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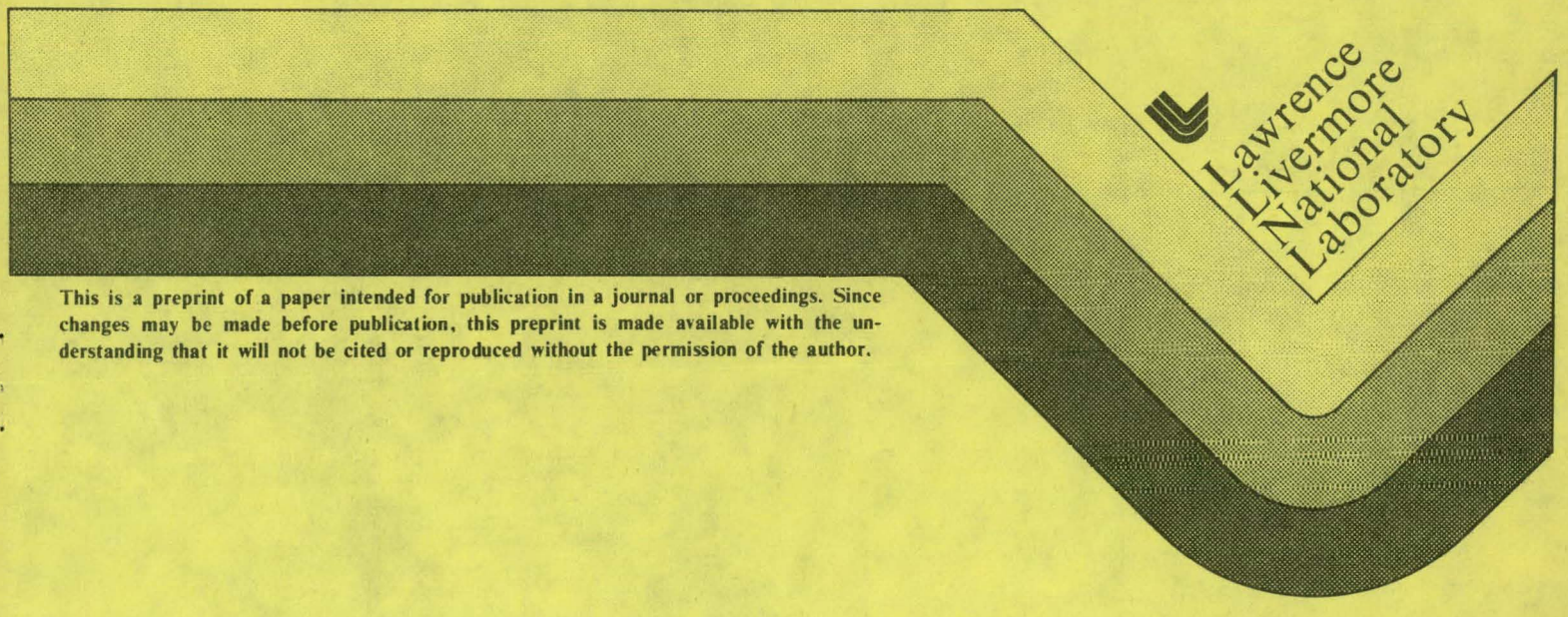

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Adaptive-grid methods for time-dependent partial differential equations

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Abstract

This paper contains a survey of recent developments of adaptive-grid algorithms for time-dependent partial differential equations. Two lines of research are discussed. One involves the automatic selection of moving grids to follow propagating waves. The other is based on stationary grids but uses local mesh refinement in both space and time. Advantages and disadvantages of both approaches are discussed. The development of adaptive-grid schemes shows promise of greatly increasing our ability to solve problems in several spacial dimensions.

1. Introduction

It has been common practice for many years to use adaptive grids and methods of varying orders of accuracy in the integration of ordinary differential equations [11]. Until recently, this has not been the case for time-dependent partial differential equations, but it seems likely that multidimensional computations will be very costly or even impossible without the development of adaptive-grid methods. In this paper we survey briefly two lines of current research, and we suggest some promising future developments.

Hyperbolic partial differential equations are known to exhibit propagating waves [22], of both characteristic and subcharacteristic nature. Consequently, numerical computation on a fixed grid tends to be costly - a fine grid is required everywhere. Admittedly, it is not always necessary to resolve the behavior in the wave front, and special methods have been developed for such cases. We omit these special problems from our discussion, and hence, we exclude shock tracking as done, for example, by deNeef [8], Zhu [28], and Salas [17]. We also exclude special algorithms for computing shocks and contact discontinuities on fixed grids, such as the methods of Glimm [7], Boris and Book [4,5], and Woodward and Colella [25]. We concentrate on problems for which the solution must be computed accurately in the frontal region, such as chemical combustion [9] and the accretion of matter to form a star [21, 24].

One approach to adaptive grids is to use a fixed number of grid points and to let them move with whatever fronts are present. We discuss work in this direction

in Section 2, including the work of Dwyer and his coworkers [9] on combustion and the work of Winkler [21, 24] on star and galaxy formation. We also describe the general moving-grid algorithm of Miller and his coworkers [12, 14, 15]. The other approach is the use of local mesh refinement, and in Section 3 we describe the work of Bolstad [3] and Berger and Gropp [1, 2, 13]. In Section 4 we point out the respective advantages of the moving-grid and local-mesh-refinement approaches, and we point out some directions for future development.

2. Moving-grid schemes

The most direct way to set up a moving grid is to do it via a coordinate transformation. Thus, with the notation $\partial_x = \partial/\partial_x$, a hyperbolic system

$$\partial_t u + \partial_x f(u) = F(u) \tag{2.1}$$

may be transformed into

$$\partial_t u + \partial_\xi u \, \partial_t g + \partial_\xi f(u) \, \partial_x g = F(u) \tag{2.2}$$

by means of the transformation $\xi = g(x,t)$. Extensions to higher-order equations and to several dimensions are obvious. The numerical method for solving (2.1) then consists of a construction somehow of the mapping function g and a finite-difference or finite-element approximation to (2.2) on a fixed, uniform grid. In typical applications of this method the (ξ,t)-coordinate system follows a traveling wave, so that $\partial_t u$ in (2.2) is small. Consequently, it is desirable to use an implicit method for (2.2) with long time steps and to couple the construction of g directly with the solution of (2.2), and all of the methods described in this section do so.

Implementations of the moving-grid algorithm differ in their choice of a difference scheme for (2.2), but more importantly, they differ in the algorithm used to define g. One possible choice is to use Lagrangian coordinates, and this is useful if we want to follow the motion of the material. The criteria for g are problem dependent, and so far, no robust algorithm for its construction exists. It is possible to make good choices of g in special problems, however, and in this section we present two such special problems. We begin with Dwyer's method for combustion [9], and then we discuss Winkler's method for computing the formation of stars [21, 24]. We close this section with a description of Miller's method [12, 14, 15], which is more general than the others.

Let us mention here that several authors, including Rai and Anderson [16] and Yanenko and his coworkers [26, 27] have used similar ideas in fluid-dynamical

computations. We do not expand on this application because there is some validity to the claim that in such problems there is no need to put many grid points in the wave fronts, and that special difference schemes on fixed grids are adequate.

In one dimension the equations of a combusting gas mixture are a modification of (2.1) in that second-derivative terms representing viscosity and heat diffusion must be added [23, pp. 2-4]. From a qualitative point of view it is clear that it is a good idea to select a grid which is stationary with respect to the flame front. Thus, we need to know the flame speed accurately. Now, the flame speed depends strongly on the behavior of the solution in the flame region. Consequently, we need a fine grid in the flame region. Combustion problems have the special property that the rate of chemical rection depends very strongly on the temperature [23, p.4]. In fact, a flame front may be identified numerically as a region of large temperature gradient. In the work of Dwyer [9] the basic idea is to select the mapping $\xi = g(x,t)$ so as to make $|\partial_\xi T|$ nearly constant, where T denotes the temperature. Some variation in $|\partial_\xi T|$ must be permitted, for otherwise, there would be no grid points in regions of constant temperature, such as might be present in large unburned regions. It is also noted in [9] that in flame-initation regions, it may happen that u is changing rapidly, even though $|\partial_x T|$ is small. Therefore, [9] recommends monitoring of a linear combination of $|\partial_\xi T|$ and $|\partial_\xi^2 T|$ in such flames.

Some two-dimensional computations with this method are also reported in [9], but only in some special, essentially one-dimensional geometries. A set of fixed grid lines is drawn so that they will be approximately orthogonal to the flame front throughout its course, and the one-dimensional moving-grid algorithm is used on each of these grid lines. Examples of geometries where this approach is inadequate are also given in [9].

Another application of the moving-grid method (2.2) is the computation of the formation of a star or galaxy [21, 24]. We begin with a description of the physical processes leading to the formation of a star, which is assumed to be spherically symmetric. We have an extended, diffuse cloud of matter which is being pulled by the force of gravity onto a protostar at the center. As the protostar grows, it becomes hotter and denser, until thermonuclear fusion begins. Since we are interested only in the growth of the protostar, we want to use a grid which moves with the surface of the protostar and not with the falling particles [24]. The speed of the moving surface depends on the rate of accumulation of falling matter, on the gravitational forces acting the protostar, and on the outward pressure of the light radiated by the protostar.

Because several processes are important, it is not sufficient to select the mapping g by monitoring changes in a single variable. In fact, Winkler [24] chooses g so as to make

$$\sum \log^2 (|\partial_\zeta u_i|/|u_i|)$$

nearly constant as a function of ξ. The need for the relative rates $|\partial_\xi u_i|/|u_i|$ is dictated by the extremely large changes in such things as particle velocity, density, and temperature across the surface of the protostar. The choice of $\log^2$ came about through numerical experience [24]. It is clear that Winkler's mapping algorithm is a generalization of Dwyers [9].

In [21] Tscharnuter and Winkler report on a three-dimensional computation using a modification of this method to study the evolution of a galaxy. A spherical coordinate system is used with a fixed, uniform grid for the angles. Along the radial lines moving one-dimensional grids are chosen as in the protostar computation. Thus, the method is basically one-dimensional, and spiral galaxies are not treated.

Let us comment on the choice of criterion for the construction of the mapping function in [9] and [21, 24]. From the point of view of a numerical analyst, the grid should be fine at points where the local truncation error is large, not at points where $|\partial_x u|$ or $\sum|\partial_x u_i|/|u_i|$ is large. Because of the high degree of nonlinearity in the problems treated in [9, 21, 24], $|\partial_x u|$ is probably a pretty good estimator of the local truncation error. It is easy, though, to find examples of problems in which $|\partial_x u|$ is a poor estimate of the local truncation error. One such example is any second-order accurate scheme for a linear, hyperbolic equation. Similarly, a glance at the figures from Sod's gas-dynamical computations [18] shows that in the middle of a rarefaction wave $|\partial_x u|$ may be large, but the error is small. This point should be kept in mind when the methods of [9, 21, 24] are applied in other settings.

We turn now to the moving grid method of Keith Miller and his coworkers [12, 14, 15], which does use the local truncation error as a consideration in the construction of the grid. In this method an approximate solution to (2.1) is written as a piecewise linear spline in x over a grid which varies in time. The spline u and the grid are chosen so as to minimize

$$\|\partial_t u + \partial_u f(u) - F(u)\|^2 + \text{penalty} \quad . \tag{2.3}$$

The Euler equation for minimizing (2.3) is a discretization of (2.2), coupled to a discretization of a partial differential equation

$$L(u, \partial_t, \partial_\xi)G = 0 \tag{2.4}$$

for the function G such that $x = G(\xi,t)$ is the inverse mapping to $\xi = g(x,t)$.

As is explained in [14], a penalty function is needed in (2.3) for two reasons. One reason is that the method is ill posed without a penalty. In fact, without the penalty, the line $t = t_o$ is tangent to a characteristic curve for (2.2), (2.4) at every point (x_o, t_o) at which $\partial_x^2 u = 0$. The paper [14] gives examples of nonuniqueness of solutions. The other reason for the penalty

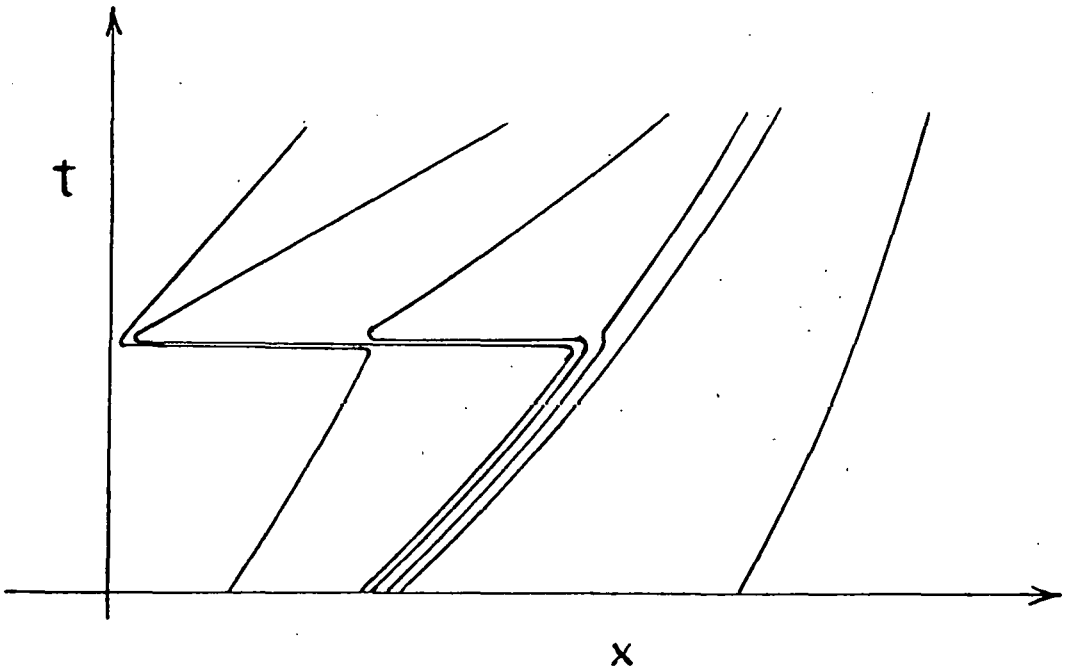

Figure 1. Moving grids

function in (2.3) is that without it, for a scalar equation (2.1) with F = 0 the (ξ,t)-coordinates follow the characteristic curves of (2.1). Such behavior has some advantages, of course, but it also means that grid points accumulate at a shock. Thus, the penalty function also serves to keep the grid points sufficiently well separated. Examples of penalty functions for specific problems are given in [12, 14, 15].

One advantage of Miller's method over that of Dwyer and Winkler is that Miller's method may be extended directly to higher dimensions. Much work remains to be done on the choice of penalty functions in higher dimensions, however. Another advantage of Miller's method is that the transformation of the equation from (2.1) to (2.2) is not done explicitly, but comes about automatically. This can be very useful for higher-order equations in several dimensions.

The primary disadvantage of the methods discussed in this section is that the number of grid points is fixed throughout the entire course of the computation. Thus, if the grid is following one wave front and another one arises somewhere, no new grid is created for the new wave, but rather the old grid has to adjust itself abruptly. A situation of this sort would occur in a combustion problem if a rarefaction wave were to enter from a boundary after the flame had started. A representative grid for this problem is shown in Figure 1.

In fact, this rigidity in the number of grid points is not inherent in the method but is primarily a question of computer science, namely, facility in the manipulation of data structures. The difficulty arises from the fact that, so far,

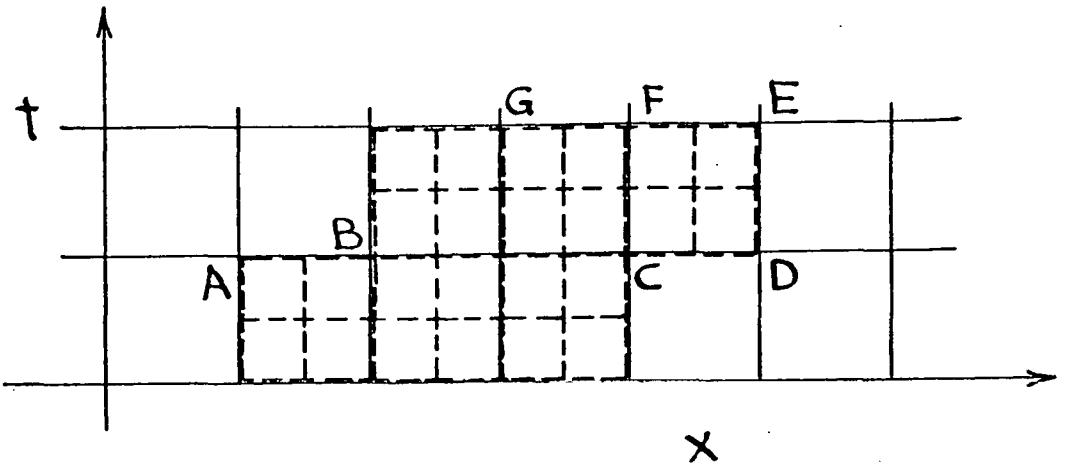

Figure 2. Local mesh refinement

the computer programs for the method are all written in FORTRAN, a language in which the manipulation of data structures is extremely awkward. It would be far easier to add and delete grids if the program were written in a language such as PASCAL, SIMULA, or possibly VAL.

3. Local mesh refinement

In this section we describe the local-mesh-refinement algorithm of Oliger and his students, Berger, Bolstad, and Gropp. This method does use a flexible data structure. Descriptions of the method in the open literature may be found in the works of Gropp [13] and of Berger, Gropp, and Oliger [2]. The theses of Berger [1] and Bolstad [3] will contain further discussion of the method, but they are not yet finished. We should point out that the publication dates for these papers do not correspond exactly with the chronological order in which the work was done. In fact, Bolstad's work [3] predates the others. It is for one-dimensional problems, and its data structures cannot be used in two dimensions. Gropp's paper [13] is a test of whether the method is reasonable at all in two dimensions. In the later papers [1, 2] the test for refinement is improved and the fine grids are permitted to have arbitrary orientation.

Let us briefly describe one time step of a one-dimensional version of the algorithm. Suppose that an approximate solution u is given at time $t = t_0$. We first compute the solution at time $t = t_0 + \Delta t$ by using a difference scheme on a coarse grid over the whole domain. This grid is denoted by solid lines in Figure 2. We then locate regions of low accuracy, using estimates of local truncation error, for example. We create fine grids on these regions of low

accuracy, and to be certain of capturing waves on the fine grids, we extend the fine grids a little way into the region of adequate accuracy. A fine grid is shown by broken lines in Figure 2. We provide initial and boundary data on the fine grid as follows. If fine-grid data is available from the previous time step, we use it (segment BC in Figure 2). Otherwise, we create initial data on the fine grid by interpolating coarse-grid data, as on segment CD in Figure 2. Similarly, the boundary data, such as for DE in Figure 2, are obtained by interpolation. Unused fine-grid data is purged (segment AB in Figure 2). After the integration on the fine grid, the values at coarse grid points interior to fine grids (segment GF in Figure 2) are replaced by projections of fine-grid values.

Let us make a few remarks about the implementation of the algorithm. In the computations done to date the ratio $\Delta t/\Delta x$ is the same on the fine grids as on the coarse grid. This is because the test problems have all involved explicit methods for hyperbolic equations. Note that the algorithm is recursive, so that it is possible to have many levels of refinement. Experience indicates [1, 3] that three levels is a good number with Δx on each fine grid taken to be 1/4 of the Δx for the next coarser grid. We also point out that at any time level there may be any number of fine grids. (Only a certain number will fit, of

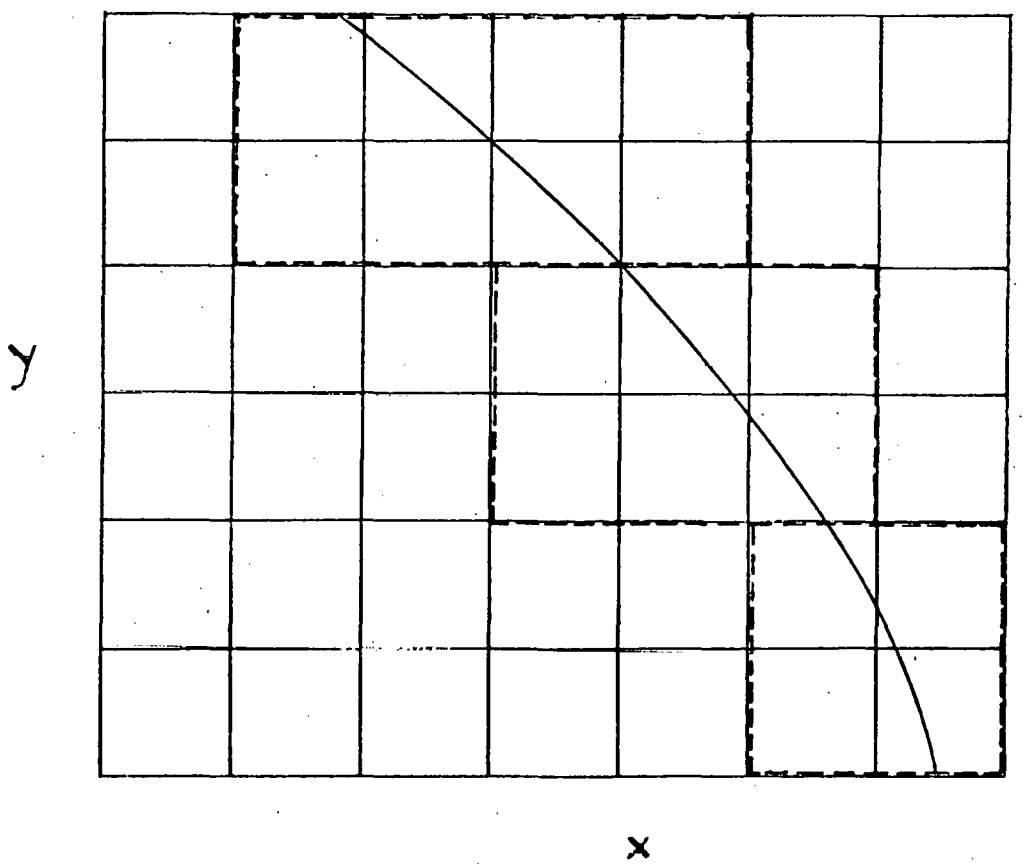

Figure 3. Parallel fine grids

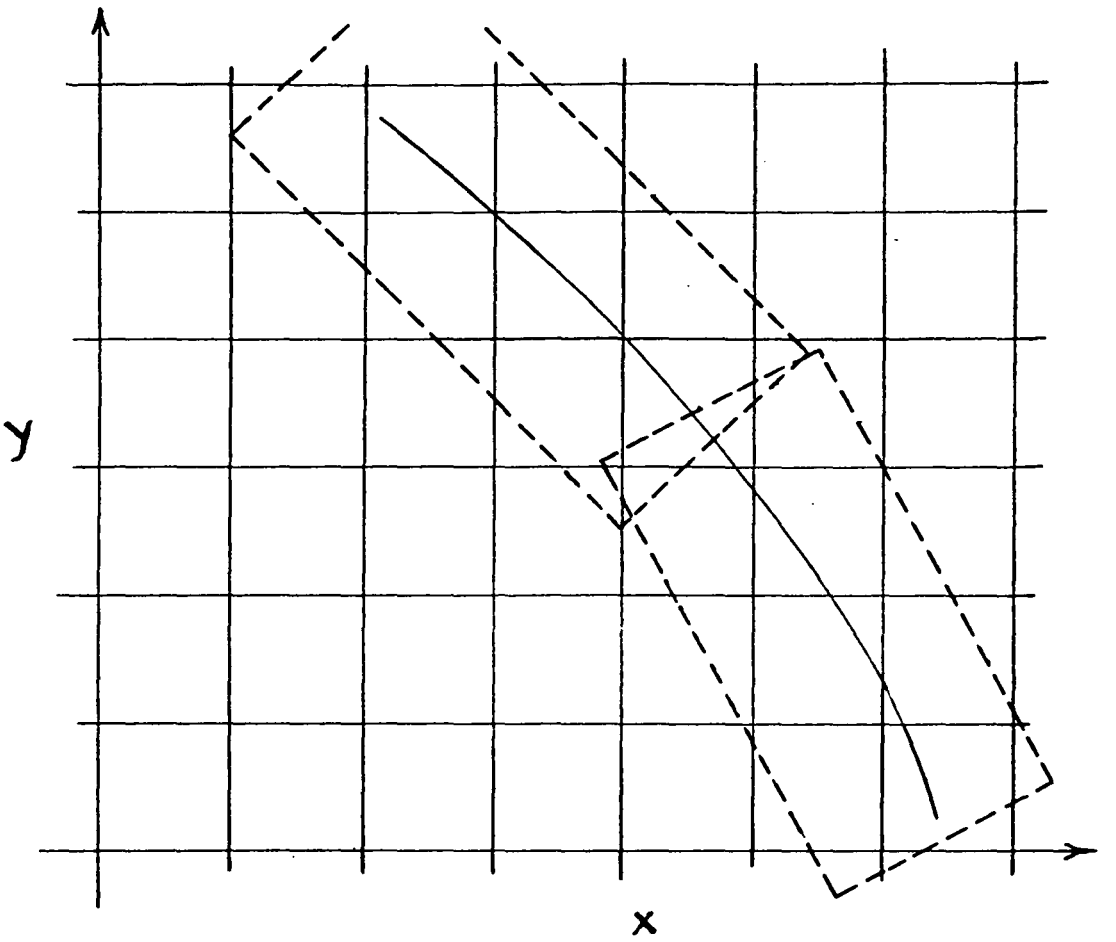

Figure 4. Fine grids with arbitrary orientation

course.) Consequently, the data structure is a tree, and it is appropriate to organize it via a linked list. Finally, we remark that on a multiprocessor the integrations on the different fine grids may be carried out simultaneously on different components.

The method has been extended to two dimensions in two different ways. Gropp [13] aligned the fine grids with the coarse grid, and Berger [1] permits fine grids with arbitrary orientation. Gropp's approach requires a larger number of fine grids to cover a wave front moving skew to the grid. See Figure 3. Berger's approach requires fewer fine grids, but the interpolation is much more complicated, and grid overlap causes some difficulty. See Figure 4. It is not yet clear which approach is better, although some people have strong opinions on the matter.

4. Conclusions

The principal advantage of moving-grid methods over local mesh refinement is

that in local mesh refinement the numerical dispersion is as bad as it would be on a fixed fine grid. For linear hyperbolic equations numerical dispersion is characterized in [6]. For nonlinear problems the situation is different, depending on the application. For combustion problems the finest grid will have to be fine enough to resolve the flame. For gas dynamics with shocks the difference scheme on the finest grid should be one of the special schemes designed for shocks [4, 5, 25].

The main advantage of local mesh refinement is its data structure, which permits the tracking of a varying number of wave fronts. We would like to see the development of a computer program which combines the best features of both methods, say, a fixed coarse grid with an arbitrary number of moving fine grids. For specific problems and only one level of refinement this can be done now, but general software is not likely to come soon.

Another question which needs to be addressed is the generalization of these methods to arbitrary domains in two dimensions. One possible approach is to begin with one of the happings of the domain onto a union of rectangles, such as [10, 19, 20].

The authors realize that some readers will disagree with opinions expresed here, but that is to be expected in a survey of field in which rapid development is under way.

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