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Abstract

In the numerical solution of partial differential equations, by finite methods, greater efficiency can be obtained if the geometry of the grid is determined by the solution. Many techniques for adapting the grid to the numerical solution it supports, have been proposed. One such scheme for convection equations in one dimension is considered here, and its application to convection-diffusion problems is investigated.

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Notation

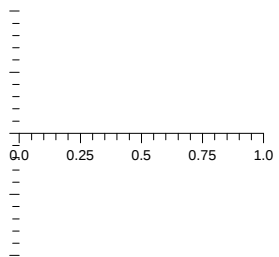
$\mathbb{R}_+$	positive real numbers
u_j^n	finite difference approximation of $u(x_j, t_n)$
$(\Delta x_j)^n$	$x_j^n - x_{j-1}^n$
$(\Delta x^{n+1})_j$	$x_j^{n+1} - x_j^n$

The subject of this dissertation is adaptive finite difference schemes, for the numerical solution of partial differential equations involving convection. A scheme is said to be adaptive if the underlying discretisation mesh (grid) undergoes changes in geometry, in response to the numerical solution it supports.

addition to convection. An attempt is made to modify the scheme presented in Chapter 3, to provide solutions to the new problem. In addition, the solution of this test problem contains a steep, moving front which the grid is required to track.

Conclusions drawn from the numerical results contained in Chapter 4 lead to further modifications to the scheme, which are considered in Chapter 5.

The modelling of partial differential equations (PDEs) which involve dominant convection terms, has long been recognised to pose significant problems for numerical solution methods. For instance, first order upwind schemes provide some desirable properties : they preserve monotonicity of the solution and give reasonably accurate phase speed. However, for these schemes, numerical diffusion is severe. This is demonstrated in Figure 1.1, which shows how the first order upwind scheme produces unwanted smearing in the solution. The initial data is shown in the first graph.



and represent a form of truncation error for the scheme. It is the largest of these terms which will be of interest here.

There is a slight subtlety involved in obtaining the modified equation [9]. This occurs when the high order time and mixed derivatives are to be eliminated. It is not valid to use the original differential equation for this purpose, which is the

$$\begin{array}{cc} \frac{n+1}{j} & \frac{n}{j} \\ \hline \end{array} \quad \begin{array}{cc} \frac{n}{j} & \frac{n}{j-1} \\ \hline \end{array}$$

$$t \quad \text{---} \quad tt \quad \text{---} \quad x \quad xx \text{---} \quad 2$$

which will be followed in the remainder of this dissertation.

Finally, there is an approach to the problem of numerical diffusion, which forms a natural complement to that of adaptive grids. This is the velocities introduced by Smolarkiewicz [8] and Margolin [6]. Here the diffusion term of the modified equation is re-written as an extra convective term. The

By imposing velocities onto grid nodes, which hold solution values, we are now attempting to solve the differential equation within a moving frame of reference. (The term $\frac{d}{dt}$ is here to be read as $\frac{d}{dt} + \mathbf{v} \cdot \nabla$.) It is important to consider how the form of the equation is changed, when its independent variables are transformed to those of the moving frame.

differential equations in the time variable. Then this system is discretised and solved using some time stepping procedure. This is the approach of the

. It is in the first of these stages that the transformation to the moving frame occurs. Hence the time transformation equation plays a rôle of little importance, and we may make the convenient choice,

$$t = \tau.$$

To obtain the transformed differential equation, we require the partial derivatives of the above coordinate transformation. These are most readily calculated by means of the Jacobian.

For the coordinate transformation,

$$x = x(\xi, \tau)$$

$$t = \tau$$

the Jacobian is readily seen to be

$$\frac{\begin{pmatrix} x \\ t \end{pmatrix}}{\begin{pmatrix} \xi \\ \tau \end{pmatrix}} = \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \tau} \\ 0 & 1 \end{pmatrix}$$

and the inverse of the Jacobian is found to be

$$\frac{\begin{pmatrix} \xi \\ \tau \end{pmatrix}}{\begin{pmatrix} x \\ t \end{pmatrix}} = \begin{pmatrix} 1 & \frac{\partial \xi}{\partial \tau} \\ 0 & 1 \end{pmatrix}$$

Hence the required partial derivatives are

$$\begin{aligned} \frac{\partial x}{\partial \xi} &= \frac{1}{\xi} & \frac{\partial x}{\partial \tau} &= -\frac{\tau}{\xi} \\ \frac{\partial t}{\partial \xi} &= 0 & \frac{\partial t}{\partial \tau} &= 1 \end{aligned} \tag{2.1}$$

Now consider the differential equation

$$u_t = \mathcal{L}u,$$

where $\mathcal{L}$ is some operator containing space derivatives only. By defining,

$$\hat{u}(\xi, \tau) = u(x, t)$$

we obtain, by use of the partial derivatives found above,

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial \hat{u}}{\partial \xi} \frac{\partial \xi}{\partial t} + \frac{\partial \hat{u}}{\partial \tau} \frac{\partial \tau}{\partial t} = \frac{\partial \hat{u}}{\partial \tau} + \frac{\partial \xi}{\partial t} \frac{\partial \hat{u}}{\partial \xi} \\ \Rightarrow \frac{\partial u}{\partial t} &= \frac{\partial \hat{u}}{\partial \tau} - \frac{x_\tau}{x_\xi} \frac{\partial \hat{u}}{\partial \xi} \end{aligned} \quad (2.2)$$

And the differential equation in the moving frame is,

$$\frac{\partial \hat{u}}{\partial \tau} = \frac{x_\tau}{x_\xi} \frac{\partial \hat{u}}{\partial \xi} + \hat{\mathcal{L}}\hat{u} \quad (2.3)$$

where $\hat{\mathcal{L}}$ is obtained by a suitable transformation of $\mathcal{L}$.

This equation often appears in a slightly different form. Since x_τ is the velocity of the moving frame, we may write

$$\dot{x} = x_\tau$$

and refer to $\dot{x}$ as the frame velocity. A further notational shorthand is also in use, where the symbol $\frac{\partial u}{\partial x}$ is used to denote $\frac{1}{x_\xi} \frac{\partial \hat{u}}{\partial \xi}$. The equation in the moving frame now reads,

$$\frac{\partial \hat{u}}{\partial \tau} - \frac{x_\tau}{x_\xi} \frac{\partial \hat{u}}{\partial \xi} = \mathcal{L}u \quad (2.4)$$

equations (2.3) and (2.4) will play an important part in the remaining chapters.

2.2 Adaptive Grids

Two broad classes of adaptive grid methods may be identified [5] :

I. Dynamic Rezone Methods

II. Static Rezone Methods

2.2.1 Dynamic Rezone Methods

In grid adaption algorithms of this class, grid node movement is bound to that of the solution. Individual grid nodes attempt to keep pace with moving features of the solution.

Example Petzold [7] has proposed the following two stage finite difference scheme.

The first stage produces grid movement which serves to minimise the time rate of change of the solution at individual grid nodes. This allows for a larger time step to be used, without loss of accuracy.

The second stage belongs properly to the static class of methods. It consists in applying refinements to the grid produced by the first stage, in order to obtain better resolution in regions of rapid spatial change.

Since this scheme contains elements of the two main classes of adaptive methods, it is worth considering it in a little more detail.

Petzold's Scheme The first stage is based on a transformation to a Lagrangian frame, due to Hyman [4]. This transformation is obtained by finding the frame

velocity which minimises the quantity

$$= \frac{\dot{x}^2}{2} + \frac{1}{2} \left(\frac{dx}{dt} \right)^2 \quad \text{where} \quad \frac{dx}{dt} = \frac{dx}{dt}$$

The notation proceeds a little more smoothly if the following definitions are made,

$$\begin{aligned} \dot{x} &= \frac{dx}{dt} \\ \ddot{x} &= \frac{d^2x}{dt^2} \\ \ddot{x} &= \frac{1}{\xi} \frac{d^2x}{dt^2} \end{aligned}$$

Then (2.4) reads

$$\ddot{x} = \ddot{x}_t + \ddot{x}_x$$

$$\begin{aligned} \ddot{x} &= \ddot{x}_t + \ddot{x}_x \\ \ddot{x} &= \ddot{x}_t + \ddot{x}_x \end{aligned}$$

$$\frac{1}{2} \left(\frac{dx}{dt} \right)^2 + \frac{1}{2} \left(\frac{dx}{dt} \right)^2$$

$$\frac{1}{2} \left(\frac{dx}{dt} \right)^2$$

take to achieve their purpose are highly problem dependent, and must be found by inspection. This reduces the possibility of the method being incorporated into a fully automatic package, a standard aim of many methods of this kind. This is a problem common to many adaptive techniques.

In addition, the grid so far does not necessarily adapt to sharp features of the solution. A second, grid enhancement, stage is required. Petzold uses a grid redistribution technique, where nodes are added or deleted from the grid, to achieve

$$u_x + (u_{xx})^2 \leq \text{preset tolerance},$$

a process which also involves a number of interpolations.

The principal technique of this class of adaptive methods is that of equidistribu-

tion, $(\quad)$,

$$(\quad) = \frac{1}{0} \quad^x \quad (\quad)$$

$$\text{where} \quad = \frac{1}{0} \quad (\quad)$$

The solution domain is assumed to be the unit interval, $0 \leq x \leq 1$. The monitor function is chosen to be some quantity related to the spatial variation of the solution.

To conclude, the Petzold scheme highlights many aspects which are of importance in designing adaptive methods :

The choice of solution properties to which the grid is to adapt

The manner in which the grid is to be altered

Can it be guaranteed that the grid will remain monotonic, that nodes will not overtake one another

3.2 Outline of the *Masterful* Scheme

The scheme is implemented on a grid which subdivides the unit interval into $J+1$ cells, or subintervals. Such a grid has J internal nodes, whose positions are free to be varied as the scheme proceeds. The nodes at either end of the interval remain fixed throughout.

$$\begin{array}{ccccccc}
 & | & & | & & | & & | & & | & & | \\
 0 = x_0 & & x_1 & & x_2 & \cdots & x_j & \cdots & x_J & & x_{J+1} = 1
 \end{array}$$

The *Masterful* scheme is constructed from a first order upwind scheme and the node adjusting algorithm [2], combined in the following steps :

Scheme

- a) Apply the upwind scheme to current solution, producing a first approximation to the solution at the next time level
- b) Apply the best-fit algorithm to piecewise linear recovered function (see section 3.3.2.) This produces new nodal positions, which are better suited to represent the solution at the new time level
- c) Use the nodal displacements to obtain a new frame of reference
- d) Apply the upwind scheme to the current solution a second time, but this time the differential equation is solved within the new frame

Consider the differential equation

$$u_t + (u^2)_x = 0 \tag{3.4}$$

The scheme advances the numerical solution of this equation, through one time interval Δt , according to the following steps :

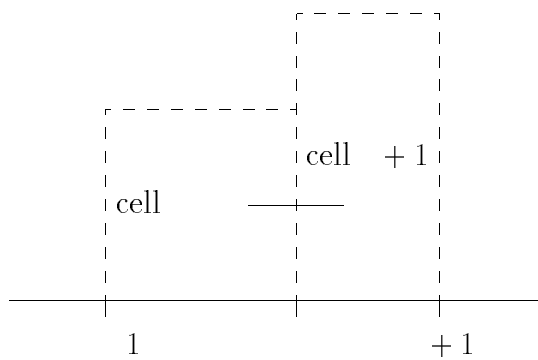
Let $u_j^* : j = 0, 1, \dots, J+1$ be the finite difference solution of (3.4) obtained by an upwind step on the data at time level t_n ,

$$u_k^* = u_k^* - \frac{\Delta t}{\Delta x} \frac{1}{2} \left(\frac{u_j^n + u_{j-1}^n}{2} \right) \quad \text{if } u_j^n \geq 0 \tag{3.5}$$

$$\text{where } \frac{1}{2} \left(\frac{u_j^n + u_{j-1}^n}{2} \right) = \begin{cases} u_j^n & \text{if } u_j^n \geq 0 \\ u_{j-1}^n & \text{if } u_j^n < 0 \end{cases}$$

$$\text{and } \frac{1}{2} \left(\frac{u_j^n + u_{j-1}^n}{2} \right) = \frac{u_j^n + u_{j-1}^n}{2}$$

The grid adaption routine is based on a technique for obtaining piecewise constant best L_2 fits, to a piecewise linear continuous function [2]. The motivation for using this procedure, is the L_2 interpretation of upwind schemes. In this formalism the region is considered to be divided into cells. Each cell contains one node, where the cell value of the solution is u_j^n .



$$\begin{array}{ccccccc}
& & & & n+1 & & n+1 \\
& & & & j & & j \\
\\
n+1 & j & & n+1 & & n & \\
& j & & j & & j & \\
\\
& & & & 2 & * & \\
& & & & j & & \\
& & & & \hline
& & & & * & & \\
& & & & j & & \\
& & & & j & n & \\
& & & & * & & * \\
& & & & j & & j+1 \\
\\
n+1 & j & & & 2 & * & \\
& & & & j & & \\
& & & & \hline
& & & & * & & \\
& & & & j & & \\
& & & & j+1 & n & \\
& & & & * & & * \\
& & & & j & & j+1
\end{array}$$

$$j - \frac{1}{2} \quad - \quad \frac{j+1}{j} \quad \frac{j}{j} \quad \frac{j+1}{j-1} \quad \frac{j}{j-1}$$

$$\begin{array}{ccccccc} n+1 & n & n & n & & n & n \\ k & k & j & j & \frac{1}{2} & \frac{1}{2} & 1 \\ & & & & \frac{j}{n} & & \end{array}$$

$$\text{where } \quad = \quad \begin{matrix} \text{if } & \frac{n}{j-\frac{1}{2}} & \cdot \frac{n}{j-\frac{1}{2}} & 0 \\ & 1 & \text{if } & \frac{n}{j-\frac{1}{2}} & \cdot \frac{n}{j-\frac{1}{2}} & 0 \end{matrix}$$

Since both upwind passes preserve monotonicity , and the grid adaption method maintains the ordering of the nodes, the scheme as a whole is also monotonicity preserving.

The first two stages of the scheme are straight forward : first obtain a prediction for the solution at the next time level ; then adjust the nodal positions to give a better fit to this new solution. The nodal displacements per time step describe the required velocity of the frame of reference. In the last stage the upwind method is to be applied in this moving frame.

— —

— — —
ξ

τ

x —
ξ

$$t = \frac{\cdot}{\xi} \tag{3.8}$$

Using (3.7), (3.6) becomes

$$- + (\cdot) - = 0$$

—

$$\frac{n}{j}$$

— —

—

—

$$\frac{n+1}{} \quad \frac{n}{} \quad \frac{n}{}$$

$$\frac{n}{j-\frac{1}{2}}$$

$$\frac{n}{} \quad \frac{n}{j-\frac{1}{2}}$$

$$\frac{n}{} \quad \frac{n}{j-\frac{1}{2}} \quad \frac{n}{j-\frac{1}{2}} \quad \frac{n+1}{} \quad \frac{n}{j-\frac{1}{2}}$$

Now ξ has been chosen such that $\xi(x_j^n, n\Delta t) = j, \quad j = 0, 1, \dots, J+1 \quad \forall n$

By applying linear interpolations to this data, the two quantities in the numerator of (3.11) are found to have the following approximations,

$$\begin{aligned}\xi^n(x_{j-\frac{1}{2}}^n) &= j - \frac{1}{2} \\ \xi^{n+1}(x_{j-\frac{1}{2}}^n) &= j - 1 + \frac{x_{j-\frac{1}{2}}^n - x_{j-1}^{n+1}}{x_j^{n+1} - x_{j-1}^{n+1}}.\end{aligned}$$

Details of the calculations involved are given in the Appendix. Combining these with

$$x_{j-\frac{1}{2}}^n = \frac{1}{2} \left(\frac{x_j^{n+1} - x_j^n}{\Delta t} + \frac{x_{j-1}^{n+1} - x_{j-1}^n}{\Delta t} \right)$$

equation (3.11) reduces to,

$$\frac{\partial \xi^n}{\partial x}(x_{j-\frac{1}{2}}^n) = \frac{1}{x_j^{n+1} - x_{j-1}^{n+1}}$$

When this is written into the upwind scheme, the resulting discretisation differs from that of (2.4) only in the calculation of the space interval. In this new scheme the grid differences are calculated at the new time level, instead of the current level. A comparison between the two discretisations is given in the next section.

3.5 Numerical Results

The schemes derived from equations (2.4) and (2.3) are here referred to as the first and second discretisations respectively.

A comparison is made between the two discretisations applied to the test

problem,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0$$

with initial data,

$$u(x, 0) = \frac{1}{2} - x.$$

The measure of the error used here is

$$\text{error} = \frac{\left\{ \sum_{j=0}^{J+1} [u(x_j^n, t_n) - u_j^n]^2 \right\}^{\frac{1}{2}}}{J+1}$$

The results, in *table* 3.1, are typical of the two discretisations. The second form of discretisation provides a slight improvement in accuracy, in most cases.

Number of free nodes	error at $t = 0.5$		Steps required	
	First discretisation	Second discretisation	First	Second
9	6.53×10^{-3}	7.77×10^{-3}	4	4
19	3.65×10^{-3}	3.03×10^{-3}	8	8
39	1.66×10^{-3}	1.30×10^{-3}	16	15
59	9.88×10^{-4}	7.72×10^{-4}	24	23
99	5.00×10^{-3}	3.89×10^{-4}	40	38

Table 3.1: error comparison

So far, the scheme, presented in Chapter 3, has only been applied to problems

$$\frac{\quad}{\quad} \quad \frac{\quad}{\quad} \quad \frac{2}{2}$$

smeared over a larger region, and less steep. Since the monotonicity preserving property of the scheme ensures sharp resolution of steep fronts for (4.1), the more rounded solutions of (4.2) should cause no extra difficulties. For this reason a test problem is chosen which possesses a moving front, in addition to the extra physical diffusion.

Before this problem can be tackled, it is first necessary to obtain a discretisa-

$$\begin{array}{ccccc} x & & \overline{\hspace{1cm}} & & t & & \overline{\hspace{1cm}} \\ & & \xi & & & & \xi \\ x & & & & t & & \end{array}$$

$$\begin{array}{ccccccc} \overline{\hspace{1cm}} & & & & \xi & t & & \tau & t \\ & & & & \tau & & & x & \xi \end{array}$$

$$\begin{array}{ccccccc} \overline{\hspace{1cm}} & & & & \xi & x & & \tau & x \\ & & & & x & \xi & & & \end{array}$$

$$\begin{array}{ccccccc} \frac{2}{\overline{\hspace{1cm}}} & & \overline{\hspace{1cm}} & & x & \xi \\ & & & & xx & \xi & & x & \xi \xi & x & & \xi \tau & x \\ & & & & xx & \xi & & x^2 & \xi \xi \end{array}$$

$$\begin{array}{ccccccc} \overline{\hspace{1cm}} & & & & x & & xx & \overline{\hspace{1cm}} & & x^2 & \frac{2}{2} \end{array}$$

$$xx$$

$$\begin{array}{ccccccc} x & \xi & & & \overline{\hspace{1cm}} & & x & \xi \end{array}$$

$$xx \quad \xi \quad x \quad \xi \xi \quad x \quad \xi \tau \quad x$$

$$xx \quad \xi \quad x^2 \quad \xi \xi$$

$$xx \quad x^3 \quad \xi \xi$$

Fourier stability analysis for a scheme of the form,

$$\frac{u_j^n}{\Delta x} + \frac{u_{j-1}^n}{\Delta x} = \frac{(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1})}{(\Delta x)^2}$$

provides an indication of the quantities which are of importance to the stability of the explicit schemes to be considered here :

$$\text{If } \frac{u_j^n}{\Delta x} \text{ and } \frac{u_{j-1}^n}{\Delta x} = \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2} \text{ then}$$

The necessary stability condition involves terms due to diffusion, as well as convection. For this particular example, $\frac{u_j^n}{\Delta x} + 2 \frac{u_{j-1}^n}{\Delta x} = 1$.

A measure of the relative importance of convection and diffusion processes, is given by the mesh Peclet number,

$$Pe = \frac{u \Delta x}{\alpha} \quad (4.5)$$

When the scheme, obtained by the method of Section 4.1.2, is implemented, some method must be found for selecting the time increment, Δt , to ensure stability. In general this value will change from step to step. It is a simple matter to select a value, of Δt , for which the condition above is satisfied by the data at the current time level. Furthermore, the adaptive scheme has the flexibility to allow Δt to be changed, if need be, to satisfy the stability requirements of the second upwind pass. This is due to the fact that, the second pass only uses the nodal displacements, u_j^n , and not the nodal velocities.

However, for the discretisation in Section 4.1.1, the matter is not so simple. The second upwind pass now involves quantities from the Jacobian of the trans-

displacement. Hence it is no longer valid to change Δt between upwind passes.

Some method must be found to select Δt , from the data at time t_n , which will guarantee the stability of both upwind passes. Such a method might be found

—

ϵ

ϵ

$$\frac{(\Delta x)^2}{\Delta t}$$

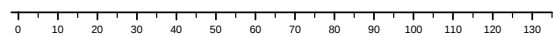
If the discretisation measure, $\left(\frac{\Delta x}{\Delta t}\right)^2$, is small in comparison to the physical diffusion strength, $\frac{D}{\Delta x}$, then the scheme models the diffusion process with great accuracy. This corresponds to a small value of Δx , and a consequently large value of Δt . It is when the value of Δt is large that convection-diffusion problems pose the greatest challenge to numerical methods.

For the current test problem, values of Δx were chosen to provide high and low mesh Peclet numbers.

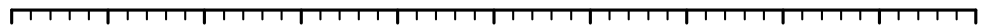
e

Figure 4.1 contains a graph showing the nodal positions, with time represented vertically. The thick line shows the position of the centre of the front, as it moves across the grid. Beneath this, is shown the numerical solution at times $t = 0, 0.25, 0.5, 0.75, 1.0$. The dotted lines show the corresponding exact solutions. This figure identifies two principal defects in the numerical solution.

First, the initial regular grid results in deterioration of the solution during the first few time steps. As the grid becomes better adapted to the solution, numerical diffusion decreases and the solution deteriorates much less during



shows that the front effectively leaves the grid at about $t = 0.7$, and the solution becomes meaningless.



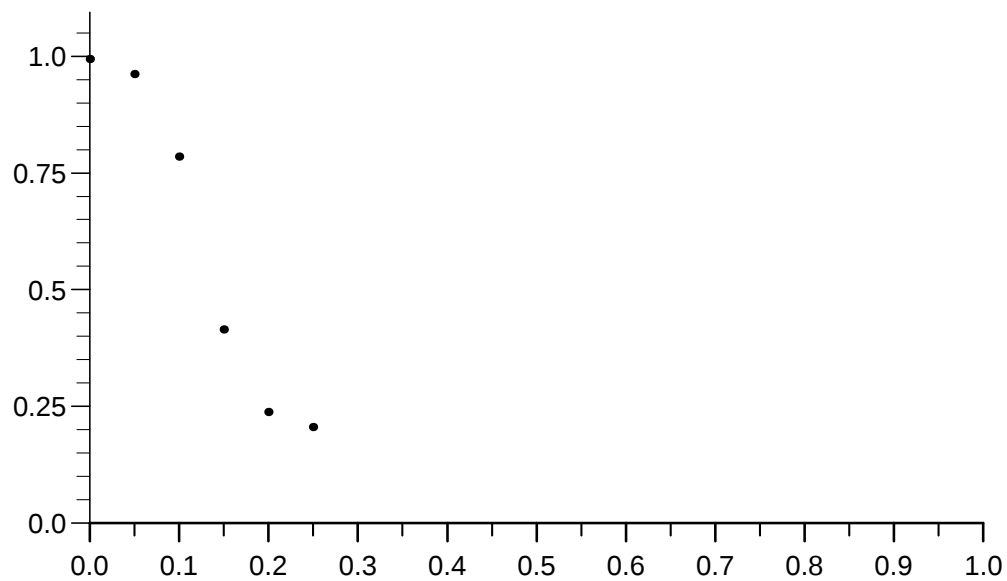
to stability of the upwind scheme. A fully implicit, unconditionally stable version of the scheme was applied to the problems presented in Chapter 4.

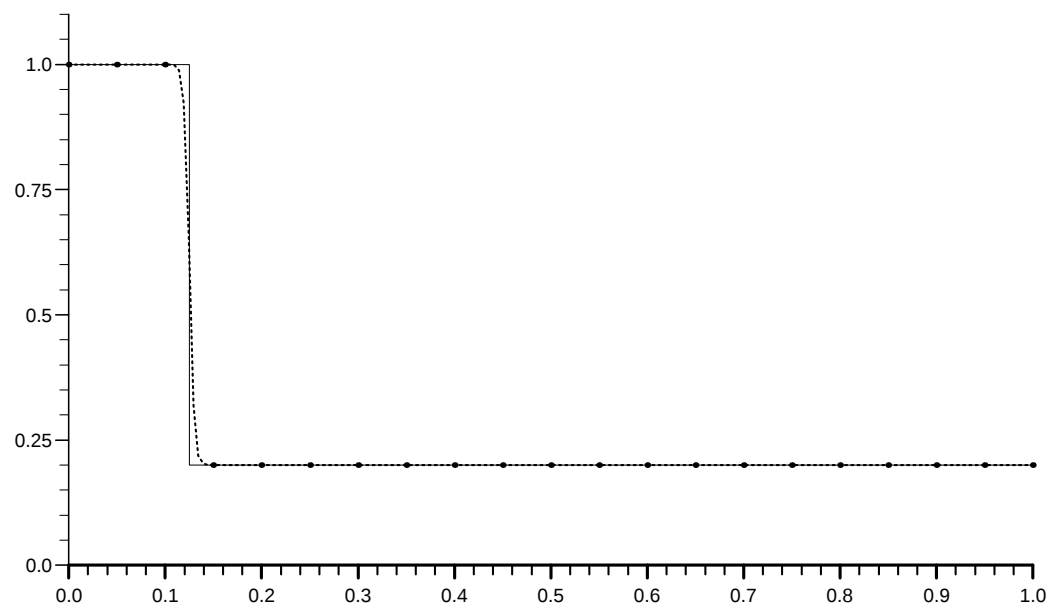
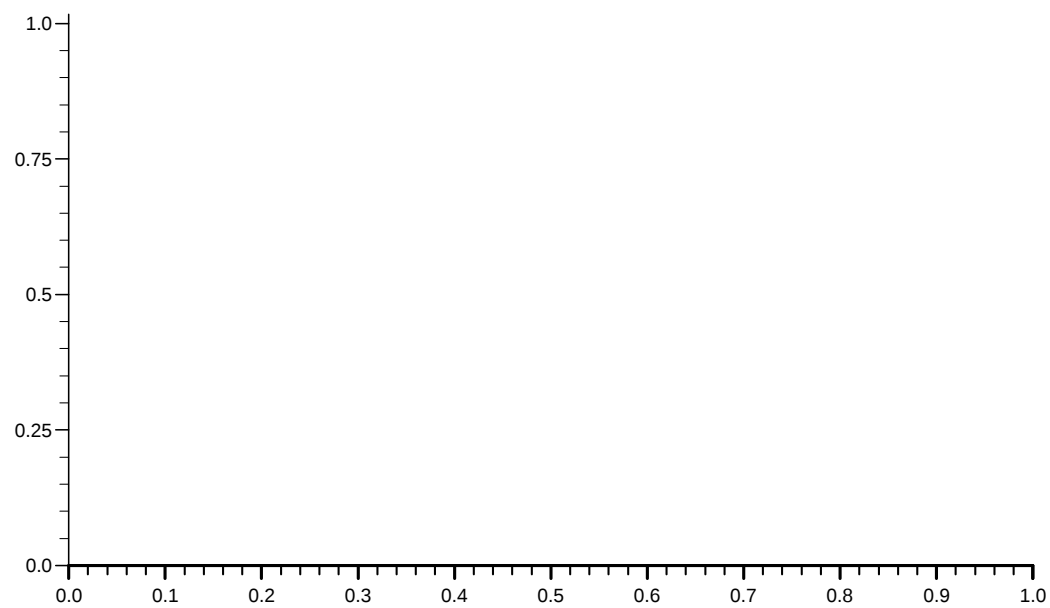
5.1.1 Results for Implicit Scheme

The fully implicit scheme requires a tridiagonal matrix to be solved at each time step. An algorithm employing LU decomposition, with forward and backward substitutions, is used for this purpose.

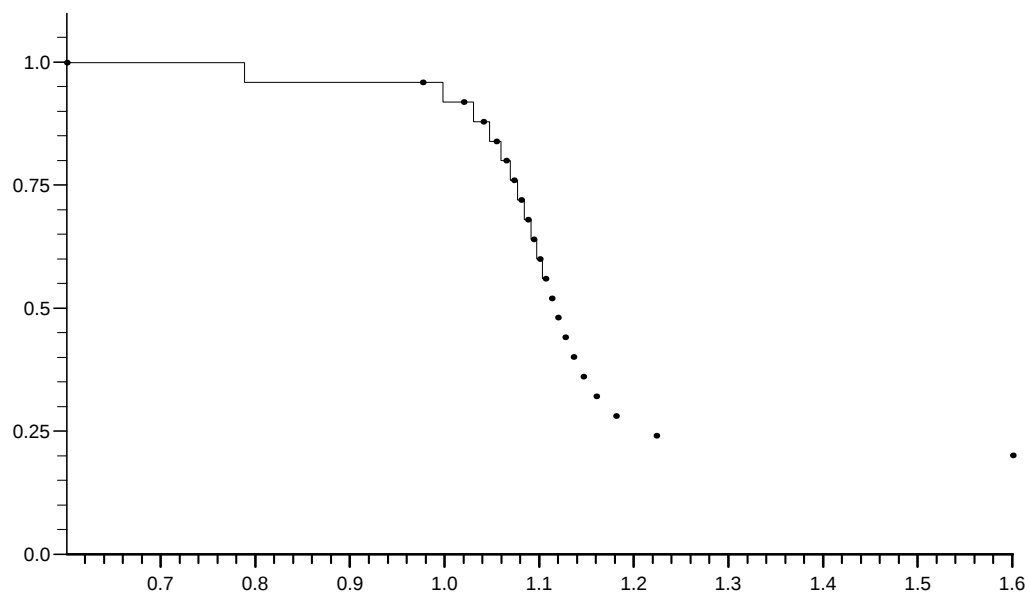
Figures 5.1, 5.2 show the result of applying the implicit scheme to the test problem of Chapter 4. In each case the time step has been selected, by trial and error, to obtain the most accurate solution.

The implicit scheme appears to offer little, if any, improvement on the explicit scheme, and will not be considered further.





moving with the speed of the front. *Figure 5.3* shows that, under these conditions, the nodes eventually move to stable positions around the front. Once the grid has reached this stable configuration, the solution displays a dramatic reduction in numerical diffusion. The remaining error, which can be seen in the lower graph (solution at $t = 1.0$), is almost entirely a remnant of the early ill-placing of nodes.



However, the grid is seen to be unable to respond to moving features in the solution, Section 4.2. This indicates that the scheme is not of the Dynamic Rezone type.

In Chapter 5, the adaptive grid is given the translational speed of the front to be tracked. This drift velocity must be found by means independent of the adaptive scheme. The numerical solution, though much improved, still suffers deterioration due to numerical diffusion on the initial, ill-adapted grid. This problem may be remedied by monitoring the goodness of fit of the grid to the solution. If the grid is not well adapted, other means must be employed to reduce numerical diffusion and maintain accuracy.

$$j$$

$$\begin{matrix} n+1 & n & n+1 \\ j & j & j \end{matrix}$$

$$\begin{matrix} & 2 \\ n+1 & j & - & \frac{2}{j} \end{matrix} \qquad +1$$

$$\begin{matrix} & 2 & & \\ +1 & - & \frac{+1}{+1} & +1 \end{matrix} \qquad +1$$

$$+1$$

$$+1$$

$$+1$$

$$\frac{+1}{}$$

$$\begin{matrix} +1 & - & \frac{+1}{} \end{matrix}$$

A similar inequality is obtained for the case $\binom{n}{j} \geq \binom{n}{j+1}$. Combining these inequalities and using the definition,

$$\binom{n}{j} = \frac{n}{j} \binom{n-1}{j-1}$$

$$\frac{\binom{n}{j-1}}{\binom{n}{j}} = \frac{n+1}{j} > \frac{\binom{n}{j}}{\binom{n}{j+1}}$$

$$\frac{n}{j-\frac{1}{2}} > \frac{\binom{n}{j-1}}{\binom{n}{j}}$$

$$\frac{n}{j-1} > \frac{n}{j-\frac{1}{2}} > \frac{n+1}{j}$$

$$n+1 > \frac{n}{j-\frac{1}{2}}$$

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