

In this dissertation we will discuss the finite difference method for approximating conservation laws with a source term presenithh.9e

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The following is a list of symbols and notation used throughout this project.

$\div x$	Step-size in x-direction.
$\div t$	Step-size in t-direction.
i	Integer denoting current step number.
n	Integer denoting current step number.
I	Total number of steps in x-direction.
N	Total number of steps in t-direction.
$x_i = i \div x$	Current position in space.
$t_n = n \div t$	Current position in time.
u	

Recently, the numerical solution of conservation laws with a source term, i.e.

$$\frac{\epsilon u}{\epsilon t} + 2 \frac{\epsilon f(u)}{\epsilon x} = R(x, t, u)$$



be accurately even

(1.3)

(1.2) and discuss
the truncation error
and second order
also be discussed
finite difference

encountered when
consider how to
deal of research has
to handle source
chapter 3, we will

In this chapter, we will look at some numerical schemes for approximating the 1-D scalar conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \quad (2.1)$$

where $u(x,t)$ is the conserved quantity and $f(u)$ is the flux. We can also rearrange (2.1) to obtain the quasi-linear form

$$\frac{\partial u}{\partial t} + a(u) \frac{\partial u}{\partial x} = 0 \quad (2.2)$$

where $a(u) = f'(u)$, which is called the wave-speed. If $a(u) = c$, where c is a constant, then (2.1) becomes the linear advection equation.

The most basic form of the conservation law is the linear advection equation

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0 \quad (2.3)$$

where c is a constant and $f(u) = cu$. Here, the constant c is known as the wave speed since $a(u) = c$. There are a variety of numerical techniques for approximating the linear advection equation, such as finite element methods and finite volume methods. Another class of numerical technique used for approximating the linear advection equation are finite difference methods. Finite difference methods

In order to obtain a first order scheme, we use a forward difference approximation in time and a backward difference approximation in space and assume both of these finite differences to be approximations at (i,n) , i.e.

$$\frac{\partial u}{\partial t} = \frac{u_i^{n+1} - u_i^n}{\Delta t} \quad \text{and} \quad \frac{\partial u}{\partial x} = \frac{u_i^n - u_{i-1}^n}{\Delta x}.$$

Substituting these into (2.3) gives

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_i^n - u_{i-1}^n}{\Delta x} = 0,$$

and hence,

$$u_i^{n+1} = u_i^n - v(u_i^n - u_{i-1}^n)$$

where $v = c \frac{\Delta t}{\Delta x}$ and is known as the Courant number. This scheme is one of the most

basic numerical approximations of the advection equation. However, it can be shown that this scheme is numerically unstable if $c < 0$, in which case we use a forward difference approximation in space and time and assume that both are approximations at (i,n) , i.e.

$$\frac{\partial u}{\partial t} = \frac{u_i^{n+1} - u_i^n}{\Delta t} \quad \text{and} \quad \frac{\partial u}{\partial x} = \frac{u_{i+1}^n - u_i^n}{\Delta x},$$

then substituting into (2.1) gives

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_{i+1}^n - u_i^n}{\Delta x} = 0.$$

Whence,

$$u_i^{n+1} = u_i^n - v(u_{i+1}^n - u_i^n).$$

This scheme is numerically unstable if $c > 0$. Separately, these schemes can become numerically unstable, but if we combine them

$$u_i^{n+1} = u_i^n - \begin{cases} v(u_i^n - u_{i-1}^n) & \text{if } v > 0 \\ v(u_{i+1}^n - u_i^n) & \text{if } v < 0 \end{cases} \quad (2.4)$$

we obtain the Upwind method with switching through $\nu = 0$. This scheme can still become unstable but only for $\nu > 1$. This will be discussed later.

Alternatively, we could obtain another first order scheme if we use a forward

$$\frac{\partial u}{\partial t} = -c \frac{\partial u}{\partial x} \quad (2.7)$$

$$\Rightarrow \frac{\partial^2 u}{\partial t^2} = -c \frac{\partial^2 u}{\partial t \partial x} = -c \frac{\partial^2 u}{\partial x \partial t} = -c \frac{\partial}{\partial x} \frac{\partial u}{\partial t} = -c \frac{\partial}{\partial x} \left(-c \frac{\partial u}{\partial x} \right)$$

so,

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}. \quad (2.8)$$

Substituting (2.7) and (2.8) into (2.6) gives

$$^1 \approx -\Delta \frac{\partial}{\partial t} + \frac{\Delta^2}{2} \frac{\partial^2}{\partial t^2} + \dots$$

but if we use central difference approximations in space and assume that both are approximations at $(i, n+1)$ instead of approximations at (i, n)

$$u_i^{n+1} = u_i^n - \frac{v}{2}(u_{i+1}^{n+1} - u_{i-1}^{n+1}) + \frac{v^2}{2}[u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}] \quad (2.10)$$

we obtain the implicit Lax-Wendroff scheme. This scheme is implicit since terms involving $n+1$ appear on the right hand side of the equation. Implicit schemes cause difficulties since we now have to solve a tri-diagonal system at each time step. Rearranging (2.10)

$$-\frac{v}{2}(1+v)u_{i-1}^{n+1} + (1+v^2)u_i^{n+1} + \frac{v}{2}(1-v)u_{i+1}^{n+1} = u_i^n$$

hence

$$\begin{array}{cccccc} b & c & 0 & \dots & 0 & 0 & u_0^{n+1} & u_0^n - a u_{-1}^{n+1} \\ a & b & c & 0 & 0 & 0 & u_1^{n+1} & u_1^n \\ 0 & a & b & c & 0 & 0 & u_2^{n+1} & u_2^n \\ & & & & & & & = \\ 0 & 0 & a & b & c & 0 & u_{l-2}^{n+1} & u_{l-2}^n \\ 0 & 0 & 0 & a & b & c & u_{l-1}^{n+1} & u_{l-1}^n \\ 0 & 0 & 0 & 0 & a & b & u_l^{n+1} & u_l^n - c u_{l+1}^n \end{array}$$

great deal more and definitely too many to look at in this section. For a more in depth discussion of finite difference schemes for the advection equation, look in Kroner[8], LeVeque[7] and Ames[14].

In Section 2.1, we discussed some finite difference schemes for approximating the linear advection equation, which is a form of the scalar conservation law

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

where $f'(u) = a(u)$. However, we can adapt the techniques discussed in Section 2.1 so that we can numerically approximate the solution of the scalar conservation law but we must be careful how we approximate (2.1) since we wish to ensure conservation.

If a scheme is non-conservative, then the scheme will move discontinuities at the incorrect wave speed. For example, if we approximated the quasi-linear form of equation (2.1) by using the finite difference method then we would obtain a non-conservative scheme. Consider inviscid Burger's equation, i.e.

$$\frac{\partial u}{\partial t} + \frac{\partial \frac{1}{2}u^2}{\partial x} = 0,$$

re-writing in quasi-linear form gives

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

and by using a forward difference approximation in time and a backward difference approximation in space and assuming that both are approximations are at (i,n) , i.e.

$$= \frac{1}{x} \quad \text{and} \quad = \frac{\sum_{i=1}^n u_i}{x}$$

To ensure conservation, we require that the method be in conservation form, i.e.

$$u_i^{n+1} = u_i^n - s \left[F(u_{i-p}^n, u_{i-p+1}^n, \dots, u_{i+q}^n) - F(u_{i-p-1}^n, u_{i-p}^n, \dots, u_{i+q-1}^n) \right]$$

where F is called the numerical flux function and is of $p + q + 1$ arguments. We can ensure conservation by numerically approximating (2.1) and using a similar approach as we did in the previous sub-section. For example, when we derived the Upwind scheme, we used a forward difference in time and either a forward or a backward difference in space depending on the value of v . Here, we take a same approach but we will apply finite differences to f instead of u , i.e.

Another method, which ensures conservation, is to approximate $v_{i+1/2}$ by replacing $a($

Name of Scheme	Scheme	Order
Upwind (first order)	$u_i^{n+1} = u_i^n - \begin{cases} s(f_i^n - f_{i-1}^n) & \text{if } v_{i+1/2} > 0 \\ s(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} < 0 \end{cases}$	1
Lax-Friedrichs	$u_i^{n+1} = \frac{1}{2}(u_{i+1}^n + u_{i-1}^n) - \frac{s}{2}[f_{i+1}^n - f_{i-1}^n]$	1
Second Order Upwind (Warming and Beam)	$u_i^{n+1} = u_i^n - \frac{s}{2} \begin{cases} (3-v_{i-1/2})(f_i^n - f_{i-1}^n) - (1-v_{i-3/2})(f_{i-1}^n - f_{i-2}^n) & \text{if } v_{i+1/2} > 0 \\ -(1+v_{i+3/2})(f_{i+2}^n - f_{i+1}^n) + (v_{i+1/2} + 3)(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} < 0 \end{cases}$	2
Leapfrog	$u_i^{n+1} = u_i^{n-1} - s(f_{i+1}^n - f_{i-1}^n)$	2
Lax-Wendroff	$u_i^{n+1} = u_i^n - \frac{s}{2}(f_{i+1}^n - f_{i-1}^n) + \frac{s}{2}[v_{i+1/2}(f_{i+1}^n - f_i^n) - v_{i-1/2}(f_i^n - f_{i-1}^n)]$	2
MacCormack Predictor- Corrector	$u_i^* = u_i^n - s(f_{i+1}^n - f_i^n)$ $u_i^{n+1} = \frac{1}{2}(u_i^n + u_i^*) - \frac{s}{2}[f_i^* - f_{i-1}^*]$	2

Table 2-1: Finite difference schemes for the 1-D conservation law.

discretisation error, which is the error caused by using finite difference approximations to approximate the derivatives of (2.3). As an example, consider the Lax-Friedrichs scheme (2.5) for the scalar conservation law

$$u_i^{n+1} = \frac{1}{2}(u_{i+1}^n + u_{i-1}^n) - \frac{s}{2}[f_{i+1}^n - f_{i-1}^n].$$

$$_i^n = \frac{1}{6} \left(t^2 \frac{\partial^3 u}{\partial t^3} - c \Delta x^2 \frac{\partial^3 u}{\partial x^3} \right) + O(\Delta x^3) + O(\Delta t^3)$$



$$\xi_{n+1} = \xi_n - \frac{v}{2} (\xi_n e^{ik\Delta x} - \xi_n e^{-ik\Delta x}) + \frac{v^2}{2} [\xi_n e^{ik\Delta x} - 2\xi_n + \xi_n e^{-ik\Delta x}]$$

and by re-arranging

$$\xi_{n+1} = (1 - v^2 + \frac{v^2}{2}(e^{ik\Delta x} + e^{-ik\Delta x}) - \frac{v}{2}(e^{ik\Delta x} - e^{-ik\Delta x})) \xi_n.$$

Using the identities

$$e^{jk\Delta x} + e^{-jk\Delta x} = 2 \cos k\Delta x$$

and

$$e^{jk\Delta x} - e^{-jk\Delta x} = 2i \sin k\Delta x$$

we may obtain

$$\xi_{n+1} = (1 - v^2 + \frac{v^2}{2}(2 \cos k\Delta x) - \frac{v}{2}(2i \sin k\Delta x)) \xi_n.$$

So, for stability we require

$$|1 - v^2 + v^2 \cos k\Delta x - vi \sin k\Delta x| \leq 1.$$

Here, we can see that the amplification factor lies on an ellipse:

$$\xi = 1 - v^2 + v^2 \cos k\Delta x - vi \sin k\Delta x$$

If we let

$$x = 1 - v^2 + v^2 \cos k\Delta x$$

and

$$y = -vi \sin k\Delta x$$

and by using the identity

$$\cos^2 k\Delta x + \sin^2 k\Delta x = 1$$

whence

$$\frac{x - (1 - v^2)}{v^2} + \frac{y}{v} = 1.$$

So, the interval of absolute stability is an ellipse with centre $(1 - v^2)$ and crosses the x-axis at $x = 1$ and $x = 1 - 2v^2$. Figure 2-3 shows the unit circle with the ellipse of the amplification factor inside the unit circle. Here, we can see that for the ellipse to stay inside the unit circle, $1 - 2v^2 \geq -1$ and $1 - v^2 \geq 0$. Hence, for the Lax-Wendroff scheme to be stable, $v \leq 1$. This condition on v

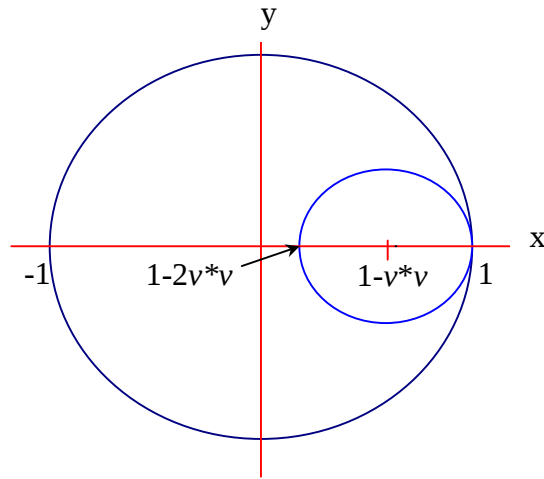


Figure 2-3: Interval of stability for Lax-Wendroff

Name of Scheme	Order (space + time)	Overall Order of Scheme	Interval Of Absolute Stability
Upwind (first order)	1 + 1	1	$ v \leq 1$
Lax-Friedrichs	2 + 1	1	$ v \leq 1$
Upwind (second order)	2 + 2	2	$ v \leq 2$
Leapfrog	2 + 2	2	$ v \leq 1$
Lax-Wendroff	2 + 2	2	$ v \leq 1$
MacCormack Predictor-Corrector	2 + 2	2	$ v \leq 1$

Table 2-2: The interval of absolute stability and the order of some schemes.

Earlier, Figure 2-2 showed the Upwind scheme becoming unstable for $v = 1.25$. This is because the Upwind scheme is stable for $0 \leq v \leq 1$, when $c > 0$, and since v lies outside the interval of absolute stability, the scheme will become unstable.

It can be show that all first order schemes suffer from dissipation which can result in a very inaccurate numerical solution. Dissipa

Earlier, we saw that this scheme had a truncation error of

$$T_i^n = \frac{\Delta t}{2} \frac{\partial^2 u}{\partial t^2} - \frac{\Delta x^2}{2\Delta t} \frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^2}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^3) + O(\Delta t^2)$$

and by using (2.8)

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

we may obtain

$$T_i^n = \frac{\Delta t}{2} c^2 - \frac{\Delta x^2}{2\Delta t} \frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^2}{6} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^3) + O(\Delta t^2).$$

So, the Lax-Friedrichs scheme is a second order approximation to

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = D \frac{\partial^2 u}{\partial x^2} \quad (2.12)$$

where $D = \frac{\Delta x^2}{2\Delta t} [1 - v^2]$. Equation (2.11) is known as the linear advection-diffusion

equation and is ill-posed if $D < 0$. In this case, equation (2.12) is well posed

since $\frac{\Delta x^2}{2\Delta t} \geq 0$ so, for (2.12) to be well posed $[1 - v^2] \geq 0 \Rightarrow |v| \leq 1$. Hence, since for

stability, $|v| \leq 1$, equation (2.12) is well posed as long as the scheme is stable. So, the

Lax-Friedrichs scheme qualitatively behaves like the solution of (2.12). Now, by

using the Fourier Transform of u with respect to x

$$\hat{u}(\xi, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x, t) e^{ix\xi} dx$$

and substituting into (2.12), we may obtain that (2.12) is an ODE with solution

$$\hat{u}(\xi, t) = \hat{u}(\xi, 0) e^{-D\xi^2 t} e^{ic\xi t}$$

and by using an inverse transform, we may obtain

$$u(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(\xi, 0) e^{-D\xi^2 t} e^{i(\omega(\xi)t - \xi x)} d\xi.$$

Here, we can see that the solution is of the form $e^{i(\omega(\xi)t - \xi x)}$, which represents a travelling wave with decreasing amplitude, $\hat{u}(\xi, 0)e^{-D\xi^2 t}$. The frequency is $\omega(\xi)$ and is dependent on the wave number ξ . In this case the frequency is $\omega(\xi) = c\xi$, this is also known as the dispersion relation. Also,

$$\frac{\omega(\xi)}{\xi}$$

is known as the phase velocity and gives us the wave speed of each wave.

For the Lax-Friedrichs scheme, the phase velocity is

$$\frac{\omega(\xi)}{\xi} = c.$$

Hence, the waves all travel at the same speed and so, the Lax-Friedrichs scheme is non-dispersive. However, the Lax-Friedrichs scheme suffers from dissipation, due to the wave travelling with decreasing amplitude. Hence, the Lax-Friedrichs scheme suffers from dissipation but not dispersion. We can also show that the Upwind scheme with $v > 0$ suffers from dissipation, since the truncation error of the scheme is

$$T_i^n = \frac{c}{2} [\Delta t c - \Delta x] \frac{\partial^2 u}{\partial x^2} + O(\Delta x^2) + O(\Delta t^2),$$

the scheme is a second order approximation to (2.12) with

$$D = \frac{c}{2} \Delta x (1 - v).$$

Hence, the Upwind scheme is also dissipative and since

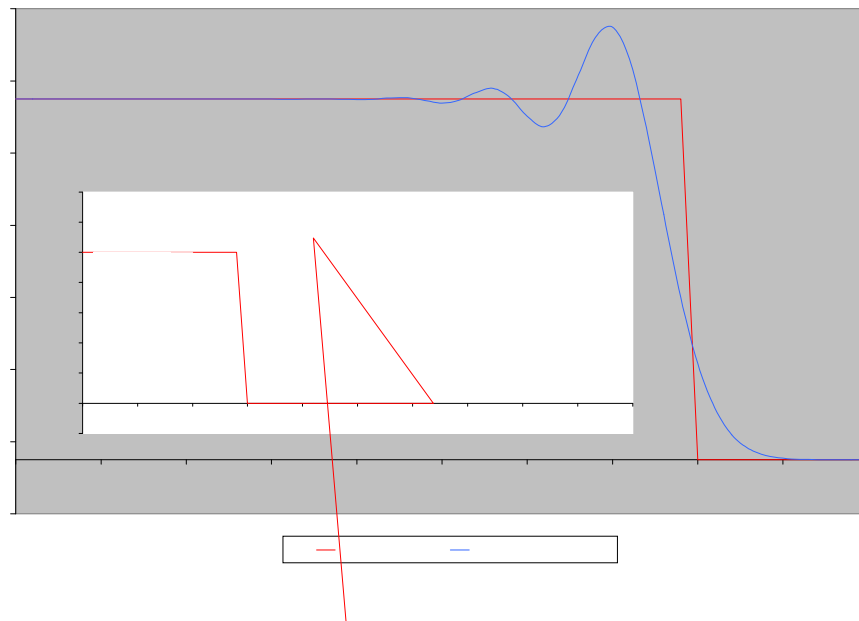
$$\frac{c}{2} \Delta x (1 - v) \left(1 + \frac{1}{v} \right) > \frac{c}{2} \Delta x (1 - v),$$

where the left-hand side represents the value of D for the Lax-Friedrichs scheme, we can see that the Lax-Friedrichs scheme is more dissipative than the Upwind scheme for $v > 0$.

Dispersion occurs when waves travel at different wave speeds and is common in all second order schemes. Figure 2-5 shows some numerical results of the Lax-Wendroff scheme applied to the advection equation with initial data

$$u(x,0) = \begin{cases} 1 & \text{if } x < 0.3 \\ 0 & \text{if } x \geq 0.3 \end{cases}$$

Here, we can see that the Lax-Wendroff scheme suffers from dispersion since oscillations are occurring in the numerical solution behind the discontinuity.



For stability, we require $|v| \leq 1 \Rightarrow v^2 \leq 1 \Rightarrow v^2 - 1 \leq 0$, which means that for $\eta < 0$,

$\frac{c}{6} \Delta x^2 \geq 0$ and since $c = 1$ and $\Delta x > 0$, verifies that $\eta < 0$ creating oscillations behind

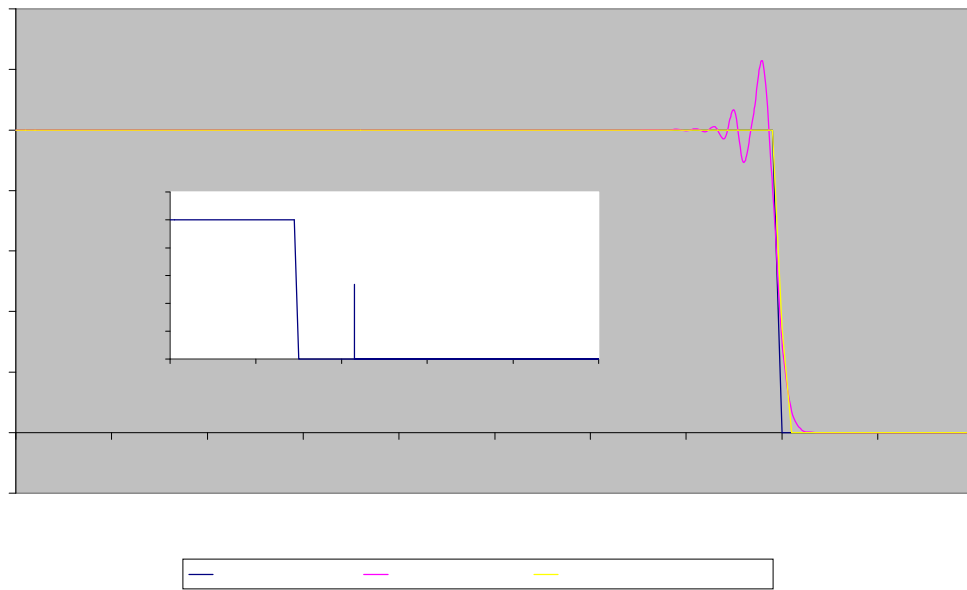
the discontinuity.

In general, all first order schemes suffer from dissipation but are non-dispersive, and all second order schemes suffer from dispersion but are non-dissipative. For a more in depth discussion on wave theory, see Whitham[9] and Ames[14].

So far we have seen that, in general, all first order schemes suffer from dissipation and all second order schemes suffer from dispersion, which creates oscillations around the discontinuity. However, there is a method which switches between a second order approximation when the region is smooth and a first order approximation when near a discontinuity. This method considerably reduces the size of the oscillations by using a first order approximation near discontinuities and is called the flux-limiter method.

Figure 2-6 shows some numerical results of the Lax-Wendroff scheme with and without the Superbee flux-limiter method applied to the scheme and with the exact solution for initial data

$$u(x,0) = \begin{cases} 1 & \text{if } x < 0.3 \\ 0 & \text{if } x \geq 0.3 \end{cases}.$$



$$u_i^{n+1} = u_i^n - \frac{s}{2}(f_{i+1}^n - f_{i-1}^n) + \frac{s}{2}[v_{i+1/2}(f_{i+1}^n - f_i^n) - v_{i-1/2}(f_i^n - f_{i-1}^n)]$$

We can re-write this equation as the first order Upwind scheme plus a second order correction term. Assuming that $v_{i+1/2} > 0$, the Lax-Wendroff scheme can be written as

$$u_i^{n+1} = u_i^n - s[f_i^n - f_{i-1}^n] - \frac{s}{2}(1 - v_{i+1/2})(f_{i+1}^n - f_i^n) + \frac{s}{2}(1 - v_{i-1/2})(f_i^n - f_{i-1}^n)$$

and we may obtain

$$F_L(u; i) = f_i^n$$

and

$$F_H(u; i) = \frac{1}{2}(1 - v_{i+1/2})(f_{i+1}^n - f_i^n).$$

Here, $F_L(u; i)$ represents the Upwind scheme and $F_H(u; i)$ represents the second order correction term. Similarly, assuming that $v_{i+1/2} < 0$, we may obtain

$$F_L(u; i) = f_{i+1}^n$$

and

$$F_H(u; i) = -\frac{1}{2}(1 + v_{i+1/2})(f_{i+1}^n - f_i^n).$$

Hence, we may obtain

$$u_i^{n+1} = u_i^n - s[F(u; i) - F(u; i-1)]$$

where

$$F(u; i) = F_L(u; i) + F_H(u; i)\phi_i$$

and

$$F_L(u; i) = \begin{cases} f_i^n & \text{if } v_{i+1/2} > 0 \\ f_{i+1}^n & \text{if } v_{i+1/2} < 0 \end{cases}$$

$$F_H(u; i) = \begin{cases} \frac{1}{2}(1 - v_{i+1/2})(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} > 0 \\ -\frac{1}{2}(1 + v_{i+1/2})(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} < 0 \end{cases}.$$

We now need to measure the smoothness of the data so that we may choose the flux-limiter to obtain second order accuracy and the TVD property. The TVD property is

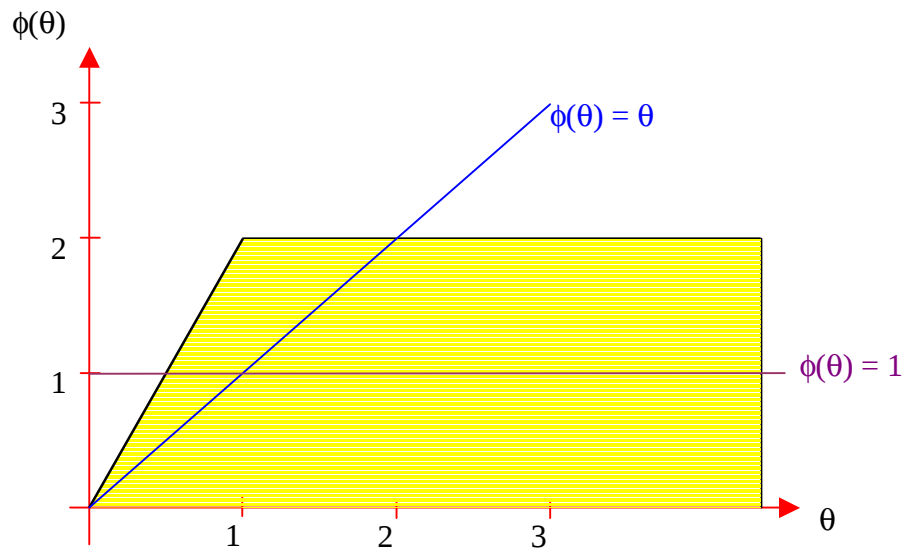


Figure 2-7: TVD region for finite difference schemes.

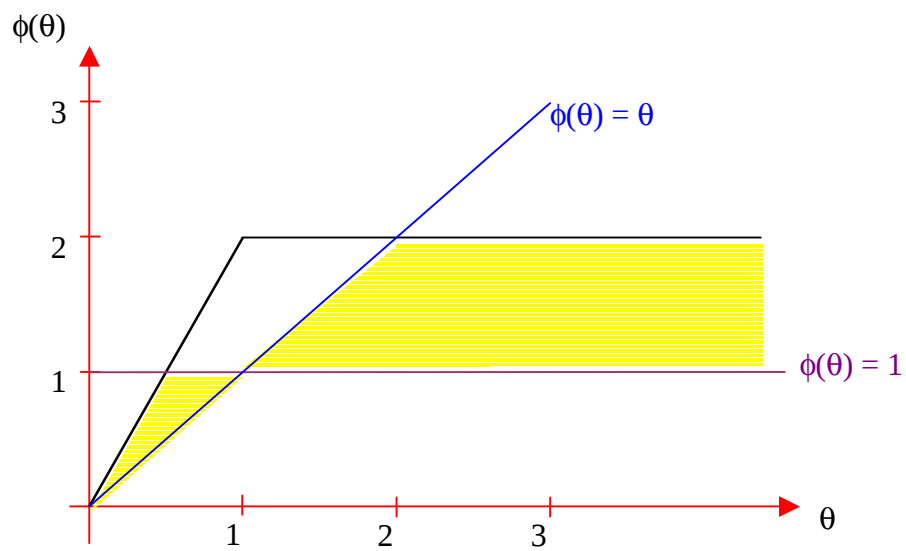


Figure 2-8: Second order TVD region for finite difference schemes.

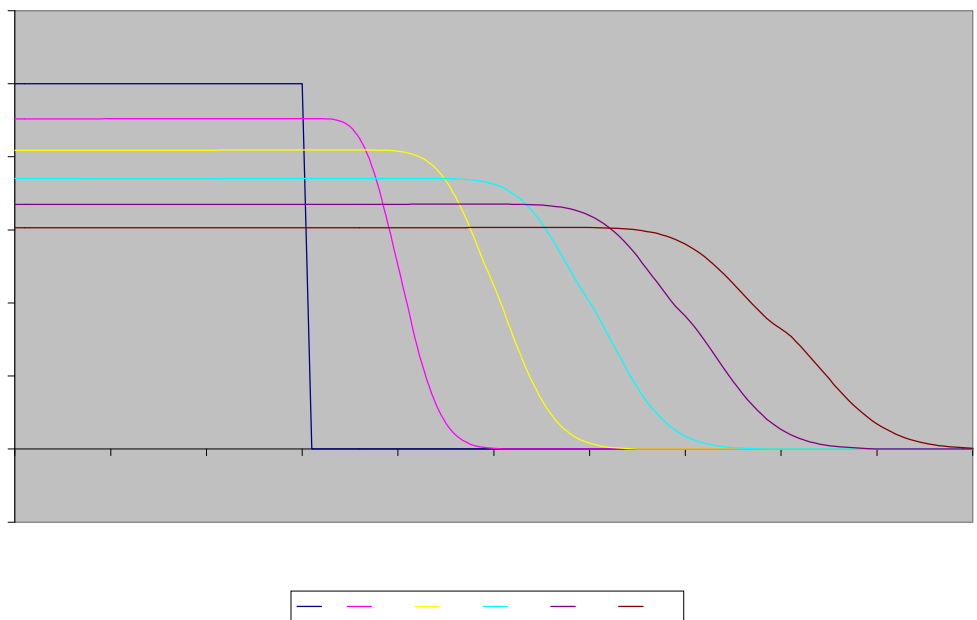
Figure 2-9: Superbee flux-limiter for finite difference schemes.

Table 2-3 lists a few flux-limiters, which

$$u(x, t) = \begin{cases} e^{-t} & \text{if } x \leq 0.3 + t \\ 0 & \text{if } x > 0.3 + t \end{cases}$$

as a test problem to illustrate some numerical results.

The most basic finite difference approach used to numerically approximate (3.1) is to ‘add’ the source term to a scheme that numerically approximates the conservation law



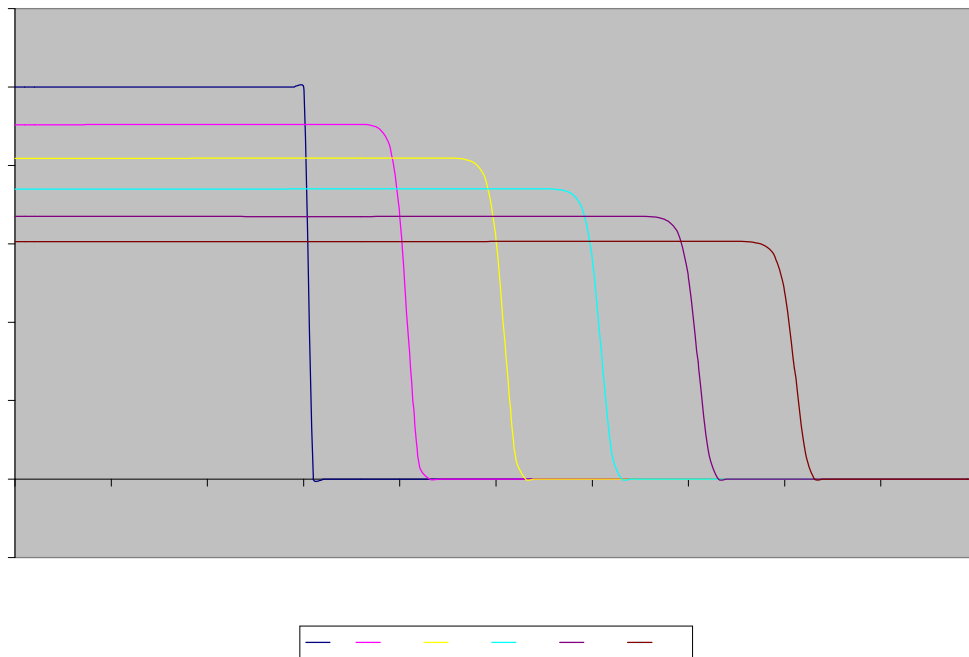
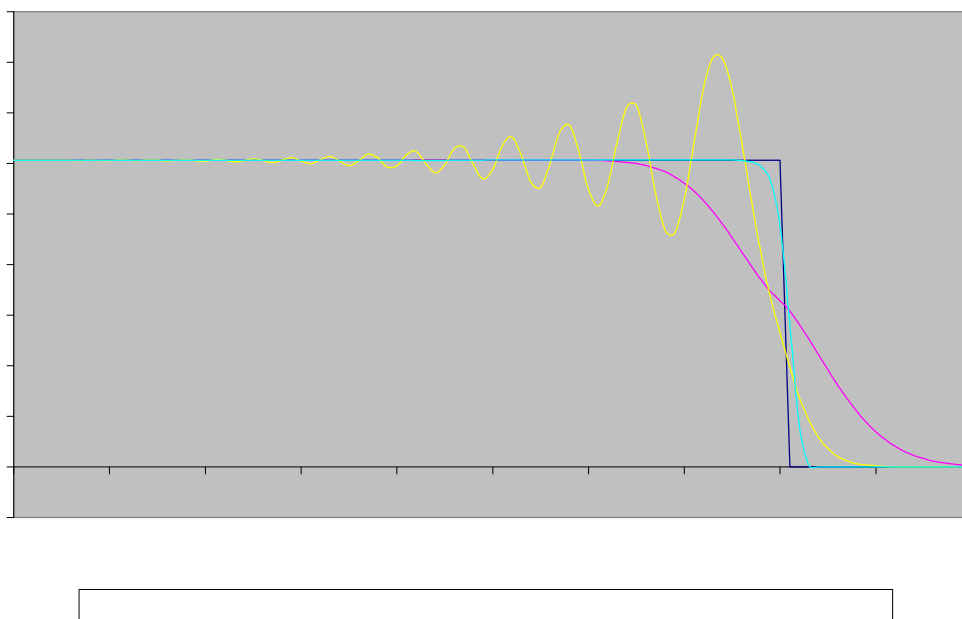


Figure 3-3: The Lax-Wendroff scheme with Superbee flux-limiter and source term 'added'.



This approach will work with all schemes discussed in Chapter 2 and, in general

$$u_i^{n+1} = u_i^{SCHEME} + \Delta t R_i^n. \quad (3.4)$$

Here, u_i^{SCHEME} represents a numerical scheme of the conservation law without a source term present. Also, by assuming the source term to be an approximation at $(i, n+1)$, we can obtain a semi-implicit scheme

$$u_i^{n+1} = u_i^{SCHEME} + \Delta t R_i^{n+1}. \quad (3.5)$$

Figure 3-1, Figure 3-2, Figure 3-3 and Figure 3-4 are all results of schemes of the form (3.4) applied to (3.2) with initial data (3.3). Figure 3-1 shows the Upwind scheme with the source term ‘added’, Figure 3-2 shows the Lax-Wendroff scheme with source term ‘added’ and Figure 3-3 shows the Lax-Wendroff scheme with Superbee flux-limiter and source term ‘added’. Figure 3-4 shows the Upwind scheme, Lax-Wendroff scheme and Lax-Wendroff scheme with Superbee flux-limiter, all with the source term explicitly ‘added’ on. Here, we can see that the Upwind scheme with source term ‘added’ suffers badly from dissipation and that the Lax-Wendroff scheme with source term added suffers badly from dispersion resulting in very large oscillations being present. The most accurate scheme was the Lax-Wendroff scheme with Superbee flux-limiter and source term ‘added’. In addition, we can see all schemes are conservative since the discontinuity was moved at the correct wave speed.

We can also use the Lax-Wendroff approach that we used in Chapter 2, Section 2, to approximate the scalar conservation law with source term. However, we must first re-write (2.11) to include the source term. Now, we can re-write (3.1) as

$$\frac{\partial u}{\partial t} + R(x, t) - \frac{\partial f(u)}{\partial x} \quad (3.6)$$

$$\Rightarrow \frac{\partial^2 u}{\partial t^2} + \left[\frac{\partial R}{\partial t} - \frac{\partial^2 f}{\partial t \partial x} + \frac{\partial R}{\partial t} - \frac{\partial^2 f}{\partial x \partial t} + \frac{\partial R}{\partial t} - \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial u} \frac{\partial u}{\partial t} \right) + \frac{\partial R}{\partial t} - \frac{\partial}{\partial x} \left(a(u) R \right) - \frac{\partial f}{\partial x} \right]$$

and we may obtain

$$\frac{\partial^2 u}{\partial t^2} + \left[\frac{\partial R}{\partial t} - \frac{\partial / a(u) R}{\partial x} + \frac{\partial}{\partial x} \left(a(u) \frac{\partial f}{\partial x} \right) \right]. \quad (3.7)$$

Now, by using Taylor's theorem

$$u_i^{n+1} \approx u_i^n + \Delta t \left(\frac{\partial u}{\partial t} \right)_i^n + \frac{\Delta t^2}{2} \left(\frac{\partial^2 u}{\partial t^2} \right)_i^n + \dots \quad (3.8)$$

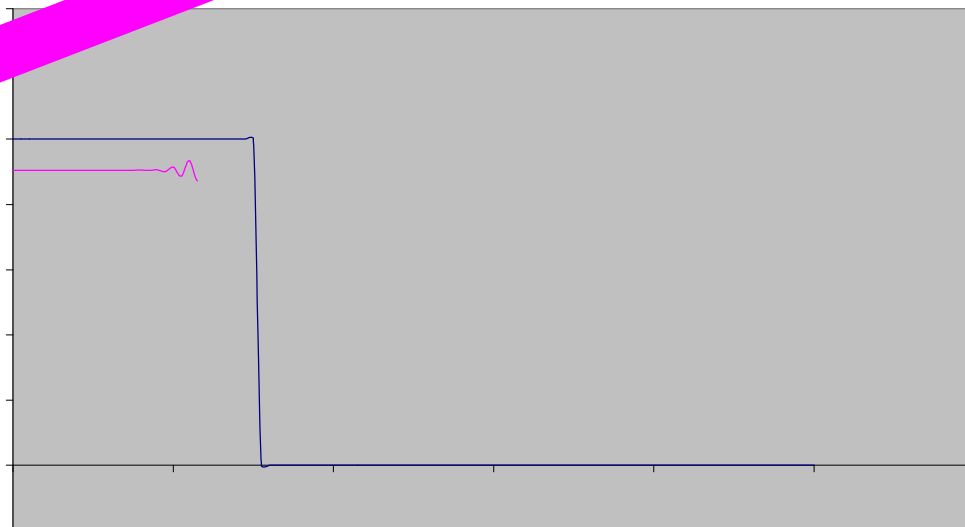
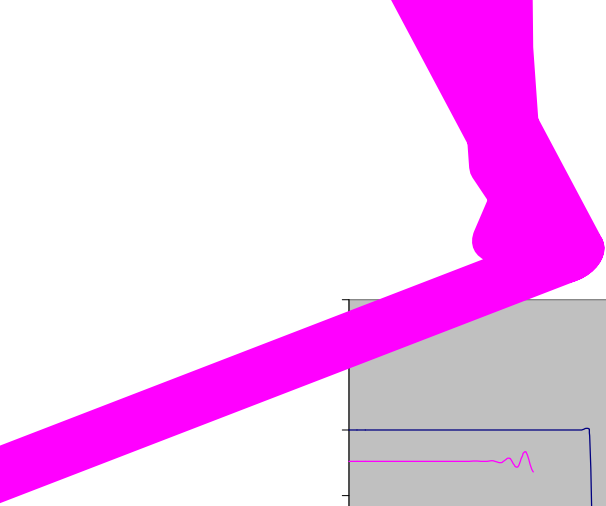
and substituting (3.6) and (3.7) into (3.8) gives

$$u_i^{n+1} \approx u_i^n + R \Delta t - \Delta t \frac{\partial f}{\partial x} + \frac{\Delta t^2}{2} \left[\frac{\partial R}{\partial t} - \frac{\partial / a(u) R}{\partial x} + \frac{\partial}{\partial x} \left(a(u) \frac{\partial f}{\partial x} \right) \right] + \dots$$

and by using central difference approximations in space and assuming that both are approximations at (i, n) then

$$\frac{\partial}{\partial t} \approx \frac{1}{2\Delta t} \left[u_{i+1/2}^{n+1} - u_{i-1/2}^{n+1} \right] - \frac{\partial}{\partial x} \left(\frac{f(u_{i+1/2}^n) - f(u_{i-1/2}^n)}{\Delta x} \right) + \frac{\partial}{\partial x} \left(a(u_i^n) \frac{f(u_{i+1/2}^n) - f(u_{i-1/2}^n)}{\Delta x} \right)$$

$$\begin{aligned}
u_i^{n+1} = & u_i^n - \frac{S}{2} \left(\frac{f_{i+1}^n - f_{i-1}^n}{f_{i+1}^n - f_i^n} + \frac{f_{i+1/2}^n - f_{i-1/2}^n}{f_i^n - f_{i-1}^n} \right) \\
& + \Delta t \left(R_i^n + \frac{\Delta t}{2} \frac{R_i^{n+1} - R_i^n}{\Delta t} - \frac{a_{i+1/2} R_{i+1/2}^n - a_{i-1/2} R_{i-1/2}^n}{\Delta x} \right)
\end{aligned}$$



$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = R(x, t) \quad (3.10)$$

which is also known as the advection transport equation. The author states that this algorithm uses a similar approach to that of the Lax-Wendroff, which can be viewed

Here we can see that (3.12) is a better approximation of the advection-diffusion equation,

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} \approx \frac{\partial}{\partial x} \left(K \frac{\partial u}{\partial x} \right) \quad \text{where} \quad K \approx \frac{\Delta x^2}{2\Delta t} (|C| - C^2),$$

and is only first order in space and time. However, we can construct a numerical estimate of the error and subtract it from (3.12) which will make the scheme second order. This approach is similar to that of the Lax-Wendroff scheme for the advection equation, which uses central differences to approximate the right hand side of (3.12) whereas MPDATA uses special properties of the Upwind scheme for approximating and compensating the error. We can re-write the error term as

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} \approx \frac{\partial (v^{(1)} u)}{\partial x}$$

where

$$v^{(1)} \approx \frac{\Delta x^2}{2\Delta t} (|C| - C^2) \frac{1}{u} \frac{\partial u}{\partial x}.$$

is a pseudo velocity. Then by using

$$u_{i+1/2} \approx \frac{1}{2} (u_{i+1} + u_i) \quad \text{and} \quad \frac{\partial u}{\partial x} \approx \frac{u_{i+1}^{(1)} - u_i^{(1)}}{\Delta x},$$

where the superscript ⁽¹⁾ denotes the first approximation of the advection equation (3.11), we may obtain the first order accurate approximation

$$V_{i+1/2}^{(1)} \approx \frac{\Delta x}{\Delta t} (|C| - C^2) \left(\frac{u_{i+1}^{(1)} - u_i^{(1)}}{u_{i+1}^{(1)} + u_i^{(1)}} \right)$$

of the pseudo velocity. In order to obtain a second order approximation, we subtract the error in the second pass

$$u_i^{n+1} \approx u_i^{(1)} - [F(u_i^{(1)}, u_{i+1}^{(1)}, V_{i+1/2}^{(1)}) - F(u_{i-1}^{(1)}, u_i^{(1)}, V_{i-1/2}^{(1)})].$$

Hence, we may now obtain the basic MPDATA algorithm

$$u_i^{n+1} \approx u_i^{(1)} - [F(u_i^{(1)}, u_{i+1}^{(1)}, V_{i+1/2}^{(1)}) - F(u_{i-1}^{(1)}, u_i^{(1)}, V_{i-1/2}^{(1)})] \quad (3.13)$$

where the pseudo velocity is

$$-\frac{1}{\lambda} \left| \frac{\partial}{\partial \lambda} \right| 0 \frac{\partial}{\partial \lambda}$$

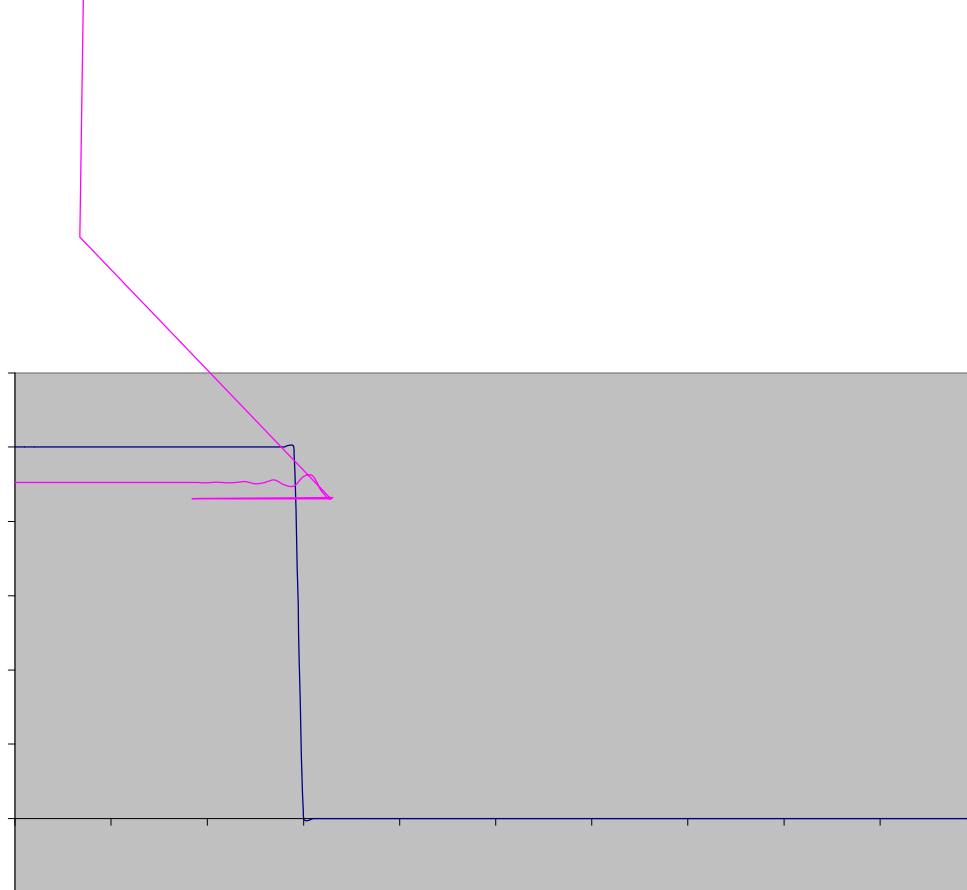
Now, by using Taylor's theorem

$$1 = \frac{1}{2} \left(\frac{1}{2} \right)^2 + \dots$$

MPDATA approach which numerically approximates (3.10) is derived by assuming the source term approximation to be at $(i, n+1/2)$ giving

$$u_i^{n+1} = MPDATA(u_i^n, C) + \Delta t R_i^{n+1/2}$$

where $MPDATA(u_i^n, C)$ corresponds to the basic MPDAT



So, the MPDATA approach is considerably less dispersive than the Lax-Wendroff approach but, near the discontinuity, the Lax-Wendroff is considerably more accurate. But overall, the MPDATA approach is a lot more accurate than the Lax-Wendroff approach for approximating (3.10). In general, the MPDATA approach (3.21) is very accurate when numerically approximating the advection-transport equation (3.10).

So far we have only looked at MPDATA algorithms for the advection-transport equation. Let us now consider MPDATA algorithms for the scalar conservation law with source term present (3.1), i.e.

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = R(x, t)$$

MPDATA can be adapted to approximate (3.1) by considering the velocity c of the advection-transport equation to no longer be a constant but to be a function of u

and Δx .

However, $w_{i+1/2}^{n+1/2}$ is unknown since w is a function of u and u is only known at the grid points (i,n) . We could approximate $w_{i+1/2}^{n+1/2}$ by using the average

$$w_{i+1/2}^{n+1/2} \approx \frac{1}{2} (w_{i+1/2}^{n+1} + w_{i+1/2}^n)$$

or by using linear interpolation

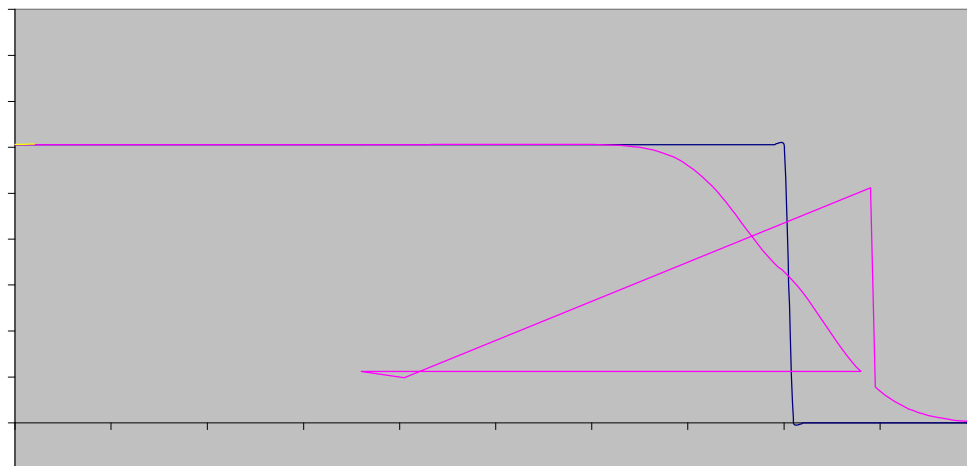
$$w_{i+1/2}^{n+1/2} \approx \frac{1}{2} (w_{i+1/2}^n + w_{i+1/2}^{n-1}).$$

If we approximate by using linear interpolation, the method would require another scheme to initially start the algorithm off, since we require a value of u at $(i,n-1)$, but if we use the average, the algorithm becomes impractical since we require the value of u at $(i,n+1)$. So far we have only considered the most basic MPDATA algorithm for the conservation law without source term and have encountered a lot of difficulties. If we now consider a source term then the corresponding MPDATA scheme is

$$u_i^{n+1} \approx MPDATA_{TM}^{\otimes} u_i^n + \frac{\Delta t}{2} R_i^n, w_{i+1/2}^{n+1/2} \Bigg] + \frac{\Delta t}{2} R_i^{n+1} \quad (3.24)$$

where $MPDATA_{TM}^{\otimes} u_i^n + \frac{\Delta t}{2} R_i^n, w_{i+1/2}^{n+1/2} \Bigg]$ corresponds to the basic MPDATA algorithm, for the conservation law without source term, discussed in Section 3.1. However, care must be taken when using this scheme since if the source term is a function of u then even more difficulties arise when using this algorithm as we will see later.

Now, by using the test problem (3.2) with initial data (3.3), we can obtain the numerical results in Figure 3-8 and Figure 3-9 and compare the numerical solution of



4 Conservation Law with Source Term $R(x,t,u)$

In Chapter 3, we discussed some finite difference schemes that numerically approximate conservation laws with a source term which is a function of x and t . In this chapter, we will discuss some finite difference schemes that numerically approximate conservation laws with a source term which is now a function of x , t and u , i.e.

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = R(x,t,u) \quad (4.1)$$

where $R(x,t,u)$ is the source term. We shall see that difficulties will arise since the source term is now a known function of u as well as x and t , resulting in the numerical approximation of the source term no longer being exact. Throughout this chapter, we will be using the following test problem considered by LeVeque and Yee[1].

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = R(u), \quad (4.2)$$

where

$$R(u) = -u(u-1) \quad u - \frac{1}{2},$$

with initial data

$$u(x,0) = \begin{cases} 1 & \text{if } x \leq 0.3 \\ 0 & \text{if } x > 0.3 \end{cases}$$

and whose exact solution is

$$u(x,t) = \begin{cases} 1 & \text{if } x \leq 0.3+t \\ 0 & \text{if } x > 0.3+t \end{cases} \quad (4.3)$$

to illustrate some numerical results.

4.1

but we would then encounter other difficulties since we only know the values of u_i^n and u_i^{n-1} , except initially when we do not know the values of u_i^{-1} . We could also

calculate the derivative analytically and then approximate the derivative, i.e. $\frac{\partial R}{\partial t}_i^n$

but the derivative of the source term may be extremely difficult to find since the source term is a function of u and u is a function of x and t . Another approach we

could take is to re-arrange $\frac{\partial R}{\partial t}_i^n$ in (4.6) by using the chain rule, i.e.

$$\frac{\partial f}{\partial t}_i^n = \frac{\partial f}{\partial u}_i^n \frac{\partial u}{\partial t}_i^n = \frac{\partial f}{\partial u}_i^n \frac{(u_i^{n+1} - u_i^n)}{\Delta t}.$$

Substituting into (4.6) gives

$$\left(\frac{\partial f}{\partial u}_i^n \right) \frac{(u_i^{n+1} - u_i^n)}{\Delta t} = \frac{\partial f}{\partial u}_i^n \frac{(u_i^{n+1} - u_i^n)}{\Delta t}.$$

We then used a forward difference approximation in space and time, to obtain

$$u_i^{n+1} = u_i^n - \frac{S}{2} (f_{i+1}^n - f_{i-1}^n) + \frac{S}{2} [v_{i+1/2} (f_{i+1}^n - f_i^n) - v_{i-1/2} (f_i^n - f_{i-1}^n)] \\ + \Delta t R_i^n + \frac{\Delta t}{2} \frac{R_i^{n+1} - R_i^n}{\Delta t} - \frac{a_{i+1/2} R_{i+1/2}^n - a_{i-1/2} R_{i-1/2}^n}{\Delta x}$$

and hence,

$$u_i^{n+1} = u_i^n - \frac{S}{2} (f_{i+1}^n - f_{i-1}^n) + \frac{S}{2} [v_{i+1/2} (f_{i+1}^n - f_i^n) - v_{i-1/2} (f_i^n - f_{i-1}^n)] \\ + \frac{\Delta t}{2} [R_i^n + R_i^{n+1}] - \frac{\Delta t}{4} [v_{i+1/2} (R_{i+1}^n - R_i^n) - v_{i-1/2} (R_i^n - R_{i-1}^n)]$$

However, if the source term is now also a function of u , then (4.8) becomes semi-implicit since we no longer know the value of R_i^{n+1} . We could replace R_i^{n+1} with (4.6) as we did in the previous sub-section, but this would only create more problems. However, we could replace R_i^{n+1} with

$$R_i^{n+1} \approx R_i^n + (u_i^{n+1} - u_i^n) \frac{\partial R}{\partial u}_i^n + \dots$$

and obtain

$$1 - \frac{\Delta t}{2} \frac{\partial R}{\partial u}_i^n u_i^{n+1} = u_i^n - \frac{S}{2} (f_{i+1}^n - f_{i-1}^n) + \frac{S}{2} [v_{i+1/2} (f_{i+1}^n - f_i^n) - v_{i-1/2} (f_i^n - f_{i-1}^n)] \\ + \Delta t R_i^n - \frac{u_i^n}{2} \frac{\partial R}{\partial u}_i^n - \frac{\Delta t}{4} [v_{i+1/2} (R_{i+1}^n - R_i^n) - v_{i-1/2} (R_i^n - R_{i-1}^n)]$$

the Lax-Wendroff approach for approximating (4.1). We can also apply flux-limiter methods to the Lax-Wendroff approach and obtain

$$1 - \frac{\Delta t}{2} \frac{\partial R}{\partial u}_i^n u_i^{n+1} = u_i^n - s[F(u; i) - F(u; i-1)] + \Delta t R_i^n - \frac{u_i^n}{2} \frac{\partial R}{\partial u}_i^n \\ - \frac{\Delta t}{4} [v_{i+1/2} (R_{i+1}^n - R_i^n) - v_{i-1/2} (R_i^n - R_{i-1}^n)] \quad (4.8)$$

where

$$F(u; i) = F_L(u; i) + F_H(u; i) \phi_i$$

and

$$F_L(u; i) = \begin{cases} f_i^n & \text{if } v_{i+1/2} > 0 \\ f_{i+1}^n & \text{if } v_{i+1/2} < 0 \end{cases}$$

$$F_H(u; i) = \frac{1}{2} \begin{cases} (1 - v_{i+1/2})(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} > 0 \\ -(1 + v_{i+1/2})(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} < 0 \end{cases}.$$

Here ϕ_i denotes the flux-limiter method, which can be any of the flux-limiters in Table 2-3. If we use (4.4) to numerically approximate the test problem (4.2), we may obtain the results shown in Figure 4-2. Here, we can see that the Lax-Wendroff approach has numerically approximated (4.2) very accurately. Also, the numerical results in 7(ve)j--r.6487--11

and by substituting into (3.24), to obtain

$$1 - \frac{\Delta t}{2} \frac{\partial R}{\partial u_i} u_i^{n+1} = MPDATA(u_i^n, C) u_i^n + \frac{\Delta t}{2} R_i^n, w_{i+1/2}^{n+1/2} + \frac{\Delta t}{2} R_i^n - u_i^n \frac{\partial R}{\partial u_i} \quad (4.9)$$

where $MPDATA(u_i^n, C)$ corresponds to the basic MPDATA algorithm with flux-limiter

$$u_i^{n+1} = u_i^{(1)} - [F(u_i^{(1)}, u_{i+1}^{(1)}, V_{i+1/2}^{(1)})\phi_i - F(u_{i-1}^{(1)}, u_i^{(1)}, V_{i-1/2}^{(1)})\phi_{i-1}]$$

whose pseudo velocity is

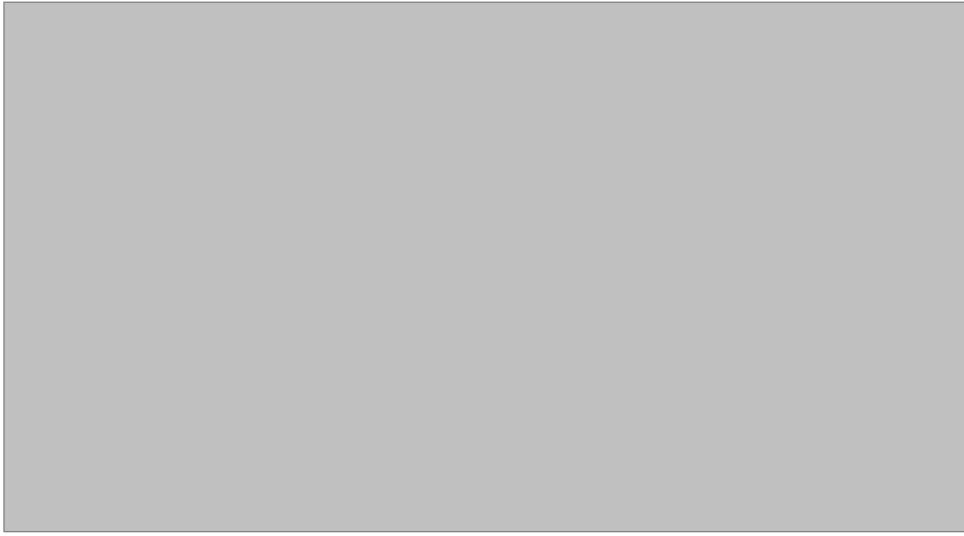
$$V_{i+1/2}^{(1)} = \frac{\Delta x}{\Delta t} (w_{i+1/2}^{n+1/2} - [w_{i+1/2}^{n+1/2}]) \frac{u_{i+1}^{(1)} - u_i^{(1)}}{u_{i+1}^{(1)} + u_i^{(1)}} - w_{i+1/2}^{n+1/2} [w_{i+3/2}^{n+1/2} - w_{i-1/2}^{n+1/2}],$$

the first order approximation is

$$u_i^{(1)} = u_i^n - [F(u_i^n, u_{i+1}^n, w_{i+1/2}^{n+1/2}) - F(u_{i-1}^n, u_i^n, w_{i-1/2}^{n+1/2})],$$

$$w_{i+1/2}^{n+1/2} = \frac{1}{2} (3w_{i+1/2}^n - w_{i-1/2}^n)$$

and ϕ_i can be any of the flux-limiters listed in Table 2-3. Here, we can see that the MPDATA approach for numerically approximating (4.1) is becoming very impractical. This is because we are approximating approximations resulting in the accuracy of the algorithm reducing rapidly and we also require another scheme to start the algorithm off. However, MPDATA can be used to accurately numerically approximate the



Here we can see that the first term on the right hand side of (4.11) can cause difficulties if the Courant number is not an integer. This is because we are using a mesh where we only know the values at the grid points $(i\Delta x, n\Delta t)$ and if v is not an integer, then the value of u required no longer lies on the mesh and is thus unknown. However, Roe[6] deduced that the only reasonable way to approximate this term is to use

$$u((i-v)\Delta x, n\Delta t) = u_i^n - v(u_i^n - u_{i-1}^n)$$

$$\alpha = \frac{1}{2}$$

then we may obtain a scheme that is second order accurate in the steady state, i.e.

$$u_i^{n+1} = u_i^n - \begin{cases} v(u_i^n - u_{i-1}^n) - \frac{\Delta t}{2} [R_i^n + R_{i-1}^n] & \text{if } v > 0 \\ v(u_{i+1}^n - u_i^n) - \frac{\Delta t}{2} [R_i^n + R_{i+1}^n] & \text{if } v < 0 \end{cases}.$$

Unfortunately, this scheme is only a first order approximation to

$$(\quad) - (\quad) (\quad) (c(t-s)s) ds$$

Scheme	Interval Of Absolute Stability ($c > 0$)	Interval Of Absolute Positivity ($c > 0$)
$\alpha = 0$	$v + \frac{\lambda \Delta t}{2} \leq 1$	$v + \lambda \Delta t \leq 1$
$\alpha = v$	$v \leq 1$ and $\frac{\lambda \Delta t}{2} \leq 1$	$v \leq 1$ and $\lambda \Delta t \leq 1$
$\alpha = \frac{1}{2}v$ (for $R(x)$ only)	$v \leq 1$ and $\frac{\lambda \Delta t}{2} \leq 1$	$\frac{\lambda \Delta t}{2} \leq 1$ and $v \leq \frac{1 - \frac{\lambda \Delta t}{2}}{1 - \frac{\lambda \Delta t}{2}}$
$\alpha = \frac{1}{2}$	$v \leq 1$ and $\frac{\lambda \Delta t}{2} \leq 1$	$v + \frac{\lambda \Delta t}{2} \leq 1$ and $\frac{\lambda \Delta t}{2} \leq v$

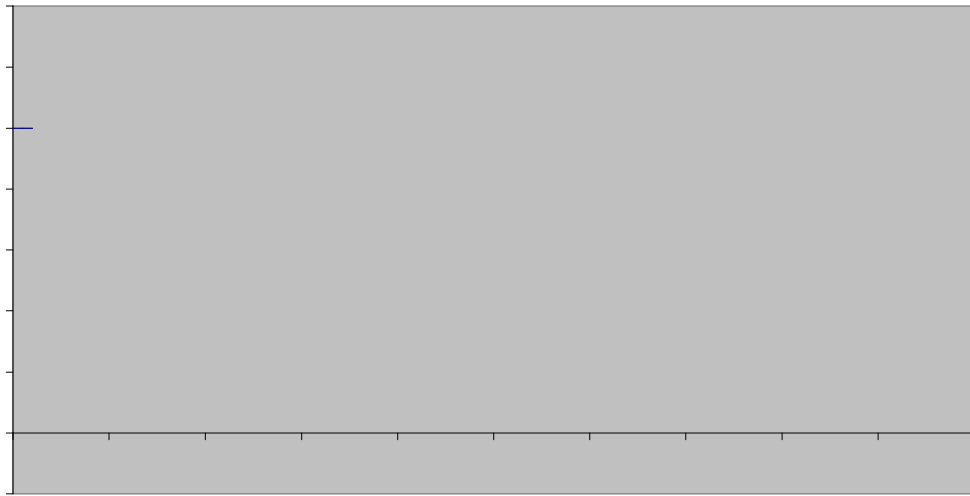
$$\begin{aligned}
u_i^{n+1} = u_i^n - & s(f_i^n - f_{i-1}^n) + \frac{s}{2} \left[(1 - v_{i+1/2}) (f_{i+1}^n - f_i^n) - (1 - v_{i-1/2}) (f_i^n - f_{i-1}^n) \right] \\
& - \Delta t R((1 - \alpha)_{X_i} + \alpha_{X_{i-1}}, (1 - \alpha)u_i^n + \alpha u_{i-1}^n) \quad \text{if } v_{i+1/2} > 0 \\
& s(f_{i+1}^n - f_i^n) - \frac{s}{2} \left[(1 + v_{i+1/2}) (f_{i+1}^n - f_i^n) - (1 + v_{i-1/2}) (f_i^n - f_{i-1}^n) \right] \\
& - \Delta t R((1 - \alpha)_{X_i} + \alpha_{X_{i+1}}, (1 - \alpha)u_i^n + \alpha u_{i+1}^n) \quad \text{if } v_{i-1/2} < 0
\end{aligned}$$

Also, we can apply the flux-limiter method to obtain

$$u^{+1} = u - s[F(u; i) - F(u; i-1)] + \Delta t \begin{cases} (1 - \alpha)R_i^n + \alpha R_{i-1}^n & \text{if } v_{i+1/2} > 0 \\ (1 - \alpha)R_i^n + \alpha R_{i+1}^n & \text{if } v_{i-1/2} < 0 \end{cases} \quad \text{if}$$

4.2.3 Some Numerical Results for the Explicit Upwind Approach

Now, by using (4.24) to numerically approximate the test problem (4.2), we may obtain the numerical results in Figure 4-4.



4.3 Implicit Upwind Approach

Embed, Goodman and Majda[2] discussed some different approaches for numerically approximating

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = R(x, u) \quad (4.25)$$

where the source term must be of the form

$$R(x, u) = e(x)g(u).$$

They discussed the first order Engquist-Osher scheme, with switching through zero, and a second order Upwind approach based on the Engquist-Osher approach. Here, we will use the analysis of Embed, Goodman and Majda[2] to derive a first and second order implicit Upwind scheme with the source term ‘added’ implicitly.

4.3.1 First Order Implicit Upwind Approach

The first scheme that we will discuss is the implicit first order Upwind approach with the source term ‘added’ implicitly, i.e. ()

and, by re-arranging we may obtain

$$u_i^{n+1} + s(f_i^{n+1} - f_{i-1}^{n+1}) - \Delta t R_i^{n+1} = u_i^n$$

and since $R(x, u) = e(x)g(u)$

$$u_i^{n+1} + s(f_i^{n+1} - f_{i-1}^{n+1}) - \Delta t e_i g_i^{n+1} = u_i^n. \quad (4.27)$$

However, the second and third terms on the

$$\begin{array}{cccccccc}
\ll & & & & & & & \\
0 & 0 & & 0 & & & & \\
& b_0 & d_0 & & \ll & & u_0^{n+1} - u_0^n & G_0 - a_0(u_{-1}^{n+1} - u_{-1}^n) \\
& a_1 & b_1 & d_1 & 0 & 0 & u_1^{n+1} - u_1^n & G_1 \\
& 0 & a_2 & b_2 & d_2 & 0 & u_2^{n+1} - u_2^n & G_2 \\
& & & & & & & = \\
& 0 & 0 & a_{I-2} & b_{I-2} & d_{I-2} & 0 & u_{I-2}^{n+1} - u_{I-2}^n & G_{I-2} \\
& 0 & 0 & 0 & a_{I-1} & b_{I-1} & d_{I-1} & u_{I-1}^{n+1} - u_{I-1}^n & G_{I-1} \\
& 0 & 0 & 0 & 0 & a_I & b_I & u_I^{n+1} - u_I^n & G_I - d_I(u_{I+1}^n - u_{I+1}^n)
\end{array}$$

$$\begin{aligned}
& (u_i^{n+1} - u_i^n) \left[1 - \frac{s}{2}(3 - v_{i-1/2}) \right] \frac{f_i^n}{u_i} \Delta t e_i \frac{\partial g_i^n}{\partial u_i} \\
& - \frac{s}{2} (u_{i-1}^{n+1} - u_{i-1}^n) [4 - v_{i-1/2} - v_{i-3/2}] \frac{\partial f_{i-1}^n}{\partial u_{i-1}} + \frac{s}{2} (u_{i-2}^{n+1} - u_{i-2}^n) [1 - v_{i-3/2}] \frac{\partial f_{i-2}^n}{\partial u_{i-2}} \\
& = \Delta t e_i g_i^n - \frac{s}{2} [(3 - v_{i-1/2})(f_i^{n+1} - f_{i-1}^{n+1}) - (1 - v_{i-3/2})(f_{i-1}^{n+1} - f_{i-2}^{n+1})]
\end{aligned}$$

$$\begin{aligned}
a_i &= \begin{cases} -\frac{s}{2}[4-v_{i-1/2}-v_{i-3/2}] \frac{\partial f}{\partial u}_{i-1}^n & \text{if } v_{i+1/2} > 0 \\ 0 & \text{if } v_{i+1/2} < 0 \end{cases}, \\
b_i &= 1 - \Delta t e_i \frac{\partial g}{\partial u}_i^n - \frac{s}{2} \frac{\partial f}{\partial u}_i^n \begin{cases} v_{i-1/2} - 3 & \text{if } v_{i+1/2} > 0 \\ v_{i+1/2} + 3 & \text{if } v_{i+1/2} < 0 \end{cases}, \\
d_i &= \begin{cases} 0 & \text{if } v_{i+1/2} > 0 \\ \frac{s}{2}[4+v_{i+1/2}+v_{i+3/2}] \frac{\partial f}{\partial u}_{i+1}^n & \text{if } v_{i+1/2} < 0 \end{cases}
\end{aligned}$$

and

$$k_i = \begin{cases} 0 & \text{if } v_{i+1/2} > 0 \\ -\frac{s}{2}[1+v_{i+3/2}] \frac{\partial f}{\partial u}_{i+2}^n & \text{if } v_{i+1/2} < 0 \end{cases}.$$

Here, A is a penta-diagonal matrix and unfortunately requires a lot more calculations than before resulting in the interval of absolute stability and the accuracy of the scheme being reduced. However, Embid, Goodman and Majda[2] discussed using the first order tri-diagonal matrix for the second order Upwind approach based on the Engquist-Oscher scheme to increase the interval of absolute stability. Using the same approach, we can obtain the second order implicit Upwind approach, i.e.

$$- \left(\begin{array}{c} - \end{array} \right)$$

$$=$$

$$- \left(\begin{array}{c} - \end{array} \right)$$

$$a_i = \begin{cases} -s \frac{\partial f}{\partial u_{i-1}} & \text{if } v_{i+1/2} > 0 \\ 0 & \text{if } v_{i+1/2} < 0 \end{cases}, \quad d_i = \begin{cases} 0 & \text{if } v_{i+1/2} > 0 \\ s \frac{\partial f}{\partial u_{i+1}} & \text{if } v_{i+1/2} < 0 \end{cases}$$

and

$$b_i = 1 + \text{sgn}(v_{i+1/2})s \frac{\partial f}{\partial u_i} - \Delta t e_i \frac{\partial g}{\partial u_i}.$$

They also state that by using the first order matrix, the interval of absolute stability

000e5TD<007775 5TD<007775 5TD<0077diml7TD(007r m5TD<007775 5TD1.15 TD.rdsa) Wa5-95

Implicit Upwind approach with $dx = 0.01$, $dt = 0.001$ and $t = 0.5$.

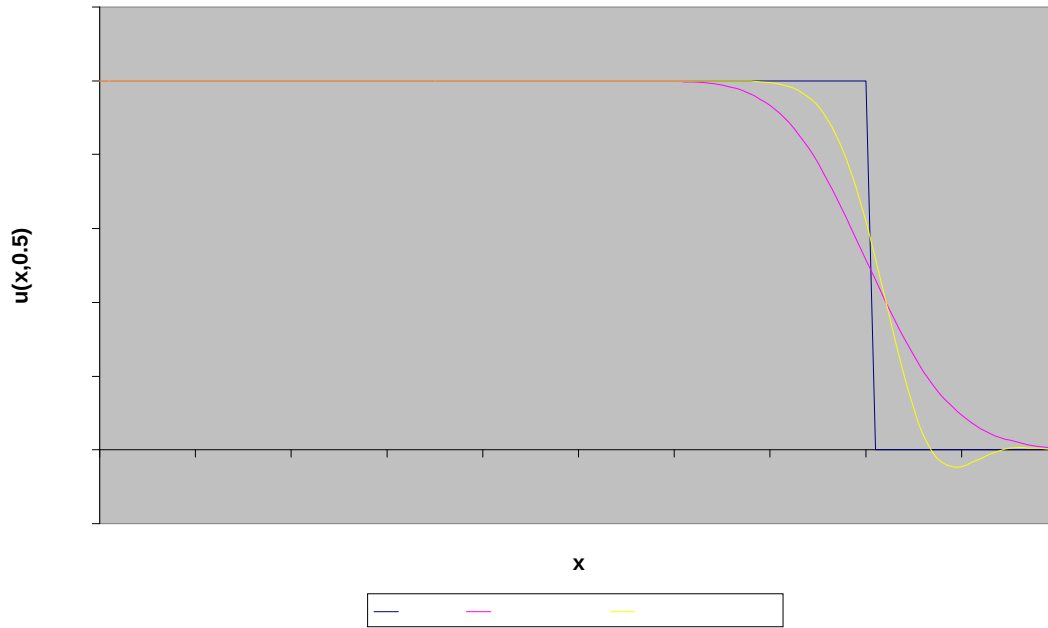


Figure 4-5: Comparison of schemes based on the implicit Upwind approach.

4.4 LeVeque and Yee's MacCormack Approach

In this sub-section we will look at how the MacCormack scheme, which is listed in Table 2-1, can be adapted to numerically approximate (4.1). This approach is frequently used and was discussed by Yee[5], LeVeque and Yee[1] and Embid, Goodman and Majda[2].

4.4.1 Explicit MacCormack Approach

We can approximate (4.1) by expanding on the explicit MacCormack scheme. The MacCormack method is the Lax-Wendroff scheme re-written in predictor-corrector form, i.e.

$$u_i^{n+1} = \frac{1}{2}(u_i^n + u_i^{(1)}) - \frac{s}{2}[f_i^{(1)} - f_{i-1}^{(1)}] \quad (4.35)$$

where

$$u_i^{(1)} = u_i^n - s(f_{i+1}^n - f_i^n)$$

for the conservation law without source term. We can adapt (4.35) to include the source terms explicitly and still maintain second order accuracy, i.e.

$$u^{n+1} = \frac{1}{2}(u^n + u^{(1)}) - \frac{s}{2}[f^{(1)} - f^n] + \Delta t \frac{R_i^{(1)}}{2}$$

4.4.2 Semi-Implicit MacCormack Approach

Yee[5] and LeVeque and Yee[1] also discuss an approach which considers the source term approximation to be at $(i,n+1)$ but still uses the explicit MacCormack scheme resulting in a semi-implicit scheme. This approach is obtained by re-writing (4.36) as

$$u_i^{n+1} = u_i^n + \frac{1}{2} [(u_i^{(2)} - u_i^{(1)}) + (u_i^{(1)} - u_i^n)]$$

where

$$(u_i^{(2)} - u_i^{(1)}) = -\frac{s}{2} [f_i^{(1)} - f_{i-1}^{(1)}] + \Delta t [R_i^{n+1}]^{(1)}$$

and

$$(u_i^{(1)} - u_i^n) = -s(f_{i+1}^n - f_i^n) + \Delta t R_i^{n+1}.$$

Now by using Taylor's theorem

$$R_i^{n+1} \approx R_i^n + (u_i^{n+1} - u_i^n) \frac{\partial R}{\partial u}_i^n + \dots$$

we may obtain

$$u_i^{n+1} = u_i^n + \frac{1}{2} [(u_i^{(2)} - u_i^{(1)}) + (u_i^{(1)} - u_i^n)]$$

where

$$(u_i^{(2)} - u_i^{(1)}) = -\frac{s}{2} [f_i^{(1)} - f_{i-1}^{(1)}] + \Delta t R_i^{(1)} + \Delta t \bar{\theta} (u_i^{(2)} - u_i^{(1)}) \frac{\partial R}{\partial u}_i^{(1)}$$

Yee[5] discusses various choices of $\bar{\theta}$ and deduces that we can obtain second order by setting $\bar{\theta} = \frac{1}{2}$. We can also apply the modified flux described in the previous sub-section by re-writing (4.38) as

$$u_i^{n+1} = u_i^{(2)} + [\phi_{i+1/2}^{(2)} - \phi_{i-1/2}^{(2)}] \quad (4.39)$$

where

$$1 - \Delta t \bar{\theta} \frac{\partial R}{\partial u}_i^n (u_i^{(2)} - u_i^{(1)}) = -s(f_{i+1}^{(1)} - f_i^{(1)}) + \Delta t R_i^{(1)},$$

$$1 - \Delta t \bar{\theta} \frac{\partial R}{\partial u}_i^n (u_i^{(1)} - u_i^n) = -s(f_{i+1}^n - f_i^n) + \Delta t R_i^n$$

and

$$\phi_{i+1/2}^{(2)} = \frac{1}{2} [|v_{i+1/2}| - v_{i+1/2}^2] (u_{i+1}^{(2)} - u_i^{(2)} - Q_{i+1/2})$$

and $Q_{i+1/2}$ is chosen from Table 4-2.

4.4.3 LeVeque and Yee's Splitting Method for the MacCormack Approach

LeVeque and Yee[1] also discuss a splitting method for the semi-implicit MacCormack approach discussed in this sub-section. The splitting method alternates between solving the conservation law with no source term

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \quad (4.40)$$

and then solving the ordinary differential equation

$$\frac{\partial u}{\partial t} = R(x, t, u), \quad (4.41)$$

i.e.

$$u_i^{n+1} = S_f(\Delta t) S_\psi(\Delta t) u_i^n$$

where $S_f(\Delta t)$ denotes the numerical solution of (4.40) and $S_\psi(\Delta t)$ denotes the numerical solution of (4.42). LeVeque and Yee[1] also state that in order to obtain second order accuracy, we can use the Strang splitting [11] to obtain

$$u_i^{n+1} = S_\psi \frac{\Delta t}{2} S_f(\Delta t) S_\psi \frac{\Delta t}{2} u_i^n \quad (4.42)$$

where $S_f(\Delta t)$ denotes the numerical solution of (4.40) and $S_\psi \frac{\Delta t}{2}$ denotes the numerical solution of (4.42). They also give a splitting method of the form (4.42) for the semi-implicit MacCormack approach with TVD discussed in the previous subsection:

$$\begin{aligned} S_\psi \frac{\Delta t}{2} : \quad & 1 - \frac{\Delta t}{4} \frac{\partial R}{\partial u}_i^n (u_i^* - u_i^n) = \frac{\Delta t}{2} R_i^n \\ & u_i^* = u_i^n + (u_i^* - u_i^n). \\ S_k(\Delta t): \quad & (u_i^{(1)} - u_i^*) = -s(f_i^* - f_{i-1}^*) \\ & u_i^{(1)} = u_i^* + (u_i^{(1)} - u_i^*) \\ & (u_i^{(2)} - u_i^{(1)}) = -s(f_{i+1}^{(1)} - f_i^{(1)}) \\ & u_i^{(2)} = u_i^* + \frac{1}{2} [(u_i^{(2)} - u_i^{(1)}) + (u_i^{(1)} - u_i^*)] \\ & [\end{aligned}$$

4.4.4 Some Numerical Results for the MacCormack Approach

If we apply (4.37), (4.39) and (4.43) with and without TVD to the test problem (4.2), we may obtain the numerical results in Figure 4-6 and Figure 4-7. Here, we can see that all three approaches give practically the same results but, as with the Lax-Wendroff approach, this will not always be the case.

Throughout this chapter, we have seen that there are a variety of methods used for approximating conservation laws with a source term present, which is a function of x , t and

5 Some Numerical Results

In this chapter, we will apply the different approaches discussed throughout this dissertation to a specific test problem (5.1) which was considered by LeVeque and Yee[1], i.e.

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = R(u), \quad (5.1)$$

where

$$R(u) = -\mu u(u-1) \quad u - \frac{1}{2},$$

with initial data

$$u(x,0) = \begin{cases} 1 & \text{if } x \leq 0.3 \\ 0 & \text{if } x > 0.3 \end{cases}$$

and whose exact solution, which is shown in Figure 5-1, is

$$u(x,t) = \begin{cases} 1 & \text{if } x \leq 0.3+t \\ 0 & \text{if } x > 0.3+t \end{cases} \quad (5.2)$$

Here, $\Delta t \mu$ determines the stiffness of (5.1) and as μ becomes greater than 1 the propagation speed of some approaches can be greatly affected. When $\Delta t \mu > 1$, the source term is said to be stiff since, for most approaches, we can no longer choose an adequate step-size in time to produce accurate results. A stiff source term moves the discontinuity to a cell boundary for each time step resulting in the discontinuity being moved at entirely the wrong speed. For example, if we apply the Lax-Wendroff approach (4.8) to the test problem (5.1), with $\mu = 1, 10, 100$ and 1000 , then we may obtain the numerical results in Figure 5-2, Figure 5-3, Figure 5-4 and Figure 5-5

respectively. Here, we can see that as $\Delta t \mu$ increases, the source term becomes stiff and the numerical approximation becomes less and less accurate. This is because as $\Delta t \mu$ increases, the discontinuity moves slower and slower which means that when the source term is stiff, the scheme is no longer conservative. However, not all of the schemes discussed in Chapter 4 will exhibit this behaviour, as we will see later.

We will use test problem (5.1) to compare the results of some of the methods discussed throughout this dissertation to ascertain which approach produces the most accurate results by seeing which approaches are conservative as the source term becomes stiff.

Name Of Approach	Reference No.	Order	Paper
Explicit ‘adding’	(4.5)	1 / 2	-
Semi-implicit ‘adding’	(4.7)	1 / 2	-
Lax-Wendroff	(4.8)	2	-
MPDATA	(4.9)	2	Smolarkiewicz + Margolin[3]
Roe’s Explicit Upwind I	(4.21)	1	Roe[6], Vazquez + Bermudez[4]
Roe’s Explicit Upwind II	(4.23)	2	Roe[6], Vazquez + Bermudez[4]
Implicit Upwind I	(4.30)	1	Embid, Goodman + Majda[2]
Implicit Upwind II	(4.34)	2	Embid, Goodman + Majda[2]
Explicit MacCormack	(4.37)	2	Yee[5], LeVeque + Yee[1], Embid, Goodman + Majda[2]
Semi-Implicit MacCormack	(4.39)	2	Yee[5], LeVeque + Yee[1]
Splitting Method (MacCormack)	(4.43)	2	LeVeque + Yee[1]

Table 5-1: Some different approaches for numerically approximating (5.1).

We will be discussing the results of the schemes listed in Table 5-1 which can also be found in Appendix A where they are written in full.

scheme being impractical for approximating conservation laws with a stiff source term.

5.2 Lax-Wendroff approach

The MPDATA approach is the first method that has ensured conservation when the source term is stiff. This is because the MPDATA approach compensates for the terms in the truncation error due to the source term approximation resulting in a conservative method even when the source term is stiff.

5.4 Roe's Upwind Approach

Now, by applying (4.21) and (4.23) to the test problem (5.1), we may obtain the numerical results in Figure 5-12. Here, we can see that by using (4.21), the method

to the discontinuity moving too slow resulting in the discontinuity being at $x = 0.6$

5.7 Overall Comparison

So far, we have looked at each approach individually but we will now compare all of the different approaches listed in Table 5-1 to see which approach produced the most accurate numerical results when applied to the test problem (5.1).

5.7.1 First Order Comparison

If we apply all the first order approaches listed in Table 5-1 to the test problem (5.1), then we may obtain the numerical results in Figure 5-18. Here, we can see that Roe's Upwind approach has obtained the most accurate numerical approximation. However, Roe's Upwind approach is not very accurate since the numerical approximation moved the discontinuity too fast resulting in the discontinuity being at $x = 0.85$ when $t = 0.5$ instead of at $x = 0.8$ when $t = 0.5$. The explicit 'adding'

aTabsc

MacCormack approach, explicit ‘adding’ approach, Lax-Wendroff approach, explicit MacCormack approach and Splitting method based on the MacCormack approach all gave similar inaccurate results. They all moved the discontinuity too slow resulting in the discontinuity being at approximately $x = 0.45$ when $t = 0.5$ instead of at $x = 0.8$ when $t = 0.5$. Also, notice how Roe’s Upwind approach failed to move the discontinuity at all. Hence, the most accurate second order scheme was the implicit Upwind approach followed by the MPDATA approach with the implicit Upwind giving very accurate results and the MPDATA approach giving accurate results. Here, most of the schemes were not conservative except for the second order implicit Upwind approach and the MPDATA approach.

5.7.3 Second Order with TVD Comparison

If we apply all the first order approaches listed in Table 5-1 to the test problem (5.1), then we may obtain the numerical results in

failed to move the discontinuity at all in the second order comparison, also produced the second most accurate set of results. However, the results of Roe's upwind approach were not very accurate since the method moved the discontinuity too fast resulting in the discontinuity being at approximately $x = 0.9$ when $t = 0.5$. The most accurate method for the second order approach with TVD was the MPDATA approach. The MPDATA approach moved the discontinuity too slow resulting in the discontinuity being at approximately $x = 0.78$ when $t = 0.5$. All of the schemes with TVD are no longer conservative when the source term is stiff.

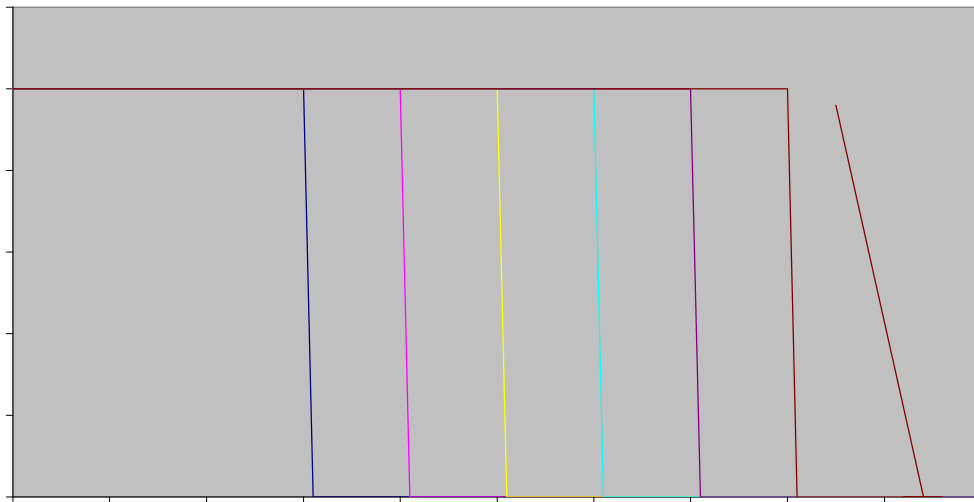
5.7.4 Conclusion

Hence, overall the second order approach with TVD did not necessarily produce more accurate results than without TVD. In fact the most accurate results were obtained by not using TVD where two of the approaches were conservative when the source term was stiff. However, some of the approaches improved when TVD was applied and others became less accurate. This is because in most cases, when TVD was applied the discontinuity would move faster. In addition, the majority of first order approaches produced extremely inaccurate results except for Roe's Upwind approach which slightly overshot the discontinuity.

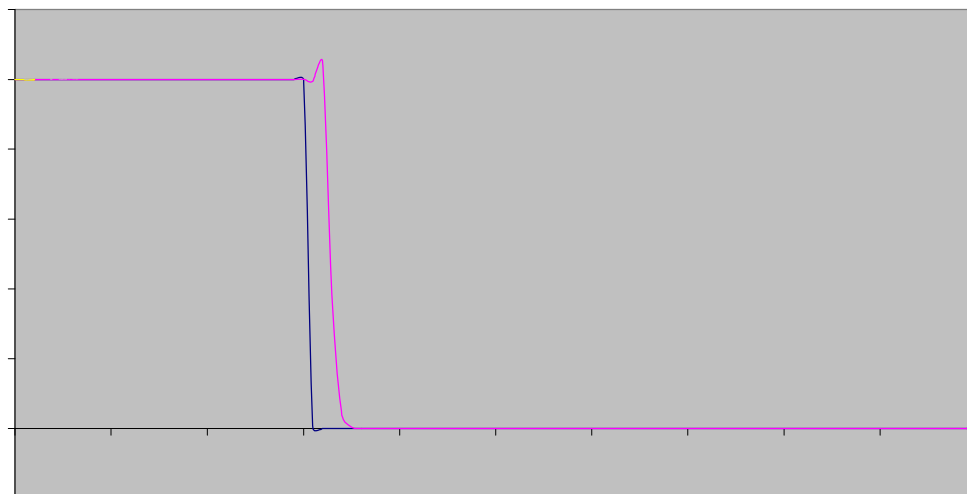
5.8 Changing the Step-Size when the Source Term is Stiff

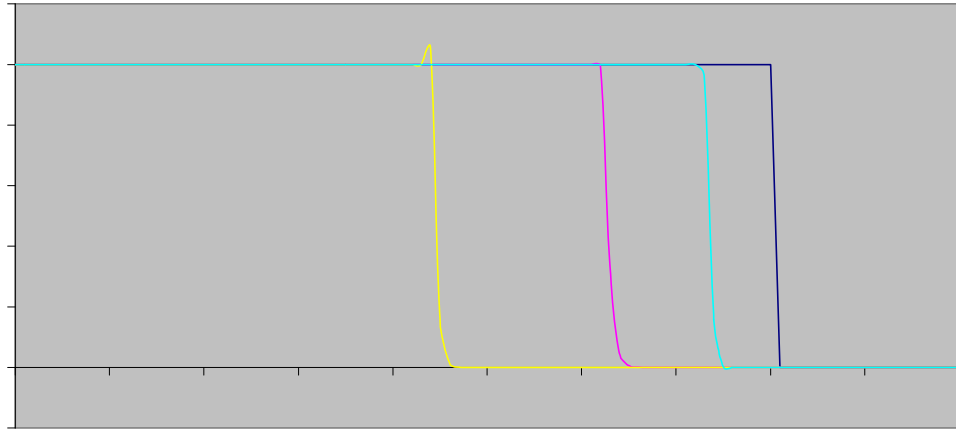
Throughout this section, we have only considered the numerical results using $\Delta x = 0.01$ and $\Delta t = 0.001$, which implies that the Courant number is $s = 0.1$. However, when the source term is stiff, the accuracy of some of the schemes can vary if the step-size is changed. For example, if we use the first order explicit Upwind approach

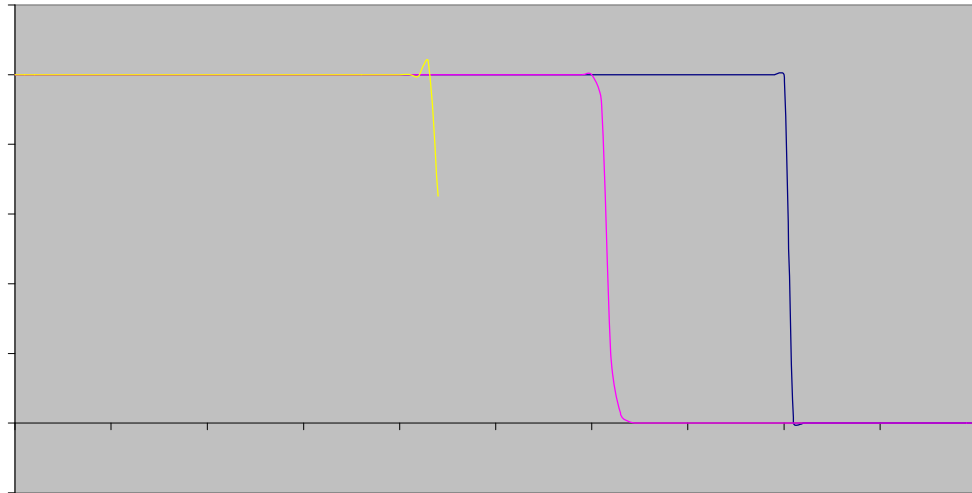
(4.21) on the test problem (5.1) with $\Delta x = 0.02$ and $\Delta t = 0.0025$, which implies that the Courant number is $s = 0.125$, then we may obtain the results in Figure 5-21. Here we would expect the results to be less accurate than the results shown in Figure 5-12 but Figure 5-21 shows that the results of the first order explicit Upwind approach are more accurate since the approach moved the discontinuity slower than in Figure 5-12. I.e. when we used $\Delta x = 0.01$ and $\Delta t = 0.001$ the explicit first order Upwind approach

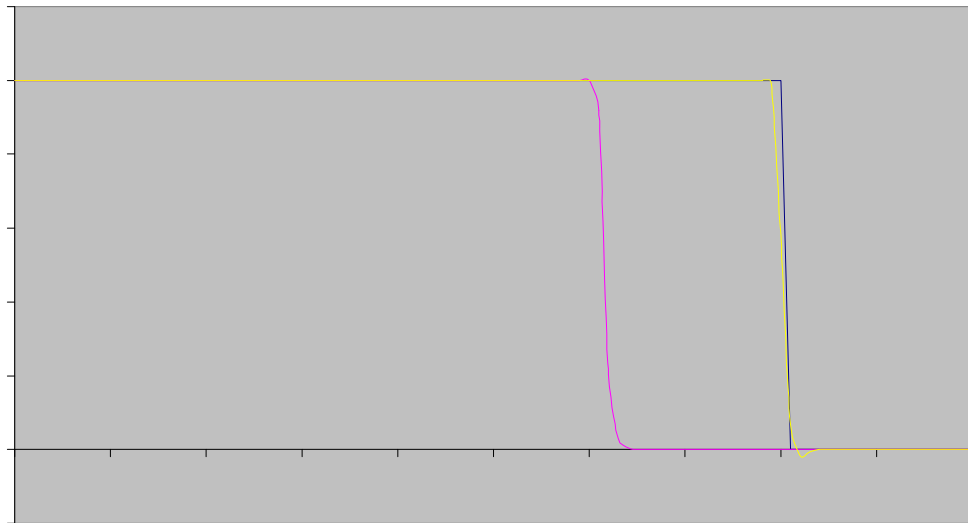


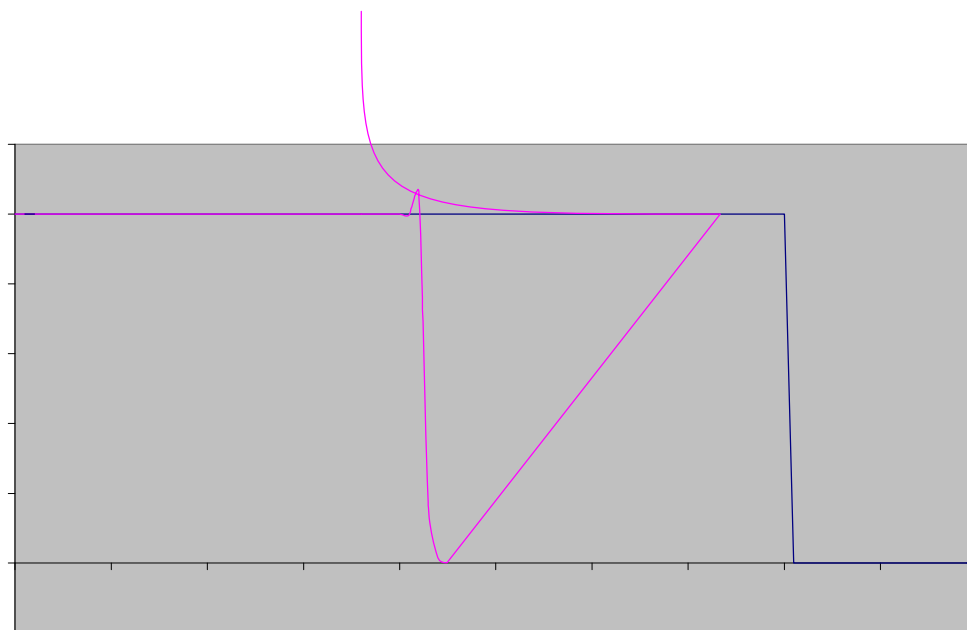












Comparison of MacCormack approach with $dx = 0.01$, $dt = 0.001$
and $t = 0.5$.

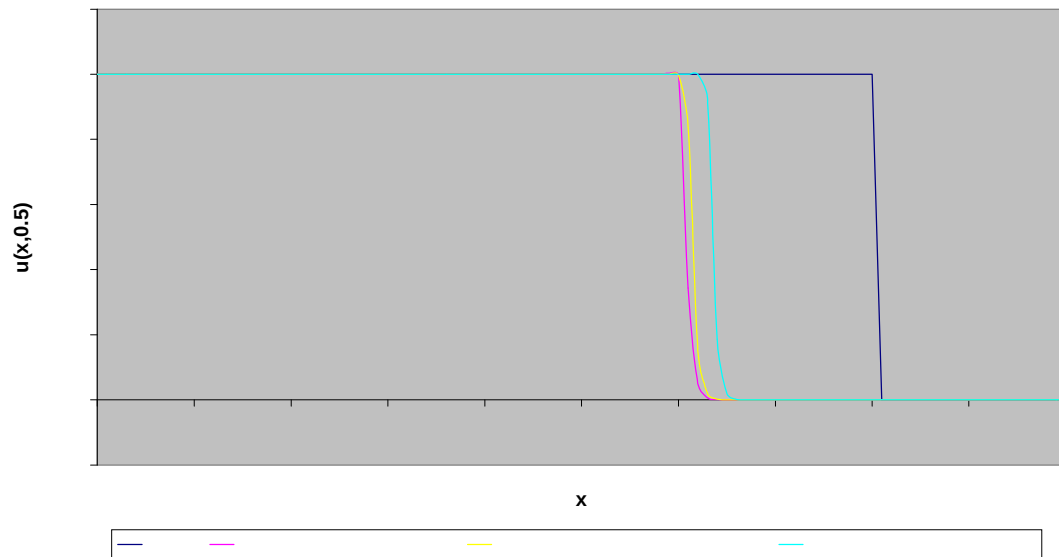
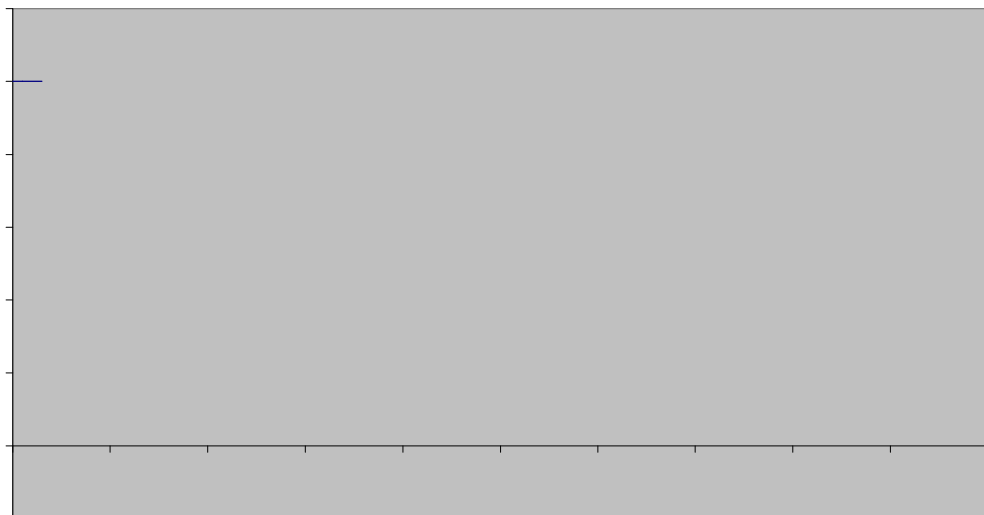


Figure 5-17: Comparison of MacCormack approach with stiff source term.



6 Conclusion

6.1 Final Comparison

Throughout this dissertation, we have discussed many techniques for numerically approximating the conservation law with and without source term, i.e.

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = R(x, t, u) \quad (6.1)$$

and encountered many difficulties, especially when the source term is a function of u . We have also seen that numerically approximating source terms accurately can be extremely difficult to do. However, we have managed to overcome the majority of the difficulties encountered and we have obtained some very accurate finite difference schemes, even when the source term is stiff.

For example, in Chapter 5, we applied the different approaches to the advection-transport equation with a stiff source term, test problem (5.2), and compared the numerical results to obtain the most accurate first order approach, second order approach and second order approach with TVD. These three most accurate approaches are compared in Figure 6-1. Figure 6-1 shows us that the most accurate approach discussed in this project was the second order implicit Upwind approach. Roe's first order upwind approach moved the discontinuity too fast but this was due to a small Courant number. If we increased the step-size, Roe's first order Upwind approach would give us more accurate results but not as accurate as the second order implicit Upwind approach. Notice how the second order MPDATA approach with TVD gave more accurate results than Roe's first order Upwind but less accurate than the second order implicit Upwind approach.

Comparison of most accurate approaches with $dx = 0.01$, $dt = 0.001$ and $t = 0.5$.

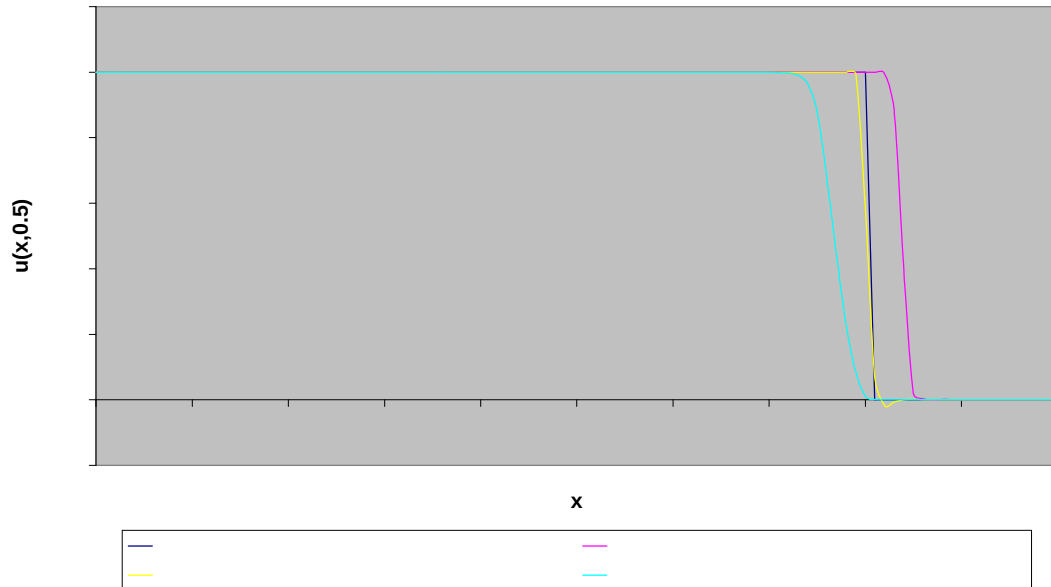


Figure 6-1: Comparison of most accurate approaches with stiff source term.

Comparison of second order Upwind with $dx = 0.01$, $dt = 0.001$ and $t = 0.5$.

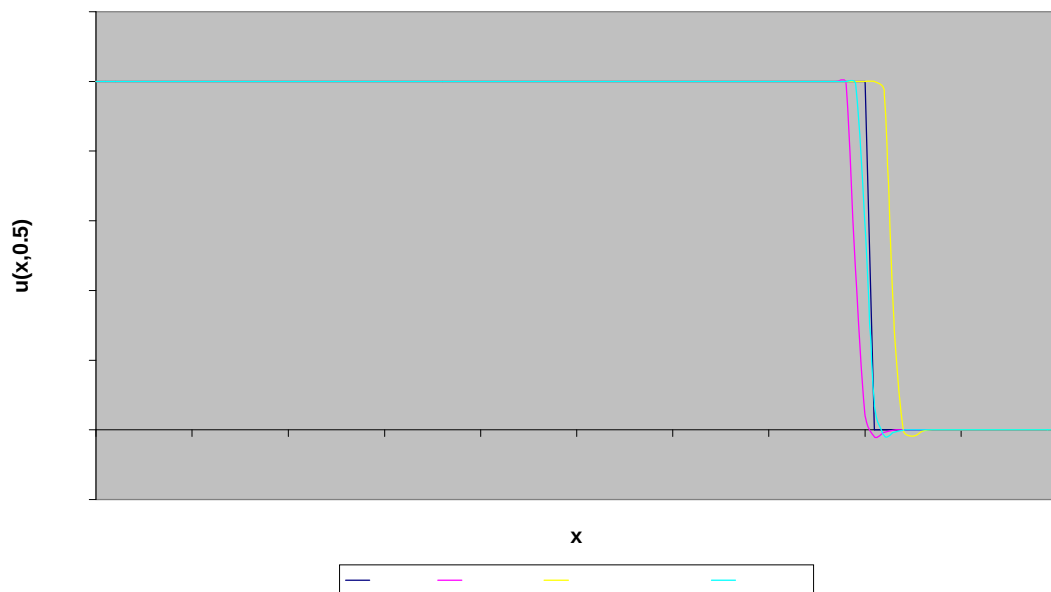


Figure 6-2: Comparison of explicit, semi-implicit and implicit second order Upwind with stiff source term.

This may be due to TVD causing the discontinuity to move faster, when the source term is stiff, or may be due to an implementation problem.

So far, we have seen that the second order implicit Upwind approach has produced the most accurate results. We have looked at a variety of techniques for numerically approximating the source term but we wish to know which technique produces the most accurate results. Figure 6-2 shows some numerical results using the second order Upwind approach applied to the test problem (5.2) but with:

1. The source term and the conservation law approximated explicitly (Explicit).
2. The source term approximated implicitly and the conservation law approximated explicitly (Semi-implicit).
3. The source term and the conservation law approximated implicitly (Implicit).

Here, we can see that the semi-implicit approach produced the least accurate results due to the method moving the discontinuity too fast and the explicit approach produced the second most accurate numerical results. This is unusual since we would expect the semi-implicit approach to be more accurate than the explicit approach. However, when we used the Lax-Wendroff approach, we saw that the semi-implicit approach was more accurate than the explicit due to the discontinuity being moved slightly faster for the semi-implicit approach, see Figure 5-8. Thus, the semi-implicit approach moves the discontinuity slightly faster which makes all approaches which move the discontinuity too slow, i.e. Lax-Wendroff with source term ‘added’, more accurate but all approaches which move the discontinuity at the correct speed or too fast, i.e. the second order Upwind approach, less accurate. The implicit approach

References

1. R.J. LeVeque and H.C. Yee, A Study of Numerical Methods for Hyperbolic Conservation Laws with Stiff Source Terms, *J. Comput. Phys.* **86**, 187 – 210 (1990).
2. P. Embid, J. Goodman and A. Majda, Multiple Steady States for 1-D Transonic Flow, *SIAM J. Sci. Stat. Comput.* **March 1984**, 21 – 41.
3. P.K. Smolarkiewicz and L.G. Margolin, MPDATA: A Finite-Difference Solver for Geophysical Flows, *J. Comput. Phys.* **140**, 459 – 480 (1998).

Appendix A

A Listing of all Numerical Schemes Discussed in Chapters 4 and 5.

All approaches numerically approximate conservation laws with a source term present, i.e.

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = R(x, t, u)$$

1. Explicit ‘Adding’ of Source Term: (First / Second Order)

$$u_i^{n+1} = u_i^{SCHEME} + \Delta t R_i^n$$

where u_i^{SCHEME} represents a numerical scheme which approximates the conservation law without a source term present and is of first / second order.

2. Semi-Implicit Adding of Source Term: (First/Second Order)

$$1 - \Delta t \frac{\partial R}{\partial u}_i^n u_i^{n+1} = u_i^{SCHEME} + \Delta t R_i^n - \Delta t u_i^n \frac{\partial R}{\partial u}_i^n$$

where u_i^{SCHEME} represents a numerical scheme which approximates the conservation law without a source term present and is of first / second order.

3. Lax-Wendroff Approach: (Second Order)

$$1 - \frac{\Delta t}{2} \frac{dR}{du}_i^n u_i^{n+1} = u_i^n - s[F(u; i) - F(u; i-1)] + \Delta t R_i^n - \frac{u_i^n}{2} \frac{dR}{du}_i^n - \frac{\Delta t}{4} [v_{i+1/2} (R_{i+1}^n - R_i^n) - v_{i-1/2} (R_i^n - R_{i-1}^n)]$$

where

$$F(u; i) = F_L(u; i) + F_H(u; i)\phi_i,$$

$$F_L(u; i) = \begin{cases} f_i^n & \text{if } v_{i+1/2} > 0 \\ f_{i+1}^n & \text{if } v_{i+1/2} < 0 \end{cases},$$

$$F_H(u; i) = \begin{cases} \frac{1}{2} (1 - v_{i+1/2}) (f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} > 0 \\ -\frac{1}{2} (1 + v_{i+1/2}) (f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} < 0 \end{cases}$$

and ϕ_i denotes the flux-limiter which can be any of the flux-limiters in Table A-1.

4. MPDATA Approach: (Second Order)

$$1 - \frac{\Delta t}{2} \frac{\partial R}{\partial u}_i^n u_i^{n+1} = MPDATA(u_i^n, C) u_i^n + \frac{\Delta t}{2} R_i^n, w_{i+1/2}^{n+1/2} + \frac{\Delta t}{2} R_i^n - u_i^n \frac{\partial R}{\partial u}_i^n$$

where $MPDATA(u_i^n, C)$ corresponds to the basic MPDATA algorithm with flux-limiter:

$$u_i^{n+1} = u_i^{(1)} - [F(u_i^{(1)}, u_{i+1}^{(1)}, V_{i+1/2}^{(1)})\phi_i - F(u_{i-1}^{(1)}, u_i^{(1)}, V_{i-1/2}^{(1)})\phi_{i-1}]$$

where

$$V_{i+1/2}^{(1)} = \frac{\Delta x}{\Delta t} (|w_{i+1/2}^{n+1/2}| - [w_{i+1/2}^{n+1/2}]^2) \frac{u_{i+1}^{(1)} - u_i^{(1)}}{u_{i+1}^{(1)} + u_i^{(1)}} - w_{i+1/2}^{n+1/2} [w_{i+3/2}^{n+1/2} - w_{i-1/2}^{n+1/2}],$$

$$u_i^{(1)} = u_i^n - [F(u_i^n, u_{i+1}^n, w_{i+1/2}^{n+1/2}) - F(u_{i-1}^n, u_i^n, w_{i-1/2}^{n+1/2})],$$

$$w_{i+1/2}^{n+1/2} = \frac{1}{2} (3w_{i+1/2}^n - w_{i+1/2}^{n-1})$$

and ϕ_i denotes the flux-limiter which can be any of the flux-limiters in Table A-1.

5. Roe's Explicit Upwind I: (First Order)

$$u_i^{n+1} = u_i^n - \begin{cases} s(f_i^n - f_{i-1}^n) - \Delta t[(1-\alpha)R_i^n + \alpha R_{i-1}^n] & \text{if } v_{i+1/2} > 0 \\ s(f_{i+1}^n - f_i^n) - \Delta t[(1-\alpha)R_i^n + \alpha R_{i+1}^n] & \text{if } v_{i-1/2} < 0 \end{cases}.$$

where $0 \leq \alpha \leq 1$ and if $\alpha = 1/2$ then the scheme is second order accurate in space.

6. Explicit Upwind II: (First Order)

$$u_i^{n+1} = u_i^n - \begin{cases} s(f_i^n - f_{i-1}^n) - \Delta t R((1-\alpha)_{X_i} + \alpha_{X_{i-1}}, (1-\alpha)u_i^n + \alpha u_{i-1}^n) & \text{if } v_{i+1/2} > 0 \\ s(f_{i+1}^n - f_i^n) - \Delta t R((1-\alpha)_{X_i} + \alpha_{X_{i+1}}, (1-\alpha)u_i^n + \alpha u_{i+1}^n) & \text{if } v_{i-1/2} < 0 \end{cases}.$$

where $0 \leq \alpha \leq 1$ and if $\alpha = 1/2$ then the scheme is second order accurate in space.

7. Roe's Explicit Upwind III: (Second Order)

$$u_i^{n+1} = u_i^n - s[F(u; i) - F(u; i-1)] + \Delta t \begin{cases} (1-\alpha)R_i^n + \alpha R_{i-1}^n & \text{if } v_{i+1/2} > 0 \\ (1-\alpha)R_i^n + \alpha R_{i+1}^n & \text{if } v_{i-1/2} < 0 \end{cases}$$

where

$$F(u; i) = F_L(u; i) + F_H(u; i)\phi_i,$$

$$F_L(u; i) = \begin{cases} f_i^n & \text{if } v_{i+1/2} > 0 \\ f_{i+1}^n & \text{if } v_{i+1/2} < 0 \end{cases},$$

$$F_H(u; i) = \frac{1}{2} \begin{cases} (1-v_{i+1/2})(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} > 0 \\ -(1+v_{i+1/2})(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} < 0 \end{cases}$$

and $0 \leq \alpha \leq 1$. If $\alpha = 1/2$ then the scheme is second order accurate in space. Also, ϕ_i

denotes the flux-limiter which can be any of the flux-limiters in Table A-1.

8. Explicit Upwind IV: (Second Order)

$$u_i^{n+1} = u_i^n - s[F(u; i) - F(u; i-1)] \\ + \Delta t \begin{cases} R((1-\alpha)_{X_i} + \alpha_{X_{i-1}}, (1-\alpha)u_i^n + \alpha u_{i-1}^n) & \text{if } v_{i+1/2} > 0 \\ R((1-\alpha)_{X_i} + \alpha_{X_{i+1}}, (1-\alpha)u_i^n + \alpha u_{i+1}^n) & \text{if } v_{i-1/2} < 0 \end{cases}$$

where

$$F(u; i) = F_L(u; i) + F_H(u; i)\phi_i,$$

$$F_L(u; i) = \begin{cases} f_i^n & \text{if } v_{i+1/2} > 0 \\ f_{i+1}^n & \text{if } v_{i+1/2} < 0 \end{cases},$$

$$F_H(u; i) = \frac{1}{2} \begin{cases} (1-v_{i+1/2})(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} > 0 \\ -(1+v_{i+1/2})(f_{i+1}^n - f_i^n) & \text{if } v_{i+1/2} < 0 \end{cases}$$

$$b_i = 1 + \text{sgn}(v_{i+1/2})s \frac{\partial f}{\partial u_i}^n - \Delta t e_i \frac{\partial g}{\partial u_i}^n$$

$$(u_i^{(2)} - u_i^{(1)}) = -s(f_{i+1}^{(1)} - f_i^{(1)})$$

$$u_i^{(2)} = u_i^* + \frac{1}{2}[(u_i^{(2)} - u_i^{(1)}) + (u_i^{(1)} - u_i^*)]$$

$$u_i^{**} = u_i^{(2)} + [\phi_{i+1/2}^* - \phi_{i-1/2}^*].$$

$$S_\psi \frac{\Delta t}{2} : \quad 1 - \frac{\Delta t}{4} \frac{\partial R}{\partial u}_i^{**} (u_i^{**} - u_i^{(2)}) = \frac{\Delta t}{2} R_i^{**}$$

$$u_i^{n+1} = u_i^{**} + (u_i^{**} - u_i^{(2)}).$$

Here,

$$\phi_{i+1/2}^{(*)} = \frac{1}{2} [|v_{i+1/2}| - v_{i+1/2}^2] (u_{i+1}^{(*)} - u_i^{(*)} - Q_{i+1/2})$$

and $Q_{i+1/2}$ can be any of the values in Table A-2.

Name of Flux-limiter	$\phi(\theta)$
Minmod	$\phi(\theta) = \max(0, \min(1, \theta))$
Roe's Superbee	$\phi(\theta) = \max(0, \min(2\theta, 1), \min(\theta, 2))$
van Leer	$\phi(\theta) = \frac{ \theta + \theta}{1 + \theta }$
van Albada	$\phi(\theta) = \frac{\theta^2 + \theta}{1 + \theta^2}$

Table A-1: Some second order flux-limiters.

Some choices of $Q_{i+1/2}$ where $\Delta_{i+1/2} = u_{i+1}^n - u_i^n$.
$Q_{i+1/2} = \min \text{mod}(\Delta_{i+1/2}, \Delta_{i-1/2}) + \min \text{mod}(\Delta_{i+1/2}, \Delta_{i+3/2}) - \Delta_{i+1/2}$
$Q_{i+1/2} = \min \text{mod}(\Delta_{i-1/2}, \Delta_{i+1/2}, \Delta_{i+3/2})$
$Q_{i+1/2} = \min \text{mod} \quad 2\Delta_{i-1/2}, 2\Delta_{i+1/2}, 2\Delta_{i+3/2}, \frac{1}{2}(\Delta_{i-1/2} + \Delta_{i+3/2})$

Table A-2: Some choices of $Q_{i+1/2}$ for the MacCormack approach.

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