BEHAVIOUR OF FINITE DIFFERENCE SOLUTION OF THE ADVECTION EQUATION

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Abstract. All finite difference equations have an equivalent partial differential equation which is the actual partial differential equation being solved. The equivalent modified partial differential equation will not be identical to the original equation being modelled. It will generally contain additional higher-order spatial terms introduced by the finite difference approximation. The behaviour of a finite difference scheme can be examined by investigating the properties of their equivalent modified partial differential equation. Analytical solutions are given for the equivalent modified partial differential equations for first, second and third-order finite difference schemes used to solve the advection equation. These analytical solutions are also used to establish the accuracy of these schemes for the simulation of problems containing discontinuous profiles.

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1. Introduction

Although finite-difference schemes can be constructed to solve partial differential equations, to be useful they must satisfy certain requirements such as (*i*) accuracy, (*ii*) stability, (*iii*) consistency, (*iv*) convergence and (*v*) efficiency [6]. Although these requirements are generally satisfied, a Taylor series expansion of the finite difference scheme will generally reveal that the finite difference scheme is a more accurate solution to a higher-order partial differential equation than the original equation it is meant to approximate. This equation can be written as a *modified equivalent partial differential equation*[8],[4]. The properties of the modified equivalent partial differential equation can be used to provide insight into the behaviour of the finite difference approximation. It also provides a theoretical estimate of the size of the dominant error term and an indication of the stability constraints for the numerical scheme.

In this paper, finite difference schemes for the solution of the constant coefficient advection equation

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = 0 \quad 0 < x < \infty, \quad t > 0 \tag{1}$$

in which c is the concentration, u is the constant fluid velocity, x is the distance and t is the time are considered. The analytical solution to this problem is simply the advection of the profile at the speed u without deformation. This equation usually dominates the transport of pollutants in groundwater and aquatic systems. In modelling these systems, it is important to understand the behaviour of finite difference analogue of equation (1). Otherwise this behaviour may obscure the true response of the system being modelled.

The modified equivalent partial differential equation for any finite difference approximations of equation (1) involving a maximum of six computational nodes over two time level is given by [5]

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + \sum_{q=2}^{\infty} \frac{u(\Delta x)^{q-1}}{q!}\eta_q(Cr)\frac{\partial^q c}{\partial x^q} = 0 \tag{2}$$

in which the cell Courant number $Cr = u\Delta t/\Delta x$ and η_q is dependent on u and the grid spacing Δt and Δx used in the numerical scheme.

The finite difference approximation is first-order accurate and it introduces artificial diffusion if the modified partial differential equation has a non-vanishing term $\eta_2(Cr)$. Numerical diffusion has the affect of smearing the profile. The forward time upwind [6] scheme is an example of a first-order scheme where $\eta_2(Cr) = (Cr - 1)$. Another is the Lax-Friedrichs scheme where $\eta_2(Cr) = (Cr^2 - 1)/Cr$. Both these schemes introduce numerical diffusion and the modified equivalent partial differential equation is a diffusion equation.

The modified equivalent partial differential equation is a dispersion equation when $\eta_3(Cr) = 0$ and $\eta_3(Cr) \neq 0$ and the finite difference scheme is second-order accurate. Second-order schemes eliminate the numerical diffusion and provide a better resolution to discontinuities in the solution than first-order schemes, however dispersion is introduced. Numerical dispersion is associated with different frequencies that make up a travelling wave, propagating at different speeds. This may result in oscillations in the numerical solution in the vicinity of steep gradients in the profile. Examples of second-order finite difference schemes are the Lax-Wendroff [3] scheme, where $\eta_3(Cr) = (1 - Cr^2)$ and the Beam-Warming [9] scheme, where $\eta_3(Cr) = -(2 - 3Cr + Cr^2)$.

The behaviour of finite difference schemes used to solve equation (1) can be established by substituting a Fourier component in space in the modified partial differential equation, and observing the evolution in time of these Fourier components or their group velocity [7].

The purpose of this paper is to demonstrate an alternative approach to describe the behaviour of finite difference schemes. This is achieved by finding analytical solutions to the modified equivalent partial differential equation. These analytical solutions are also used to establish the accuracy of these schemes for the solution of problems containing discontinuous profiles.

2. Advective-diffusion equation

The linear advective-diffusion equation is given by

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \quad 0 < x < \infty, \quad t > 0 \tag{3}$$

and the initial conditions are given by $c(x, 0) = f(x)$ for $-\infty < x < \infty$ where D is the constant diffusion coefficient. This initial value problem can be solved using the Fourier transform to provide the well known analytical solution

$$c(x,t) = \frac{c_0}{2}\operatorname{erfc}\left(\frac{x - ut}{2\sqrt{Dt}}\right) \tag{4}$$

in which erfc is the *complementary error function.* Consider a simple example, where $c_0 = u = D = t = 1$. The diffusion of a front is shown in Figure 1.

These results are similar to the results produced for the evolution of an advancing front using first-order schemes. Consider the results for the following test problem

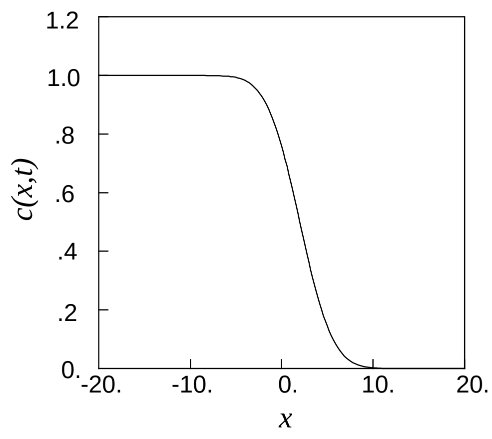

FIGURE 1. The diffusion of a step function

$$c(x, t = 0) = \begin{cases} 100 & 0 \leq x \leq 5\Delta x \\ 100\sin^2(\frac{\pi x}{20\Delta x}) & 25\Delta x \leq x \leq 45\Delta x \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

solved using the forward time upwind scheme. The step function and the *Sine-squared* wave, of width $20\Delta x$ is advected by the fluid travelling at $u = 0.5$ m/second. In the model $\Delta x = 1$ m and $\Delta t = 1$ second therefore, $Cr = 0.5$, and the simulated and analytical solutions are compared when $T = 100$ seconds. The analytical solution to this problem and the results from the first-order forward time upwind scheme is shown in Figure 2.

The simulated profile for the step function closely resembles that predicted by equation (4), the profile spreads with time.

3. Advective-dispersion equation

The linear advective-dispersion equation is given by

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = -D\frac{\partial^3 c}{\partial x^3} \quad 0 < x < \infty, \quad t > 0 \tag{6}$$

and the initial condition is given by $c(x, 0) = f(x)$ for $-\infty < x < \infty$. D is the dispersion coefficient in this equation. This equation is also known as the linearized form of the *Korteweg-deVries* equation which plays an important role in the theory of water waves (see for example Whitham[10], p. 366).

Using the Fourier transform in space, then equation (6) becomes

$$\frac{dC(\alpha, t)}{dt} + ui\alpha C(\alpha, t) = i\alpha^3 DC(\alpha, t) \quad t > 0$$

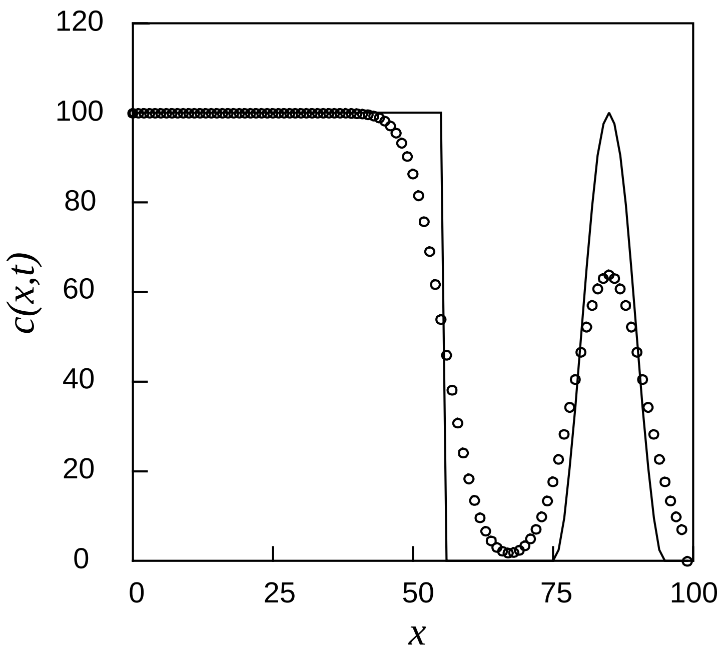

FIGURE 2. Analytical and forward time upwind solution of the advection equation

with the initial conditions $\mathcal{F}\{f(x,0)\} = C(\alpha,0) = \mathcal{F}(\alpha)$ where $\mathcal{F}$ is the Fourier transform in space. The solution of this homogeneous first-order differential equation is

$$C(\alpha,t) = \mathcal{F}(\alpha)\exp(i\alpha^3 Dt - i\alpha ut))$$

Taking the inverse Fourier transform of this expression and substituting the Fourier transform for $f(x)$, then

$$c(x,t) = \frac{1}{(3Dt)^{1/3}}\int_{-\infty}^{\infty} f(\xi)\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[i\left(\frac{\mu^3}{3}+\frac{\mu(x-\xi-ut)}{(3Dt)^{1/3}}\right)\right]d\mu\right]d\xi \tag{7}$$

where $\mu = (3Dt)^{1/3}\alpha$. The inner integral is an integral representation of the *Airy's function* $\mathrm{Ai}(x)$ defined by

$$\mathrm{Ai}(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left(i\left[\tau^3/3+\tau z\right]\right)d\tau \tag{8}$$

which was obtained from equation 10.4.32 in Abramowitz and Stegun [1].

A plot of the Airy functions, $\mathrm{Ai}(x)$ and $\mathrm{Ai}(-x)$ are shown in Figure 3.

Making use of equation (8), then equation (7) becomes

$$c(x,t) = \frac{1}{(3Dt)^{1/3}}\int_{-\infty}^{\infty} f(\xi)\mathrm{Ai}\left(\frac{x-\xi-ut}{(3Dt)^{1/3}}\right)d\xi \tag{9}$$

which is an integral representation of the solution of the initial boundary value problem. If $f(x) = c_0$, for $x < 0$ and 0 otherwise, then equation (9) becomes

$$c(x,t) = \frac{c_0}{(3Dt)^{1/3}}\int_{-\infty}^{0}\mathrm{Ai}\left(\frac{x-\xi-ut}{(3Dt)^{1/3}}\right)d\xi. \tag{10}$$

This solution indicates that for a moving front at $x = ut$, oscillations should be observed for negative ξ and the profile decays exponentially for positive ξ. This is illustrated by

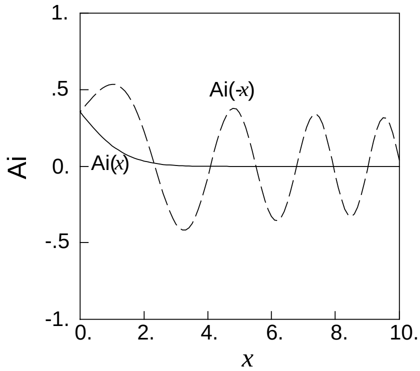

FIGURE 3. Airy functions $\mathrm{Ai}(x)$ and $\mathrm{Ai}(-x)$

considering a simple example, where $u = t = c_0 = 1$ and $D = 1/3$. Introducing a new variable $\zeta = x - \xi - 1$, then equation (10) becomes

$$c(x,t) = \int_0^\infty \mathrm{Ai}(\zeta)d\zeta - \int_0^{x-1} \mathrm{Ai}(\zeta)d\zeta. \tag{11}$$

This can be simplified by making use of equation 10.4.82 in Abramowitz and Stegun [1] where

$$\int_0^\infty \mathrm{Ai}(z)dz = \frac{1}{3}$$

then equation (11) becomes

$$c(x,t) = \frac{1}{3} - \int_0^{x-1} \mathrm{Ai}(\zeta)d\zeta.$$

Evaluating the integral numerically, the resulting concentration profile is illustrated in Figure 4.

These results are typical of those obtained for the solution of the advection equation using second-order schemes in which D is positive. Oscillations are observed behind the advancing front and the profile decays exponentially forward of the front. This is the case for the second-order Lax-Wendroff scheme, the results of which are shown in Figure 5 for the above test problem, equation (5).

If the diffusion coefficient is negative, the linear advective-dispersion equation is written in the form

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^3 c}{\partial x^3} \quad 0 < x < \infty, \quad t > 0$$

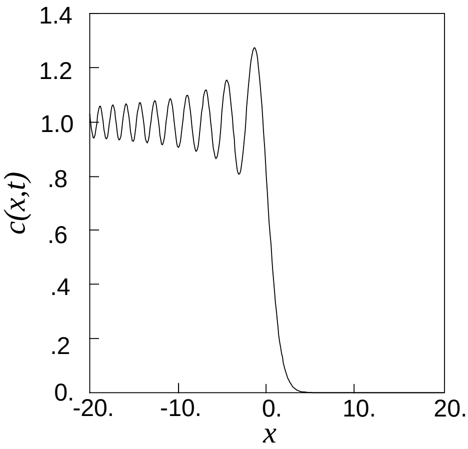

FIGURE 4. The dispersion of a step function for positive dispersion coefficient, D

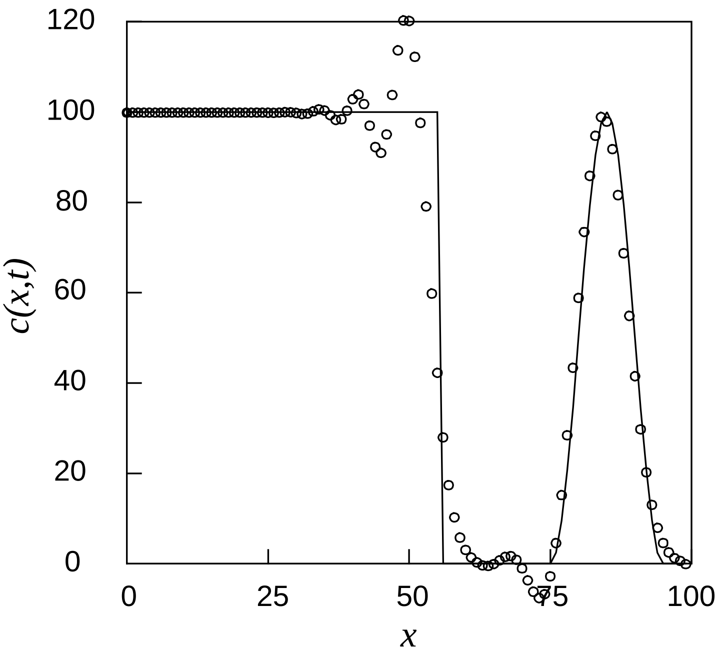

FIGURE 5. Analytical and Lax-Wendroff solution of the advection equation

with the initial conditions $c(x, 0) = f(x)$ for $-\infty < x < \infty$. This equation has an analytical solution analogous to equation (10) given by

$$c(x,t) = \frac{c_0}{(3Dt)^{1/3}} \int_{-\infty}^{0} \mathrm{Ai}\left(\frac{ut + \xi - x}{(3Dt)^{1/3}}\right) d\xi \tag{12}$$

for the initial conditions $f(x) = c_0$ for $x < 0$ and 0 otherwise. Using the test problem, where $u = t = c_0 = 1$ and $D = 1/3$, then equation (12) becomes

$$c(x,t) = \int_0^\infty \mathrm{Ai}(-\zeta)d\zeta - \int_0^{x-1} \mathrm{Ai}(-\zeta)d\zeta \tag{13}$$

which can be simplified by making use of equation 10.4.83 in Abramowitz and Stegun [1]

$$\int_0^\infty \mathrm{Ai}(-z)dz \simeq \frac{2}{3}.$$

Equation (13) becomes

$$c(x,t) = \frac{2}{3} - \int_0^{x-1} \mathrm{Ai}(-\zeta)d\zeta.$$

Evaluating the integral numerically, the resulting concentration profile is illustrated in Figure 6.

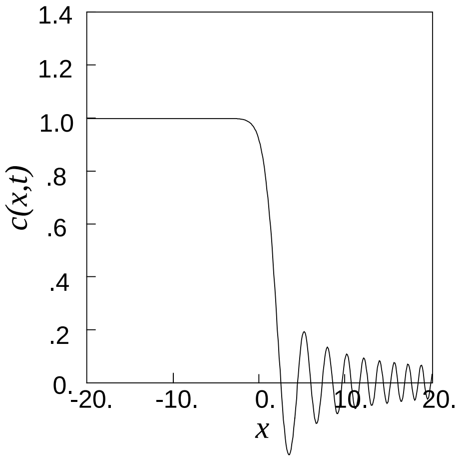

FIGURE 6. The dispersion of a step function for negative dispersion coefficient, D

In this case the analytical solution indicates that oscillations are observed prior to the arrival of the advancing front. Similar profiles are observed for the solution of the advection equation using second-order schemes such as the Beam and Warming schemes. The solution of the test problem using the Beam and Warming scheme is illustrated in Figure 7.

As predicted oscillations occur downstream of the disturbance.

There is however a major distinction between the results shown in Figures 4 and 6 and those obtained from a second-order numerical scheme. Since a numerical scheme has a finite domain, boundary conditions are imposed on the initial value problem. These boundary conditions must be satisfied. Therefore, the oscillations are dampened so that the boundary conditions are satisfied. These constraints do not exist in the analytical solution where the oscillations extend to infinity. Other higher-order even terms introduced by the finite difference approximation may also dampen these oscillations.

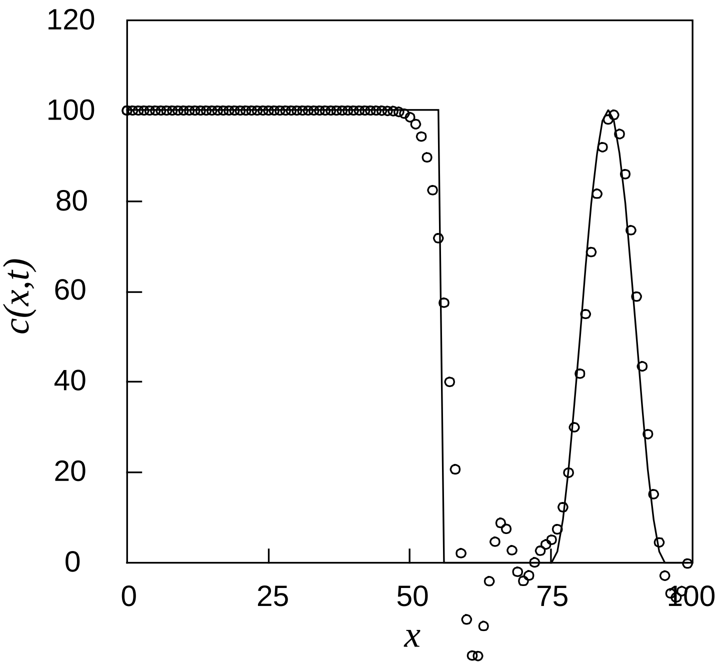

FIGURE 7. Analytical and Beam and Warming solution of the advection equation

4. Higher-order equations

The above procedure can be generalised for any higher-order scheme. Only the third-order scheme is considered here. In this case

$$c(x,t) = \int_{-\infty}^{\infty} f(\xi)\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\left(-\alpha^4 Dt + i\alpha(x-\xi-ut)\right) d\alpha\right] d\xi.$$

If $f(x) = c_0$, for $x < 0$ and 0 otherwise then

$$c(x,t) = c_0 \int_{-\infty}^{0}\left[\frac{1}{\pi}\int_{0}^{\infty} \exp\left(-\alpha^4 Dt\right)\cos\left(\alpha(x-\xi-ut)\right) d\alpha\right] d\xi \tag{14}$$

which makes use of the identity; $e^z = e^x e^{iy} = e^x(\cos(y) + i\sin(y))$ and $\int_{\infty}^{-\infty}\sin(y)dy = 0$. The inner integral has been evaluated numerically for $D = 1$, $t = 1$ and $ut = \xi$. The results are shown in Figure 8. The function is symmetrical about $x = 0$ and oscillatory with the amplitude of the oscillations damping rapidly.

Solving equation (14) numerically for $u = t = c_0 = 1$ and $D = 1/3$, produced the results shown in Figure 9.

The simulated profile is symmetrical with oscillations occuring both upstream and downstream of the discontinuity. These results are typical of the results produced by third-order schemes which do not use shape preserving interpolation or flux limiters. Using the test problem, the results from the third-order Holly and Priessmann [2] scheme are shown in Figure 10.

Oscillations occur in the simulated profile both upstream and downstream of the discontinuity. In addition, these oscillations are symmetrical about the discontinuity.

The simple analysis demonstrated above has successfully predicted the behaviour of finite difference approximations of the advection equation. It also demonstrates the importance of investigating the properties of the modified equivalent partial differential

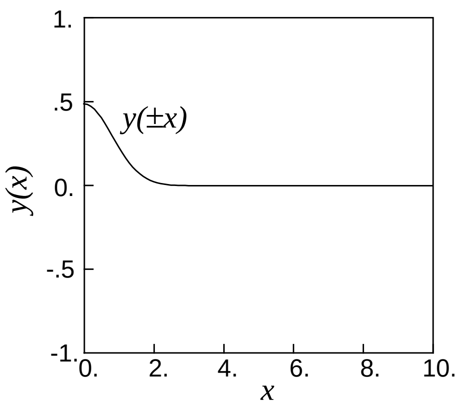

FIGURE 8. Evaluation of the inner integral in equation (14)

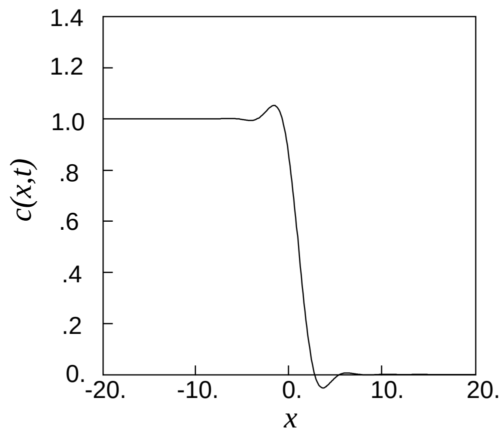

FIGURE 9. Analytical solution to the fourth-order equivalent modified partial differential equation

equation in assessing the behaviour of the finite difference scheme, and not the governing equation. This analysis can be generalised to higher-order finite difference schemes.

The analytical solutions provided can be used to evaluate the accuracy of finite difference schemes for the solution of equation (1) when there is a discontinuity in the concentration profile.

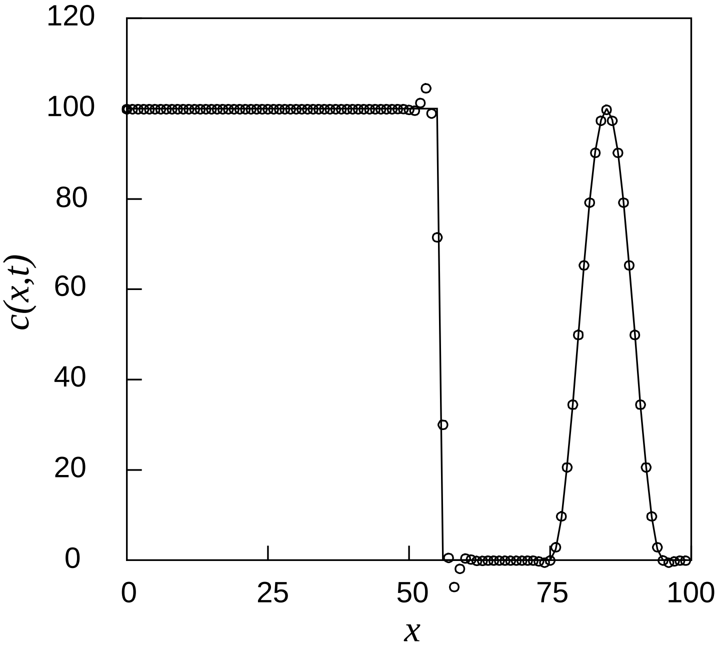

FIGURE 10. Analytical and Holly and Preissmann solution of the advection equation

5. Accuracy in the presence of a discontinuity

The predicted accuracy of a numerical scheme using traditional techniques, such as the modified equivalent partial differential equations is dramatically reduced in the presence of a discontinuity in the initial or boundary conditions.

The L_1 norm is used as a measure of the error between the exact and numerical solutions of the advection equation.

5.1. **First-order schemes.** The modified equivalent partial differential equation of a first-order finite difference approximation of the advection equation is an advective-diffusion equation. The analytical solution to the constant coefficient advective-diffusion equation is given by equation (4). Using $\mathrm{erfc}(z) = 1 - \mathrm{erf}(z)$, then the L_1 norm is given by

$$\| f(x) - c(x,t) \|_{L_1} = \int_{-\infty}^{\infty} \left| f(x) - \frac{1}{2} + \frac{1}{2}\mathrm{erf}\left(\frac{x-ut}{2\sqrt{Dt}}\right)\right| dx.$$

From the boundary condition $f(x) = 1$ for $x \le 0$ and 0 elsewhere, then

$$\begin{aligned} \| f(x) - c(x,t) \|_{L_1} &= \int_{-\infty}^{0} \left| \frac{1}{2} + \frac{1}{2}\mathrm{erf}\left(\frac{x-ut}{2\sqrt{Dt}}\right)\right| dx \\ &+ \int_{0}^{\infty} \left| -\frac{1}{2} + \frac{1}{2}\mathrm{erf}\left(\frac{x-ut}{2\sqrt{Dt}}\right)\right| dx. \end{aligned} \quad (15)$$

Since $\mathrm{erf}(-z) = -\mathrm{erf}(z)$ and making use of $| z | = | -z |$ then equation (15) becomes

$$\| f(x) - c(x,t) \|_{L_1} = \int_{0}^{\infty} \left| \mathrm{erfc}\left(\frac{x-ut}{2\sqrt{Dt}}\right)\right| dx.$$

Let $z = (x - ut)/2/(Dt)^{1/2}$, then

$$\| f(x) - c(x,t) \|_{L_1} = 2\sqrt{Dt} \int_{-ut/2/(Dt)^{1/2}}^{\infty} | \operatorname{erfc}(z) | \, dz$$

or simply

$$\| f(x) - c(x,t) \|_{L_1} = C_1 \sqrt{Dt}.$$

The L_1 norm behaves like $t^{1/2}$. The dispersion coefficient, D is a function of u, Δx and Δt in first-order schemes. When Cr and u are given, then $D = C_2 \Delta x$ and the L_1 norm becomes

$$\| f(x) - c(x,t) \|_{L_1} = C_1 \sqrt{\Delta x t}$$

in which C_2 is a constant. The error decays only like $\Delta x^{1/2}$ even though the method is formally 'first-order accurate'.

5.2. **Second-order schemes.** Standard second-order finite difference schemes introduce a dispersion term. The analytical solution of the advective-dispersion equation for a unit step function is given by equation (9) in which $f(\xi)$ is the initial conditions.

Using the L_1 norm as a measure of the error between the exact and numerical solution of the advection equation, then

$$\| f(x - ut) - c(x,t) \|_{L_1} = \int_{-\infty}^{\infty} \left| f(x - ut) - \frac{1}{(3Dt)^{1/3}} \int_{-\infty}^{\infty} f(\xi) \operatorname{Ai}\left(\frac{x - \xi - ut}{(3Dt)^{1/3}} \right) d\xi \right| dx.$$

Since[1]

$$\frac{1}{(3Dt)^{1/3}} \int_{-\infty}^{\infty} \operatorname{Ai}\left(\frac{\xi}{(3Dt)^{1/3}} \right) d\xi = 1$$

and introducing the change in variable $\zeta = x - \xi - ut$ then

$$\begin{aligned} \| f(x - ut) - c(x,t) \|_{L_1} &= \frac{1}{(3Dt)^{1/3}} \int_{-\infty}^{\infty} \left| \int_{-\infty}^{\infty} f(x - ut) \right. \\ &- \left. f(x - \zeta - ut) \operatorname{Ai}\left(\frac{\zeta}{(3Dt)^{1/3}} \right) d\zeta \right| dx. \end{aligned}$$

From the boundary conditions, let

$$f(x) = \begin{cases} 1 & x < 0 \\ 0 & x \geq 0 \end{cases}$$

Substituting, $z = x - ut$, $a = z/(3Dt)^{1/3}$ and $b = \zeta/(3Dt)^{1/3}$, then

$$\begin{aligned} \| f(x - ut) - c(x,t) \|_{L_1} &= (3Dt)^{1/3} \int_{-\infty}^{\infty} \left| \int_{-\infty}^{\infty} \operatorname{Ai}(b) \Big(f(a(3Dt)^{1/3}) \right. \\ &- \left. f((3Dt)^{1/3}(a - b)) \Big) \, da \right| db. \end{aligned}$$

Since in this case

$$f(a(3Dt)^{1/3}) - f((3Dt)^{1/3}(a - b)) = f(a) - f(a) - f(a - b)$$

then

$$\| f(x - ut) - c(x,t) \|_{L_1} = (3Dt)^{1/3} \int_{-\infty}^{\infty} \left| \int_{-\infty}^{\infty} \operatorname{Ai}(b) \left[f(a) - f(a - b) \right] da \right| db.$$

The integral has a finite value, therefore

$$\| f(x-ut) - c(x,t) \|_{L_1} \leq C_1(3Dt)^{1/3} \tag{16}$$

This suggests that at best, a second-order scheme behaves like $t^{1/3}$ if a discontinuity exists in the initial conditions.

The behaviour of second-order numerical schemes for which the dispersion coefficient D is known, can now be established by substituting for D in equation (16). Generally, $D \propto \Delta x^2$ for a given Cr and u and equation (16) becomes

$$\| f(x-ut) - c(x,t) \|_{L_1} \leq C_2 \Delta x^{2/3} t^{1/3}$$

in which C_2 is a constant. Therefore the L_1 norm decays like $\Delta x^{2/3}$ for second-order accurate schemes. These results have been confirmed using numerical experiments. For example the rate of convergence of the forward time upwind, Lax-Wendroff and the third-order Holly and Priessmann schemes, shown in Figure 11 were obtained for the following problem; $c(x,0) = c_0$ for $0 \leq x \leq 45$ m, $c(0,t) = c_0$, $c(L,t) = 0$, $c_0 = 100$, $u = 0.25$ m/second and $L = 200$ m. Fifteen data sets containing between 201 to 20001 computational nodes ($\Delta x = 1$ to 0.001 m). The L_1 norm between the analytical and numerical solution when, $T = 200$ seconds was calculated using all the computational points. The Courant number, $Cr = 0.25$ remains constant for all data sets.

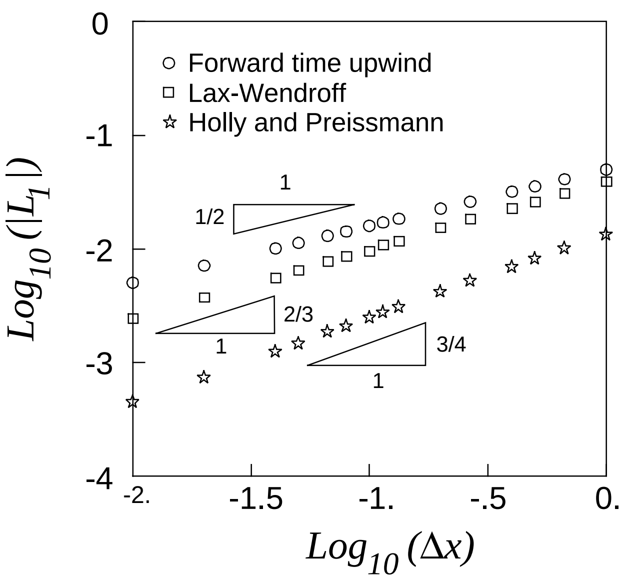

FIGURE 11. Rate of convergence of several finite difference schemes for the solution of the advection of a discontinuous profile

These numerical results confirm the above predictions. The L_1 norm for the first-order scheme behaves like $\Delta x^{1/2}$ and for the second-order scheme like $\Delta x^{2/3}$. The numerical results also suggest that for the third-order scheme the L_1 norm decays like $\Delta x^{3/4}$.

6. CONCLUSIONS

Analytical solutions have been provided for the modified partial differential equations of first, second and third-order finite difference approximation of the linear advection equation. These analytical solutions reveal that first-order schemes introduce numerical diffusion, which smears the profile and second-order schemes introduce numerical dispersion. Oscillation are only observed after the arrival of a front for second-order schemes with positive dispersion coefficients. When the dispersion coefficient is negative oscillations are only observed before the arrival of the front. For third-order schemes oscillations are symmetrical about the discontinuity. These analytical solutions were used to show that the formal accuracy of finite difference schemes is dramatically reduced if there is a discontinuity in the initial or boundary conditions. It has been shown that Qth-order accurate finite difference schemes will approximate a discontinuity with $O(\Delta x^{Q/(Q+1)})$ in the L_1 norm sense. Therefore, a front can only be modelled to first-order accuracy at best, which of course, is the best that can be expected.

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