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A note on the grid movement induced by MFE

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A Note on the Grid Movement Induced by MFE *)

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Moving-grid methods in one space dimension have become popular for solving several kinds of parabolic and hyperbolic partial differential equations involving fine scale structures such as steep moving fronts and emerging steep layers, pulses, shocks, etc.. In two space dimensions, however, application of moving-grid methods is less trivial than in 1D. For some methods, e.g., those based on equidistributing principles, it is not even clear how to extend the underlying grid selection procedure to 2D. The moving-finite-element (MFE) method does not suffer from this drawback; its mathematical extension to 2D is trivial. However, because of the intrinsic coupling between the discretization of the PDE and the grid selection, the application of MFE, as for any other method, is not without difficulties. In this paper we describe the node movement induced by MFE for various PDEs and we indicate some problems concerning the grid structure that can result from this movement.

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1. Introduction

During the last decade, moving-grid methods in one space dimension have become popular for solving several kinds of parabolic and hyperbolic Partial Differential Equations (PDEs) involving fine scale structures such as steep moving fronts, emerging steep layers, pulses, shocks, etc.. Moving-grid methods use nonuniform space grids, and move the grid continuously in the space-time domain while the discretization of the PDE and the grid selection procedure are intrinsically coupled. Examples are provided by the Moving-Finite-Element (MFE) method of Miller[10, 12], and by the Moving-Finite-Difference (MFD) method discussed in Verwer et al.[17] (see also references therein). The latter is, in contrast with MFE, restricted to problems in one space dimension.

In two space dimensions, however, application of moving-grid methods is less trivial than in 1D. For instance, there are many possibilities to treat the one-dimensional boundary and to discretize the spatial domain each having their own difficulties for specific PDEs. Therefore, 2D moving-grid methods have mostly been applied only to special types of PDEs. The MFE method ([6, 8, 11]), considering its general approach, allows in principle a large class of problems to be dealt with. However, because of the intrinsic coupling between the discretization of the PDE and the grid selection, the application of MFE, as for any other method, is not without difficulties. The main difficulty we are referring to is the threat of grid distortion. Grid distortion can occur in many different ways due to the quite complex solution behaviour of 2D-evolution problems. For example, sharp layer regions could develop propagating through the domain, or rotating pulses could emerge and die out again.

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The purpose of this note is to describe the node movement induced by MFE for various PDEs and to indicate some problems concerning the grid structure that can result from this movement.

A standard way of describing moving-grid methods, is the introduction of a transformation of the three dependent variables x, y (space), and t (time) into new variables ξ, η, and τ (usually one chooses $t = \tau$). The effect of the transformation may be to stretch the coordinates in a steep region, so that the transformed derivatives are small compared with the old ones. Of course, many of the difficulties that the spatial discretization yields are now shifted to the problem of how to define the mapping. After having applied the transformation, we obtain the so-called Lagrangian form of the PDE. Within this new formulation the time-derivatives of the spatial variables x and y appear. It is clear, that before using a numerical scheme to discretize the model, one has to define extra equations for these quantities. There are various approaches to take care of this. First, one can use a 2D extension of the equidistribution principle, see, e.g., Brackbill & Saltzman[5], or Dwyer[9]. This idea is either very difficult to work out and to implement, due to the complicated structure of the formulas, or, in a simpler form, it can only be applied to a small class of models. Second, one can use the method of characteristics. This method can, however, only be applied to certain scalar hyperbolic equations. For systems in 2D the use of this method is problematical if possible at all. We would like to focus our attention on the MFE method, which defines the transformation in terms of a residual minimization. For scalar hyperbolic equations MFE is related to the method of characteristics (see, e.g., Baines[2, 3]). This link with the characteristics of the PDE is very useful in one dimension. For in that case all 'disturbances', i.e., shocks, pulses, etc., can merely follow the characteristics. So, once the user has located the grid points at the right positions, the characteristics do the rest. This has the advantage that MFE needs very few points to follow such solutions. In two dimensions it may work properly as well, for the same reasons (see, e.g., Miller[11], or Carlson & Miller[6]). However, in some situations one has to be very careful in applying this method. We will illustrate this with some examples. For parabolic equations the node movement induced by MFE is less understood. For 1D scalar equations one can derive asymptotic relations for the node movement and for the node distribution, indicating that for parabolic equations MFE strives after an equidistribution of second and first order derivatives. An example gives some indication that these results possibly also hold in 2D.

The paper is divided into four sections. In Section 2 we briefly describe MFE in two space dimensions, its relation to the method of characteristics for hyperbolic equations and results on the grid movement that can be derived for the parabolic case. Section 3 contains two examples of hyperbolic PDEs with a typical solution behaviour. For these two examples it is shown that MFE yields a severely distorted grid, although the computed solution remains accurate. However, this distortion can lead to a breakdown of the numerical time-stepping procedure. Section 3 also contains an example of a parabolic equation for which MFE strives after a transformation equidistributing second order derivatives. Finally, Section 4 is devoted to some conclusions.

2. The movement of the nodes in MFE

Let us consider the scalar PDE

$$\frac{\partial u}{\partial t} = L(u), \quad (x,y) \in \Omega, \quad t > 0, \tag{2.1}$$

with initial and boundary conditions

$$u\,|_{t=0} = u^0(x,y), \quad (x,y) \in \Omega,$$
$$B(u, \nabla u)\,|_{\partial\Omega} = g(t), \quad t > 0,$$

where u^0 and g are given functions, and L represents a differential operator involving only spatial derivatives up to second order. In general, the solution $u(x,y,t)$ of (2.1) may have a very complex behaviour. Even for a restricted situation (a scalar linear PDE with simple boundary conditions), one can have severely varying u-values in space (x,y) and time t. Some examples in this context are steep moving fronts and emerging and rotating pulses.

A common approach to handle these phenomena is to introduce a transformation which maps the variables x, y, and t into new variables ξ, η, and τ. Such a transformation can be defined as, e.g.,

$$
\begin{aligned}
x &= x(\xi, \eta, \tau) \\
y &= y(\xi, \eta, \tau) \\
t &= \tau \\
u(x,y,t) &= v(\xi, \eta, \tau).
\end{aligned}
\tag{2.2}
$$

Applied to the left-hand side of equation (2.1) this gives

$$
\frac{\partial u}{\partial t} = \frac{\partial v}{\partial \tau} - u_x \frac{\partial x}{\partial \tau} - u_y \frac{\partial y}{\partial \tau},
\tag{2.3}
$$

and additionally equations for x and y must be defined. The effect of the transformation may be to stretch the coordinates in a steep region in space so that, for example, u_ξ and u_η are small in contrast with u_x and u_y. This type of transformation is strived after by methods which equidistribute first or higher order derivatives of the solution. Another effect of the transformation may be to decrease the $\partial v / \partial \tau$ as is done by the method of characteristics and by the finite difference method of Petzold ([14], in 1D). Of course, when using a transformation, most difficulties are shifted to the problem of how to define and carry out the mapping. The Moving-Finite-Element (MFE) method can, in some cases, also be shown to underly a transformation of variables (Baines[3]). Below we will discuss this method and in particular the node movement induced.

2.1. Description of MFE

MFE restricts v, x, and y to U, X, and Y from a finite-dimensional subspace. The MFE-approximations are piecewise linear on a hexagonally connected triangularization of Ω

$$
\begin{aligned}
v \approx U &= \sum_{j \in J} U_j(\tau)\, \alpha_j(\xi, \eta), \\
x \approx X &= \sum_{j \in J} X_j(\tau)\, \alpha_j(\xi, \eta), \\
y \approx Y &= \sum_{j \in J} Y_j(\tau)\, \alpha_j(\xi, \eta),
\end{aligned}
\tag{2.4}
$$

where J is the set of indices of the grid points and α_j are the standard piecewise linear hat functions. Substituted in the PDE (2.1), (2.3), this approximation gives in general a non-zero residual R, defined by

$$
R\left(\frac{\partial U}{\partial \tau}, \frac{\partial X}{\partial \tau}, \frac{\partial Y}{\partial \tau}\right) = \frac{\partial U}{\partial \tau} - U_x \frac{\partial X}{\partial \tau} - U_y \frac{\partial Y}{\partial \tau} - L(U)\,.
\tag{2.5}
$$

A least-squares minimization is performed on R with respect to the unknowns $\partial U_i / \partial \tau$, $\partial X_i / \partial \tau$, and $\partial Y_i / \partial \tau$, yielding a system of implicit ODEs

$$
\begin{aligned}
&< R, \quad \alpha_i > = 0 \\
&< R, \ - U_x \alpha_i > = 0 \\
&< R, \ - U_y \alpha_i > = 0\ , \quad \forall i \in J,
\end{aligned}
\tag{2.6}
$$

where $<,>$ is the usual L^2-innerproduct on Ω (for an elaboration of (2.6), see [3]). This ODE-system must be integrated numerically to obtain the required fully discretized solution. It is known, that this system may become very stiff. For integration in time, therefore, a suitable stiff ODE-solver must be used.

In practical applications, regularization terms (penalty functions) will be added before the minimization procedure is carried out. These penalties prevent that the parametrization of $\dot{U}$, $\dot{X}$, and $\dot{Y}$ becomes degenerate (see [8]). Further, they produce forces on the grid movement to prevent the triangles from getting too thin or from loosing their orientation. In our experiments we use the penalty functions, but in this section we will not discuss their influence on the grid movement, since the penalties are not the 'driving forces' behind the movement.

Although the Gradient Weighted version of MFE (see, e.g., [6, 19]) is more robust than MFE for steep solutions, the phenomena observed below will be essentially the same for GWMFE.

2.2. Relation of MFE with the method of characteristics

Only a few theoretical properties of the resulting ODE system (2.6) are known. One important property is the relation of MFE, in both 1D and 2D, with the method of characteristics for the scalar hyperbolic PDE with

$$L(u) = -\beta_1(u,x,y,t)\frac{\partial u}{\partial x} - \beta_2(u,x,y,t)\frac{\partial u}{\partial y}. \tag{2.7}$$

It is easy to derive that for linear β_1 and β_2, while setting aside boundary effects, the ODE system (2.6) is equivalent to

$$\begin{aligned} \dot{X}_i &= \beta_1(U_i, X_i, Y_i, t), \\ \dot{Y}_i &= \beta_2(U_i, X_i, Y_i, t), \\ \dot{U}_i &= 0, \qquad i \in J. \end{aligned} \tag{2.8}$$

This simple formulation holds for nonlinear β_1 and β_2 in 1D as well (see, e.g., Baines[2, 3]). So, the ODE system is identical to the discretized system of characteristic ODEs for the PDE (2.1). In the case that

$$L(u) = -\beta_1\frac{\partial u}{\partial x} - \beta_2\frac{\partial u}{\partial y} + \epsilon\Delta u, \tag{2.9}$$

one can expect, that for small ϵ, MFE results in a grid movement more or less the same as (2.8). (In one dimension one can even quantify the perturbation of the characteristics produced by the diffusion term (see below).)

In 1D this relation with the characteristics is very useful. For, in that case, shocks and pulses have only one degree of freedom to move: they propagate along the characteristic curves of the PDE. In many cases in two space dimensions, this characteristic behaviour is also very beneficial (cf. [7, 11]). However, there are some situations in 2D for which this behaviour will give problems. The main purpose of this note is to illustrate this. We will discuss some of these problems in Section 3.

2.3. Node movement for parabolic equations

Theoretically, little or none is known about the grid movement in 2D induced by MFE when applied to parabolic PDEs. In one space dimension, however, it is possible to get some insight by examining the asymptotic node movement and the asymptotic node distribution for the scalar PDE

$$\frac{\partial u}{\partial t} = \mu\frac{\partial^2 u}{\partial x^2} + F(x,u,t), \tag{2.10}$$

where F can also contain spatial derivatives of u. Defining $\mathcal{F}$ by

$$\frac{d\mathcal{F}}{dx} = F \tag{2.11}$$

and making some assumptions with respect to the smoothness of u, F and x and the rate of convergence of U, one can derive, in an analogous way as is done by Thrasher and Sepehrnoori[15], that the asymptotic node movement satisfies the relation

$$\dot{x} = -\frac{\partial\mathcal{F}}{\partial u} + \mu\,(2\frac{u_{xxx}}{u_{xx}} - 3\frac{\xi_{xx}}{\xi_x}), \tag{2.12}$$

where ξ is defined by a transformation analogous to (2.2), but now restricted to one space dimension.

This relation is valid only in intervals without points with a zero asymptotic node density or with zero curvature. Grid points cannot pass a point with zero curvature (cf. Baines[3]), with the consequence that grid points are confined to regions between two zero-curvature points (the so-called anti-cluster property of singular points).

If $\mu \neq 0$, then equation (2.12) can be integrated to obtain the asymptotic node distribution

$$\xi_x = K(t)\,|u_{xx}|^{2/3}\exp\left(\frac{1}{3\mu}\int(-\mathcal{F}_u - \dot{x})dx\right). \tag{2.13}$$

For $\mu = 0$ and $F = F(u,t)$ equation (2.12) means that a grid point will propagate along the characteristic $\dot{x} = -\mathcal{F}_u$ and is *not* dependent on the grid distribution. This is the situation as described in Section 2.2. For $\mu \neq 0$ one can easily derive asymptotic node distributions for restricted choices of F. For instance, the node distribution of the so-called shifting pulse, which we used as an example in [19], once every point travels with the velocity of the pulse, is given by

$$\xi_x = K(t)\,|u_{xx}|^{2/3} \tag{2.14}$$

which can be derived from (2.13) provided that $\dot{x} = \dot{x}(t)$ and $F = F(x,t)$. So once every point travels with the velocity of the pulse, the nodes should be distributed by MFE according to (2.14) and the plots in [19] show indeed that MFE approximately equidistributes some power of the second derivative of the solution.

For convection-diffusion equations like (2.9), one can derive from (2.13), assuming that $\dot{x} = 0$, $u_t = 0$ and $F = F(u,t)$, a steady-state distribution

$$\xi_x = K(t)\,|u_{xx}|^{2/3}\,|u_x|^{1/3}, \tag{2.15}$$

indicating that in this case a combination of first and second order derivatives is equidistributed.

3. Numerical examples

3.1. *Example I ('Anisotropy')*

Our first example is an anisotropic wave front (see Whitham[18, p.254]). In short, anisotropy means that a difference exists between the directions of the characteristic curves of the PDE (the movement of the 'fluid'-particles) and the movement of the wavefront. This phenomenon can not occur in one space dimension. In 2D, anisotropy may give rise to a distorted MFE grid eventually leading to a breakdown of the numerical time-stepping procedure.

Probably the best way to illustrate this effect is by giving a PDE-example. Consider, for this purpose,

$$\frac{\partial u}{\partial t} = -\beta_1\frac{\partial u}{\partial x} - \beta_2\frac{\partial u}{\partial y} + \epsilon\Delta u, \tag{3.1}$$

on the domain $\Omega = (0,1)\times(0,1)$, with

$$\beta_1 = u,$$

$$\beta_2 = \left(\frac{3}{2} - u\right),$$

$$u|_{t=0} = u_{\text{exact}}|_{t=0},$$

$$u|_{\partial\Omega} = u_{\text{exact}}|_{\partial\Omega},$$

and

$$u_{\text{exact}} = \frac{3}{4} - \frac{1}{4}\frac{1}{1+\exp\left(\dfrac{-4x+4y-t}{32\epsilon}\right)}.$$

The exact solution of this model problem (a scalar version of the system in [4, p.89]) describes a wavefront with a steep transition area of thickness $O(\epsilon)$, that moves, under an angle of 135^o with the positive x-axis, from the middle of Ω to the upper left corner. For $\epsilon \downarrow 0$ the transition area becomes steeper, and for $\epsilon = 0$ a pure hyperbolic situation is created with a discontinuous moving shock.

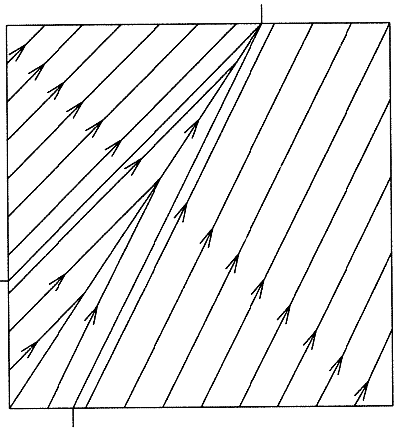

FIGURE 3.1. Node movement by characteristics from $t = 0$ to $t = 1$.

Formulation (2.8) reveals that the method of characteristics, and, to a great extent MFE as well, at first will send the grid points to the upper right corner of the domain. This can be seen very easily by writing out the equations (2.8) for this case ($\epsilon = 0$):

$$\text{for } y > x + t \qquad (3.2.a)$$
$$\dot{X}_i = U_i(t) \approx \frac{3}{4},$$
$$\dot{Y}_i = \frac{3}{2} - U_i(t) \approx \frac{3}{4},$$

and

$$\text{for } y < x + t \qquad (3.2.b)$$
$$\dot{X}_i = U_i(t) \approx \frac{1}{2},$$
$$\dot{Y}_i = \frac{3}{2} - U_i(t) \approx 1.$$

The characteristic movement from $t = 0$ until $t = 1$ is pictured in Figure 3.1. This grid movement will lead to a coarse grid in the lower left corner of Ω, since all grid points are moved to the upper right corner. Further, at later points in time, a congestion of grid points near the upper side of the domain Ω will arise, due to the boundary effects. Since, in that area, the relative distance between the nodes will become very small, the penalty functions should keep the points from moving into each other and thus the ease with which the ODE system (2.6) can be solved (if at all), will become very dependent upon the correct choice of the penalty functions. It could easily result in a drastic drop of performance only caused by inadmissible triangle orientations during the Newton process. It must be noted, however, that for $\epsilon \downarrow 0$ MFE will resemble the method of characteristics more and more, resulting in an almost exact solution in each grid point. In Figure 3.2 a boundary layer of points is shown,

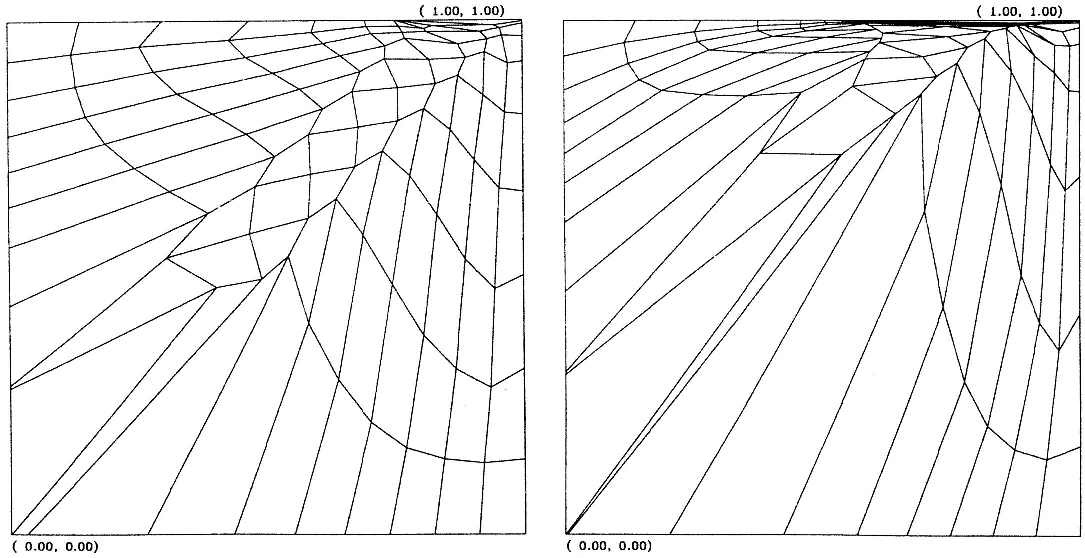

FIGURE 3.2. MFE grid for Example I at $t = 0.5$ and 1.0.
Dividing each quadrilateral by the diagonal from upper left to lower right gives the MFE triangles.

obtained by applying MFE to problem (3.1) with $\epsilon = 5.10^{-3}$ and a uniform starting grid of 11×11 moving grid points. At $t \approx 1.02$ the computational process breaks down because of the unacceptable triangle orientations. This could be prevented by taking larger penalty values resulting in a less accurate solution.

It is obvious that for these situations a procedure to delete and create nodes could be added to MFE to prevent a congestion of grid points and to keep the finite element approximation of the solution accurate enough. Also for this special case, a solution to eliminate the anisotropy in the PDE could be found. One could think of applying a transformation to the PDE that describes a rotation of the variables over an angle $\phi = 135^o$. In the new variables the characteristic curves and the direction of the normal to the wave front would coincide (the anisotropy would then cease to exist). In general situations, however, it is, a priori, unclear how to choose ϕ, especially ϕ could even be time-dependent. So far, it has not been possible to reformulate MFE in a proper way to generate such a transformation automatically.

3.2. Example II ('Grid rotation')

Our second example, copied from [13], is concerned with the fact that in 2D an unwanted rotation of the grid can occur. To illustrate this, consider

$$\frac{\partial u}{\partial t} = -\beta_1 \frac{\partial u}{\partial x} - \beta_2 \frac{\partial u}{\partial y}, \tag{3.3}$$

on the domain $\Omega = (-0.5, 1.5) \times (-0.5, 1.5)$, with

$$\beta_1 = +\pi(y - \tfrac{1}{2}),$$

$$\beta_2 = -\pi(x - \tfrac{1}{2}),$$

$$u|_{t=0} = \exp(-80[(x - \tfrac{1}{2})^2 + (y - \tfrac{3}{4})^2]),$$

and

$$u|_{\partial\Omega} = 0.$$

Although the boundary condition is mathematically not consistent with the initial condition, it is expected that this will give no problems in numerical computations, since the difference is less than the machine precision.

The exact solution describes a pulse that moves around in circles with a constant speed. During this movement the shape of the pulse does not change. The characteristic curves are circles with centre $(\frac{1}{2}, \frac{1}{2})$, which can be derived immediately from (2.8) and (3.3):

$$\dot{U}_i = 0 \quad \text{and}$$
$$(X_i - \tfrac{1}{2})^2 + (Y_i - \tfrac{1}{2})^2 = r_i^2, \quad 0 < r_i < 1,$$

with $\dot{r}_i = 0, \ \forall i$.

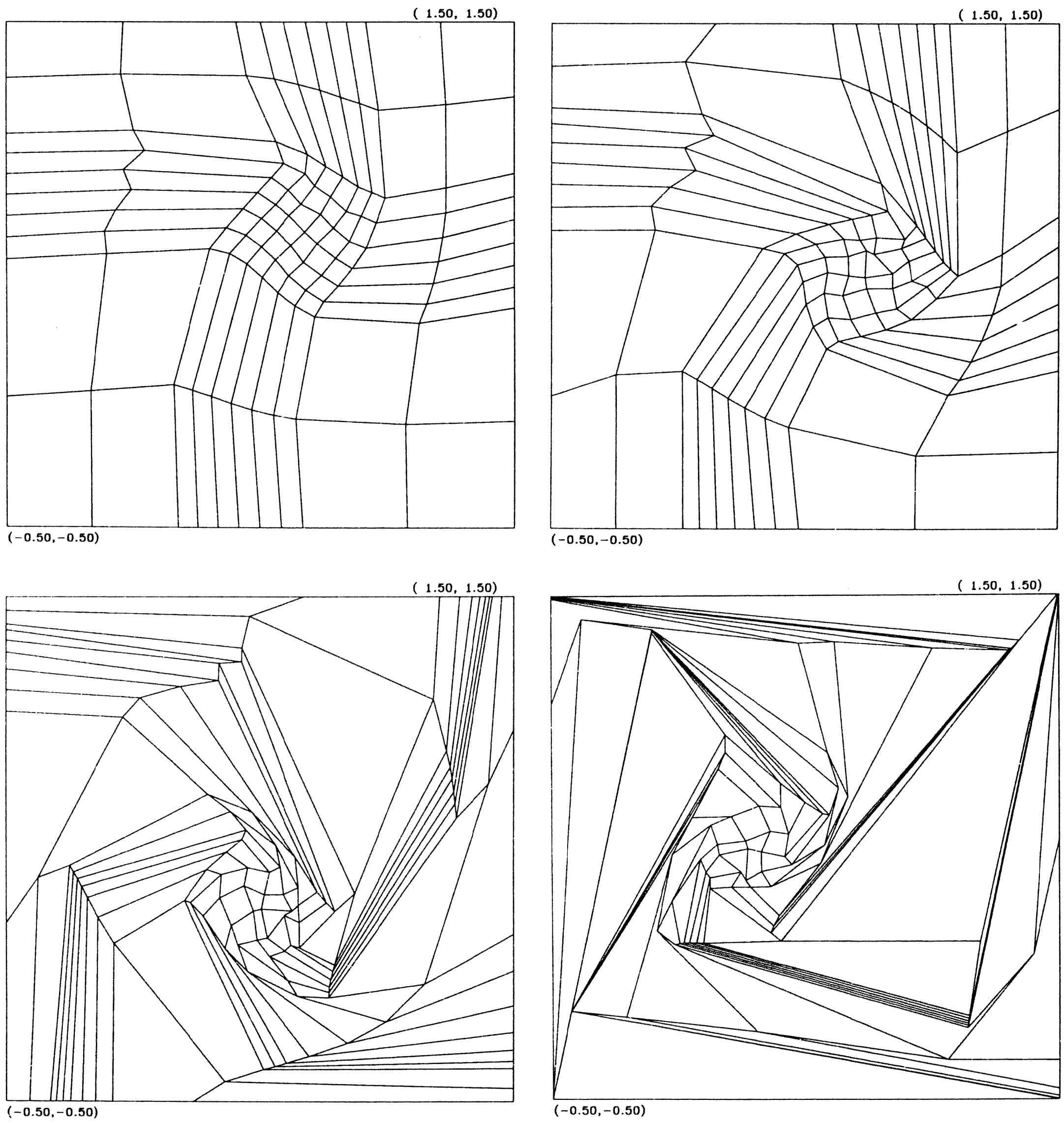

FIGURE 3.3. MFE grid for Example II at $t = 0.25$, 0.5, 1.0 and 1.5.
Dividing each quadrilateral by the diagonal from upper left to lower right gives the MFE triangles.

In contrast with the previous example, the movement of the grid points might be called ideal. They follow the steep parts of the solution in an optimal way and MFE benefits by this property, resulting in a good approximation. However, since we fixed the corner points of the square, the grid will exhibit an unwanted spiral structure. This occurs when the pulse has moved down to the lower region of Ω. A consequence of this effect is the so-called line tangling, a 2D version of node crossing in 1D. The numerical procedure will breakdown whenever this occurs, again because of inadmissible triangle orientations during the Newton process. In this case, however, larger penalty values can only delay but not prevent the breakdown. We show this spiral effect in Figure 3.3, where we pictured the grids, produced by MFE, at various time values. The starting grid consists again of 11×11 points of which 5×5 are distributed uniformly around the cone in $(0.25,0.75) \times (0.5,1.0)$. At $t \approx 1.52$ the computation breaks down. Again the MFE approximation in each grid point is rather accurate and the performance of MFE in the time stepping process is satisfying until the spiral structure leads to line tangling.

Note that in this case annihilation and creation of points, based on the accuracy of the MFE approximation, would be no cure for the grid distribution problem. Of course, there are some other means to check this effect, again for this special case. First, one could allow the grid points on the boundary to move with the internal points (i.e., 'move around the corner'). For instance, one could replace Ω by a circular domain. The grid then would produce no longer spirals, but circles, and the problem would be solved without any trouble. Another trick to avoid that the numerical procedure breaks down, is described by Mueller & Carey[13]. They add an extra penalty term to the method, which brings on an anti-rotation to the grid movement. This regularization term, however, has only a limited working: with any choice of the constant, appearing in the penalty, there remains some point of time for which the line tangling takes place. Only, with larger penalty values the method would collapse at a later moment in the time-integration. But, larger penalty values also result in a worse resolution of the pulse, yielding larger errors during the computation.

3.3. Example III ('Parabolic pulse')

In the two previous examples we encountered difficulties in applying MFE due to its strong relation with the method of characteristics for hyperbolic equations. Next, we give an example of a PDE with an exact solution very similar to that of model (3.3), but now the PDE has a parabolic character. It has already been treated by several authors ([1, 16]), and is defined by

$$\frac{\partial u}{\partial t} = \Delta u + f(x,y,t), \tag{3.4}$$

on the domain $\Omega = (-0.5,1.5) \times (-0.5,1.5)$, with

$$u\,|_{t=0} = u_{\text{exact}}\,|_{t=0},$$

$$u\,|_{\partial\Omega} = u_{\text{exact}}\,|_{\partial\Omega},$$

The source $f(x,y,t)$ is chosen so that the exact solution is

$$u_{\text{exact}} = \exp(-80[(x-r(t))^2 + (y-s(t))^2]),$$

where

$$r(t) = (2+sin(\pi t))/4, \quad s(t) = (2+cos(\pi t))/4.$$

This solution is a rotating pulse and thus very similar to the solution of Example II. However, in contrast with the hyperbolic Example II, the grid points do not move according to a principle like (2.8). In particular, MFE, applied to (3.4), shows no spiral effect. The points are not stuck to their position on the pulse and the grid structure remains more or less the same during the time-stepping. This is illustrated in Figure 3.4, where we pictured the grid at several points in time. Although the error of the approximation is higher than in Example II (this can be repaired by increasing the number of points), the procedure does not break down because of grid tangling. On the contrary, once the grid

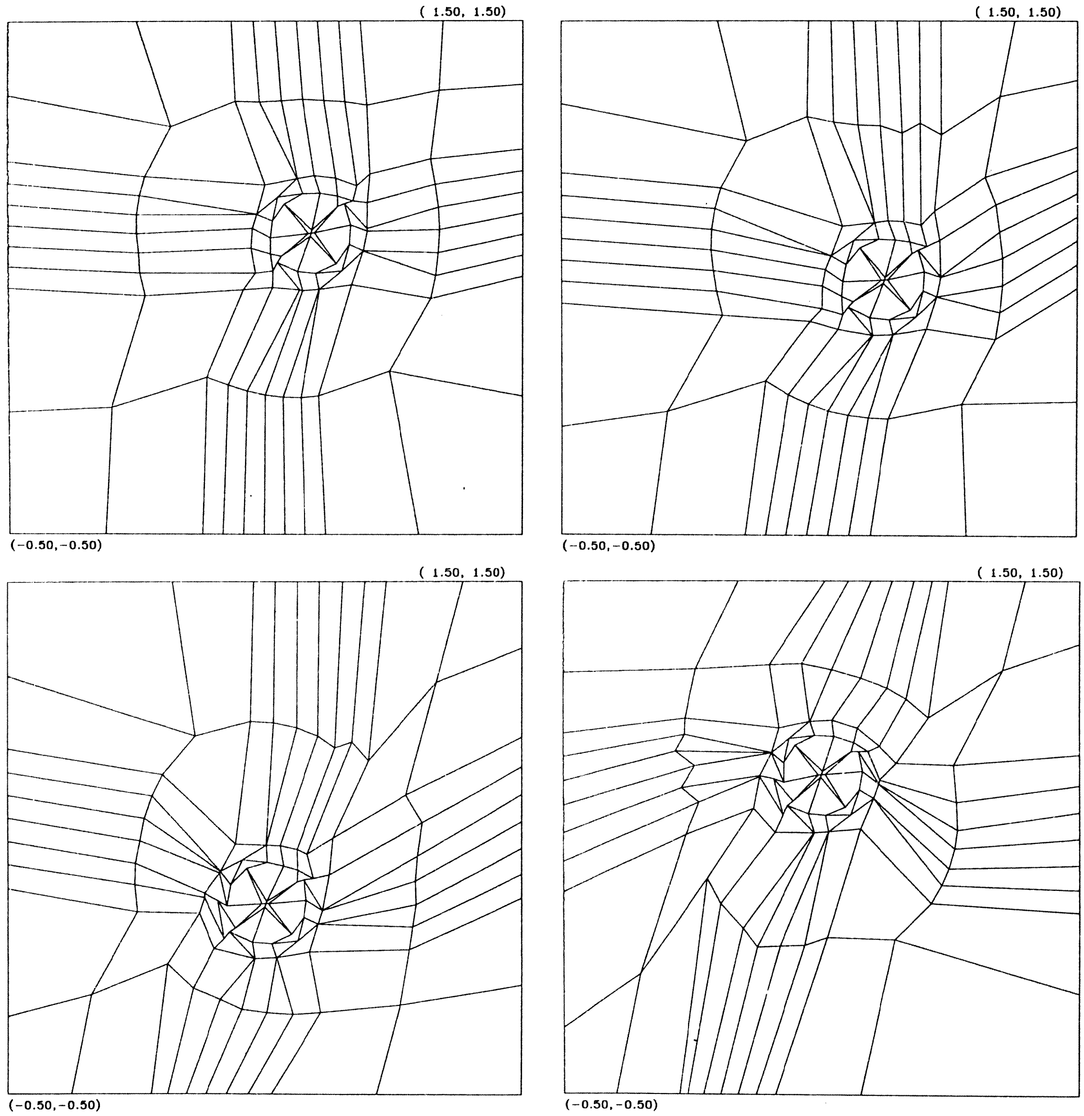

FIGURE 3.4. MFE grid for Example III at $t = 0.25$, 0.5, 1.0 and 2.0.
Dividing each quadrilateral by the diagonal from upper left to lower right gives the MFE triangles.

has been forced around the cone, the time stepping process is satisfying, although the penalty choice is also in this case of influence.

Finally, noteworthy is that the concentration of triangles in regions with large second order derivatives indicates a similar equidistribution behaviour as stated in Section 2.3 for one dimension.

4. Conclusions

For hyperbolic or strongly convection dominated convection-diffusion equations, the grid points are moved by MFE in a way similar to the method of characteristics. This results in a very good approximation of the solution but sometimes also in distorted grids, because the grid movement is independent of the grid distribution. Such grids then eventually cause the numerical time-stepping to fail. A procedure to delete and create points could in some cases be a remedy, but will on the other hand complicate the method considerably.

For scalar parabolic equations one can show that in 1D the MFE movement of a grid point does depend on the grid distribution. MFE approximates a transformation striving after equidistribution of derivatives of the solution. An example showed that possibly this remains valid also in 2D.

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