodes in convection and convection-diffusion equations.

Finally, it should be made clear that very little of the analysis given in this report goes over to systems of equations. For systems of conservation laws a possibility is to use a characteristic decomposition method to furnish the scalar equations required to make use of the present approach. However it is not clear at present how the main benefits, namely, high resolution and error control, can be made consistent with the practical limitations of working with several grids at once. The compromise of a single moving grid is the most attractive alternative, which again involves a projection ([27],[4],[13], but more work needs to be carried out on understanding the averaging process needed to select the movement before the benefits of such an approach become clear.

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