Numerical Solution of the 1-D Advection-Diffusion Equation Using Standard and Non-Standard Finite Difference Schemes

A.R.APPADU[1]
Department of Mathematics and Applied Mathematics, University of Pretoria, Pretoria, 0002, SOUTH AFRICA.
Email: Rao.Appadu@up.ac.za, biprao2@yahoo.com

Abstract
In this work, three numerical methods have been used to solve the one-dimensional advection-diffusion equation with constant coefficients. This partial differential equation is dissipative but not dispersive. We consider the Lax-Wendroff scheme which is explicit, the Crank-Nicolson scheme which is implicit as well as a Non-Standard Finite Difference scheme [14]. We solve a 1-D numerical experiment with specified initial and boundary conditions, for which the exact solution is known using all these three schemes using some different values for the space and time step sizes denoted by h and k respectively for which the Reynolds number is 2 or 4. Some errors are computed namely, the error rate with respect to the L_1 norm, dispersion and dissipation errors. We have both dissipative and dispersive errors and this indicates that the methods generate artificial dispersion though the partial differential considered is not dispersive. It is seen that the Lax-Wendroff and NSFD are quite good methods to approximate the 1-D advection-diffusion equation at some values of k and h. Two optimisation techniques are then implemented to find the optimal values of k when $h = 0.02$ for the Lax-Wendroff and NSFD schemes and this is validated by numerical experiments.

1 Introduction

The significant applications of advection-diffusion equation lie in fluid dynamics [13], heat transfer [12] and mass transfer [9]. The 3-D advection-diffusion equation is given by

$$\frac{\partial u}{\partial t} + A\ \frac{\partial u}{\partial x} + B\ \frac{\partial u}{\partial y} + C\ \frac{\partial u}{\partial z} = \alpha\ \Big(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\Big). \tag{1}$$

The coefficient of diffusivity is denoted by α and is computed as $\alpha = \dfrac{C_T}{p\ D_p}$, where p, D_p and C_T denote the pressure, specific heat of the fluid at constant pressure and thermal conductivity respectively. Also A, B, C are the velocity components of the fluid in the directions of x, y and z respectively. Eq. (1) is also referred to as the convection-diffusion equation. The three terms $A\ \dfrac{\partial u}{\partial x}$, $B\ \dfrac{\partial u}{\partial y}$ and $C\ \dfrac{\partial u}{\partial z}$ are called the advective or convective terms and the terms $\alpha\dfrac{\partial^2 u}{\partial x^2}$, $\alpha\dfrac{\partial^2 u}{\partial y^2}$ and $\alpha\dfrac{\partial^2 u}{\partial z^2}$ are called the diffusive or viscous terms.
In this paper, we consider the one-dimensional convection-diffusion equation given by

$$\frac{\partial u}{\partial t} + a\ \frac{\partial u}{\partial x} = \alpha\frac{\partial^2 u}{\partial x^2}, \tag{2}$$

with $a = 1$, $\alpha = 0.01$, $0 \leq x \leq 1$ and $0 < t \leq T$.
We denote the spatial and temporal step sizes by h and k respectively. The cfl number, c is computed as $\dfrac{a\ k}{h}$ and the parameter, s is obtained as $\dfrac{\alpha k}{h^2}$.
The initial condition is $u(x, 0) = f(x)$, and boundary conditions are

$$u(0, t) = g_0(t), 0 < t \leq T,$$

$$u(1,t) = g_1(t), 0 < t \leq T,$$

where f, g_0 and g_1 are known functions.

There has been little progress in obtaining analytical solution to the 1-D advection-diffusion equation when initial and boundary conditions are complicated, even with α and a being constant [7]. This is the reason why numerical solution of Eq.(2) is important.

The paper is organised as follows. In section 2, we study the damping and dispersive characteristics of some numerical methods for the 1-D advection diffusion equation. In section 3, we show how to quantify the errors from the numerical results into dissipation and dispersion errors by using a technique devised by Takacs [20]. In section 4, we describe the numerical experiment that we have considered and show how to choose the parameters k and h to run the numerical experiments. Sections 5 and 6 describe some explicit and implicit methods, and we study their dissipative and dispersive properties. Also, we tabulate the errors when the methods are used to solve the numerical experiment described in section 6. In section 7, we present a Non-Standard Finite Difference (NSFD) scheme and analyse its spectral properties and also use it to solve the numerical experiment. In section 8, we find the optimal value of k when $h = 0.02$ for the Lax-Wendroff and NSFD schemes and validate these using the numerical experiment. Section 9 highlights the salient features of the paper.

2 Dissipative and Dispersive Characteristics of numerical methods

Dissipation is defined as the constant decrease with time of the amplitude of plane waves as they propagate in time. If the modulus of the amplification factor, denoted by AFM is equal to one, a disturbance neither grows nor damps [8]. The modulus of the amplification factor is also a measure of the stability of a scheme. If this value is greater than one, this creates instability while damping is present whenever the value is less then one [17]. When the modulus of the amplification factor exceeds one, this indicates an unstable mode [4].
Since our partial differential equation is $u_t + a\ u_x = \alpha\ u_{xx}$, we will have dissipation and this is caused because of the term u_{xx} and such dissipation is called implicit dissipation. We can also have artificial dissipation which is caused due to the numerical method.

We let the amplification factor of the scheme approximating Eq. (2) be

$$\xi = \xi_1 + I\ \xi_2. \tag{3}$$

Then the modulus of the amplification factor, denoted by AFM is computed as $|\xi|$. We now show how the relative phase error (RPE) of a given numerical scheme approximating Eq. (2) is obtained.
A perturbation for u is obtained by substituting u by $\exp(I\ (w_1\ t - \theta x))$ where t and x represents time and space respectively, θ is the wavenumber and w_1 is the dispersion relation [18].
We then obtain

$$I\ w_1 - a\theta I + \alpha\theta^2 = 0, \tag{4}$$

where $I = \sqrt{-1}$, with on simplification gives

$$w_1 = a\ \theta + \alpha\theta^2 I. \tag{5}$$

Hence, the dispersion relation is given by

$$w_1 = a\ \theta + \alpha\theta^2\ I. \tag{6}$$

The exact phase velocity is computed as $\frac{\Re(w_1)}{\theta}$ which simplifies as θ. We next obtain the numerical phase velocity.
From Eq. (3), we have $\xi = \xi_1 + I\ \xi_2$. We can express ξ as $\exp(-bk)$ [18] where b is the exponential growth rate.
Therefore, we have $\exp(-bk) = \xi_1 + I\ \xi_2$ which implies

$$b = \frac{1}{k}\ \log\Big(\frac{\xi_1 - I\ \xi_2}{\xi_1^2 + \xi_2^2}\Big). \tag{7}$$

The numerical phase velocity is computed as $\frac{\Im(b)}{\theta}$ and is equal to

$$-\frac{1}{k\ \theta}\tan^{-1}\Big(\frac{\xi_2}{\xi_1}\Big). \tag{8}$$

The phase angle, w is computed as $w = \theta h$ where θ is the wavenumber and h is the spatial step. The relative phase error (RPE) is a measure of the dispersive character of a scheme. This quantity is a ratio and measures the velocity of the computed waves to that of the physical waves. Hence, we have

$$RPE = -\frac{1}{k\ \theta a}\tan^{-1}\Big(\frac{\Im(\xi)}{\Re(\xi)}\Big). \tag{9}$$

Since $w = \theta h$ and $c = \frac{a\ k}{h}$, we can express Eq. (9) as

$$RPE = -\frac{1}{c\ w}\tan^{-1}\Big(\frac{\Im(\xi)}{\Re(\xi)}\Big). \tag{10}$$

If the RPE is greater than one, the computed waves appear to move faster than the physical waves [11] thus causing phase lead. A ratio less than one implies that the computed waves will move slower than the physical waves, causing phase lag.

3 Quantification of errors from numerical results [20, 1, 2]

In this section, we describe how Takacs [20] quantifies errors from numerical results into dispersion and dissipation errors.
The Total Mean Square Error is calculated as

$$\frac{1}{N}\sum_{i=1}^{N}(u_i - v_i)^2$$

where, u_i represents the analytical solution and v_i, the numerical (discrete) solution at a given grid point, i.
The Total Mean Square Error can be expressed as

$$\frac{1}{N}\sum_{i=1}^{N}(u_i - v_i)^2 = \frac{1}{N}\sum_{i=1}^{N}(u_i)^2 + \frac{1}{N}\sum_{i=1}^{N}(v_i)^2 - \frac{2}{N}\sum_{i=1}^{N}u_i\ v_i. \tag{11}$$

Next,

$$\frac{1}{N}\sum_{i=1}^{N}(u_i-\overline{u_i})^2=\frac{1}{N}\sum_{i=1}^{N}\Big((u_i)^2-2u_i\ \overline{u_i}+(\overline{u_i})^2\Big) \tag{12}$$

and

$$\frac{1}{N}\sum_{i=1}^{N}(v_i-\overline{v_i})^2=\frac{1}{N}\sum_{i=1}^{N}\Big((v_i)^2-2v_i\ \overline{v_i}+(\overline{v_i})^2\Big). \tag{13}$$

The Total Mean Square Error can be further expressed as

$$\begin{aligned}\frac{1}{N}\sum_{i=1}^{N}(u_i-\overline{u_i})^2+\frac{1}{N}\sum_{i=1}^{N}(v_i-\overline{v_i})^2+\frac{2}{N}\sum_{i=1}^{N}u_i\ \overline{u_i}+\frac{2}{N}\sum_{i=1}^{N}v_i\ \overline{v_i}\\ -\frac{1}{N}\sum_{i=1}^{N}(\overline{u_i})^2-\frac{1}{N}\sum_{i=1}^{N}(\overline{v_i})^2-\frac{2}{N}\sum_{i=1}^{N}u_i\ v_i.\end{aligned} \tag{14}$$

The expression in (14) can be rewritten as

$$\sigma^2(u)+\sigma^2(v)+2\ (\bar{u})^2+2\ (\bar{v})^2-(\bar{u})^2-(\bar{v})^2-\frac{2}{N}\sum_{i=1}^{N}u_i\ v_i, \tag{15}$$

where $\sigma^2(u)$ and $\sigma^2(v)$ denote the variance of u and v respectively, $\bar{u}$ and $\bar{v}$ denote the mean values of u and v respectively.

Thus, the Total Mean Square Error is given by

$$\sigma^2(u)+\sigma^2(v)+\Big((\bar{u})^2-2\ \bar{u}\bar{v}+(\bar{v})^2\Big)+\Big(2\ \bar{u}\bar{v}-\frac{2}{N}\sum_{i=1}^{N}u_i\ v_i\Big) \tag{16}$$

which on further simplification yields

$$\sigma^2(u)+\sigma^2(v)+(\bar{u}-\bar{v})^2-2\Big(\frac{1}{N}\sum_{i=1}^{N}u_i\ v_i\ -\overline{u_i}\ \overline{v_i}\Big). \tag{17}$$

Thus, we have

$$\frac{1}{N}\sum_{i=1}^{N}(u_i-v_i)^2=\sigma^2(u)+\sigma^2(v)+(\bar{u}-\bar{v})^2-2\ Cov(u,v). \tag{18}$$

But, the correlation coefficient, ρ is given by $\dfrac{Cov(u,v)}{\sigma(u)\ \sigma(v)}$. Hence, the Total Mean Square Error can be written as

$$\frac{1}{N}\sum_{i=1}^{N}(u_i-v_i)^2=\sigma^2(u)+\sigma^2(v)+(\bar{u}-\bar{v})^2-2\ \rho\ \sigma(u)\ \sigma(v), \tag{19}$$

which simplifies to

$$\frac{1}{N}\sum_{i=1}^{N}(u_i-v_i)^2=(\sigma(u)-\sigma(v))^2+(\bar{u}-\bar{v})^2+2\ (1-\rho)\ \sigma(u)\ \sigma(v). \tag{20}$$

On putting $\rho=1$, we get $2\ (1-\rho)\ \sigma(u)\ \sigma(v)=0$. Thus, we define $(2\ (1-\rho)\sigma(u)\ \sigma(v))$ as the dispersion error as correlation coefficient in statistics is analogous with phase lag or phase lead in Computational

Fluid Dynamics.
Consequently, $(\sigma(u) - \sigma(u))^2 + (\bar{u} - \bar{v})^2$ measures the dissipation error.

We also obtain values of the error rate with respect to the L_1 norm which is calculated as

$$E_{num} = \frac{1}{N} \sum_{i=1}^{N} |u_i - v_i|, \tag{21}$$

where u_i and v_i are the computed and exact values respectively and N is the number of spatial grid points.

4 Choice of the parameters h and k

We refer to [7] where three explicit methods are used to solve the partial differential equation

$$u_t + 0.8\ u_x = 0.008\ u_{xx}, \tag{22}$$

where

$$u(x, t = 0) = \exp\Big(- \frac{(x-2)^2}{8}\Big), \tag{23}$$

$$g_0(t) = \sqrt{\frac{20}{20+t}}\ \exp\Big[- \frac{(5+4t)^2}{10\ (t+20)}\Big], \tag{24}$$

and

$$g_1(t) = \sqrt{\frac{20}{20+t}}\ \exp\Big[- \frac{2\ (5+2t)^2}{5\ (t+20)}\Big]. \tag{25}$$

Tests were carried out for three values of the cell Reynolds number, $R_\Delta = \frac{c}{s}$, namely $R_\Delta = 2, 4, 8$ [7]. Since $c = \frac{0.8\ k}{h}$ and $s = \frac{0.008\ k}{h^2}$, we can express R_Δ in terms of h, in that case we have $R_\Delta = 100\ h$. Thus, for $R_\Delta = 2, 4, 8$, the corresponding values of h are 0.02, 0.04 and 0.08 respectively.
Since $c = \frac{0.8\ k}{h}$ and $h = 0.02, 0.04, 0.08$, we have the following relationships between c and k namely $c = 40\ k$, $c = 20\ k$ and $c = 10\ k$.
Then three values of c were chosen as 0.16, 0.32 and 0.64 and then the corresponding values of k determined as 0.004, 0.008, 0.016, 0.032, 0.064. For these values of k, the number of time-steps, M are calculated as $M = \frac{1}{k}$ and hence, M take the following values namely 250, 125, 62.5, 31.25 and 16.625 respectively. However, we note that M can only be an integer. Hence, an improvement can be made when choosing c and k while keeping $R_\Delta = 2, 4, 8$ and $h = 0.02, 0.04, 0.08$.

We next refer to [16] where both explicit and implicit methods were used for numerical solution of the one-dimensional advection-diffusion equation in a region bounded by $0 \le x \le 1$ and $0 \le t \le 1$ [9], with $a = 1$, $\alpha = 0.01$ and with the following initial and boundary conditions:

$$u(x, 0) = \exp\Big(- \frac{(x+0.5)^2}{0.00125}\Big), \tag{26}$$

$$u(0, t) = \frac{0.025}{\sqrt{0.000625 + 0.02\ t}}\ \exp\Big(- \frac{(0.5-t)^2}{(0.00125 + 0.04t)}\Big), \tag{27}$$

$$u(1,t) = \frac{0.025}{\sqrt{0.000625 + 0.02\ t}}\ \exp\Big(-\frac{(1.5-t)^2}{(0.00125+0.04t)}\Big). \tag{28}$$

The exact solution is given by

$$u(x,t) = \frac{0.025}{\sqrt{0.000625 + 0.02\ t}}\ \exp\Big(-\frac{(x+0.5-t)^2}{(0.00125+0.04t)}\Big). \tag{29}$$

The values of h and k used were 0.02 and 0.004 respectively for all the numerical methods considered in [16].

In our work, we use we consider both implicit and explicit schemes to solve

$$u_t + 1.0\ u_x = 0.01\ u_{xx},$$

subject to boundary conditions given by (26), (27) and (28).
We consider two values for R_Δ, say, 2 and 4. Thus, we have $R_\Delta = 100\ h$ as $a = 1$ and $\alpha = 0.01$. For $R_\Delta = 2$ and 4, we have $h = 0.02$ and 0.04 respectively. Hence, $c = \dfrac{k}{0.02}$ and $c = \dfrac{k}{0.04}$ and therefore we have $c = 50\ k$ and $c = 25\ k$.

We consider the case when $c = 50\ k$. If we choose $c = 0.25$, 0.50 and 1.0, then the values taken by k are 0.01, 0.02 and 0.04 respectively.
Next we consider, $c = 25\ k$. If we choose, $c = 0.25$, 0.5 and 1.0, we have $k = 0.01$, 0.02 and 0.04 respectively.
Hence, for $h = 0.02$, the values taken by k are 0.005, 0.01 and 0.02. For $h = 0.04$, k can take the values 0.01, 0.02 and 0.04. Some of these possibilities might give rise to an unstable scheme and must be ignored.
However, for implicit methods, all the 6 combinations of k and h are possible and we can also consider the case when $c = 2.0$ instead of only the three cases, namely, $c = 0.25$, 0.5 and 1.0.

5 Construction of explicit and implicit finite difference methods

We can approximate $\dfrac{\partial u}{\partial x}$ as

$$\frac{(1-\gamma)\ (u_i^n - u_{i-1}^n) + \gamma(u_{i+1}^n - u_i^n)}{h}, \tag{30}$$

or,

$$\frac{(1-\gamma)\ (u_i^{n+1} - u_{i-1}^{n+1}) + \gamma(u_{i+1}^{n+1} - u_i^{n+1})}{h}. \tag{31}$$

Hence, an approximation for $\dfrac{\partial u}{\partial x}$ is

$$(1-\phi)\ \Big[\frac{(1-\gamma)\ (u_i^n - u_{i-1}^n) + \gamma(u_{i+1}^n - u_i^n)}{h}\Big] + \phi\Big[\frac{(1-\gamma)\ (u_i^{n+1} - u_{i-1}^{n+1} + \gamma(u_{i+1}^{n+1} - u_i^{n+1})}{h}\Big], \tag{32}$$

where h represents the spatial step size, ϕ and γ are the temporal and spatial weighting factors respectively.

An approximation for $\dfrac{\partial^2 u}{\partial x^2}$ is

$$\frac{u_{i+1}^n - 2\ u_i^n + u_{i-1}^n}{h^2}, \tag{33}$$

or

$$\frac{u_{i+1}^{n+1} - 2\ u_i^{n+1} + u_{i-1}^{n+1}}{h^2}. \tag{34}$$

Hence, a discretization for $\dfrac{\partial^2 u}{\partial x^2}$ is

$$(1-\phi)\ \Big[\frac{u_{i+1}^n - 2\ u_i^n + u_{i-1}^n}{h^2}\Big] + \phi\Big[\frac{u_{i+1}^{n+1} - 2\ u_i^{n+1} + u_{i-1}^{n+1}}{h^2}\Big]. \tag{35}$$

On plugging approximations for $\dfrac{\partial u}{\partial x}$ and $\dfrac{\partial^2 u}{\partial x^2}$ as given by (32) and (35) into Eq. (2), we obtain a family of explicit and implicit numerical schemes given by

$$u_i^{n+1} = \frac{1}{A_0}\ \Big(A_1\ u_{i-1}^n + A_2\ u_i^n + A_3\ u_{i+1}^n + A_4\ u_{i-1}^{n+1} + A_5\ u_{i+1}^{n+1}\Big), \tag{36}$$

where,

$$\begin{aligned} A_0 &= 1 - \phi[c\ (2\gamma - 1) - 2s], \\ A_1 &= (\phi - 1)\ [c\ (\gamma - 1) - s], \\ A_2 &= 1 + (\phi - 1)\ [c(1 - 2\ \gamma) + 2s], \\ A_3 &= (1 - \phi)\ [s - c\ \gamma], \\ A_4 &= \phi[s + c\ (1 - \gamma)], \end{aligned}$$

and

$$A_5 = \phi[s - \gamma c],$$

where $c = \dfrac{a\ k}{h}$ and $s = \dfrac{\alpha\ k}{h^2}$.

6 Standard Schemes

6.1 Lax-Wendroff scheme

The Lax-Wendroff scheme is given by

$$u_i^{n+1} = \frac{1}{2}\ (2s + c + c^2)\ u_{i-1}^n + (1 - 2s - c^2)\ u_i^n + \frac{1}{2}(2s - c + c^2)\ u_{i+1}^n, \tag{37}$$

and is obtained on replacing ϕ by zero and γ by $\dfrac{1-c}{2}$, in Eq. (36).
The modified equation is given by [6]

$$u_t + a\ u_x - \alpha u_{xx} + \frac{1}{6}\ a\ h^2\ (1 - c^2 - 6\ s)\ u_{xxx} + ... = 0, \tag{38}$$

and this indicates that the leading error terms are dispersive in nature.

The amplification factor and the relative phase error are obtained as

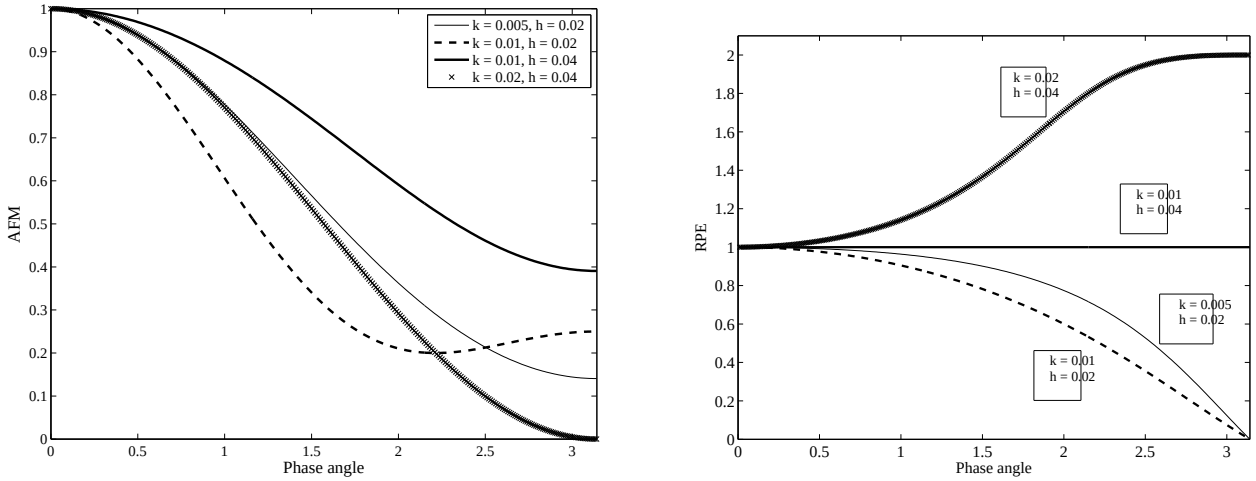
$$\xi = 1 + (2s + c^2)\ (\cos(w) - 1) - I\ c\sin(w), \tag{39}$$

and

$$RPE = \frac{1}{cw}\tan^{-1}\Big(\frac{c\sin(w)}{1 + (2s + c^2)\ (\cos(w) - 1)}\Big). \tag{40}$$

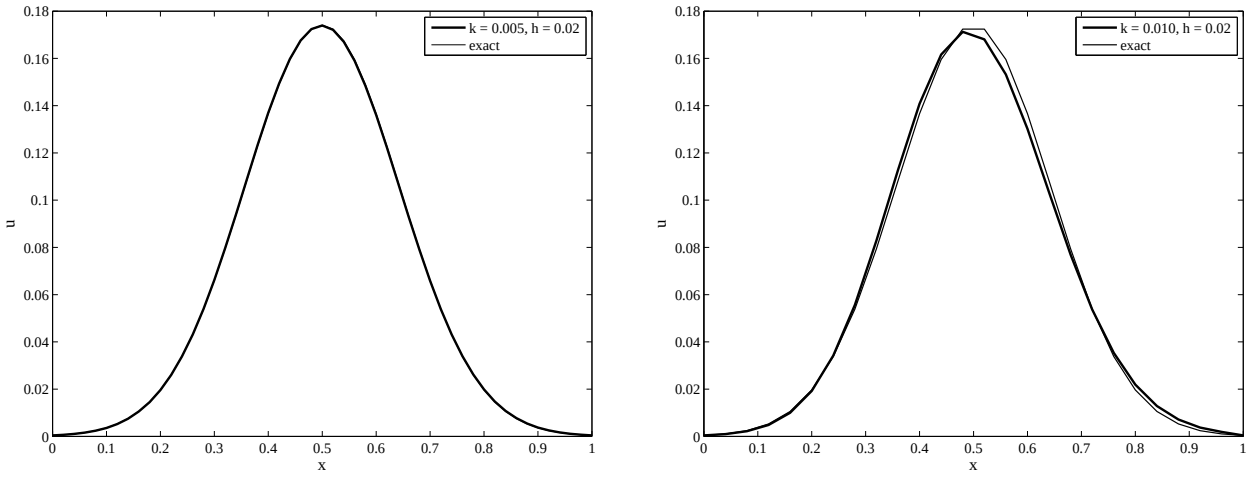
Plots of the AFM and RPE, both versus the phase angle, w for four combinations of values of k and h are shown in Figs. (1(a)) and (1(b)). The combination $k = 0.01$, $h = 0.04$ is the least dissipative one. The scheme is not dispersive when $k = 0.01$, $h = 0.04$. Phase lag behaviour is observed when $k = 0.005$, $h = 0.02$ and $k = 0.01$, $h = 0.02$. Phase lead phenomenon occurs when $k = 0.02$ and $h = 0.04$.

We tabulate the errors in Table (1) for the four combination of values of h and k. The errors are least when $k = 0.005$ and $h = 0.02$ and greatest when $k = 0.01$ and $h = 0.04$.



(a) AFM (b) RPE

Figure 1: Plot of AFM and RPE vs phase angle for the Lax-Wendroff scheme



(a) (b)

Figure 2: Comparison of numerical results with exact results using Lax-Wendroff scheme at some values of k and h.

Table 1: Errors for Lax-Wendroff scheme

k	h	cfl	E_{num}	$max\ \|u_e - u_c\|$	Error at $(0.5, 1.0)$	Diss. Error	Disp. Error
0.005	0.02	0.25	1.8166×10^{-4}	5.8157×10^{-4}	1.6348×10^{-4}	6.3582×10^{-9}	5.4502×10^{-8}
0.01	0.02	0.50	7.3296×10^{-4}	0.0024	1.6348×10^{-4}	9.1960×10^{-8}	8.9741×10^{-7}
0.01	0.04	0.25	0.0021	0.0065	0.0011	9.1500×10^{-7}	7.1622×10^{-6}
0.02	0.04	0.50	1.2252×10^{-4}	3.7946×10^{-4}	3.7946×10^{-4}	4.0896×10^{-9}	2.4477×10^{-8}

6.2 Crank-Nicolson scheme

The Crank-Nicolson method is obtained if we plug $\gamma = 1/2$ and $\phi = 1/2$ into Eq. (36). A single expression for the scheme is

$$u_i^{n+1} = \frac{1}{4\ (1+s)}\Big((c+2s)\ u_{i-1}^{n+1} - (c-2s)\ u_{i+1}^{n+1} + (c+2s)\ u_{i-1}^{n} - (c-2s)\ u_{i+1}^{n} + (4-4s)\ u_i^n\Big). \quad (41)$$

The modified equation is given by

$$u_t + a\ u_x - \alpha\ u_{xx} + \frac{1}{12}ah^2\ (2+c^2)\ u_{xxx} + ... = 0, \quad (42)$$

and this indicates that the leading error terms are dispersive in nature.

The amplification factor is given by

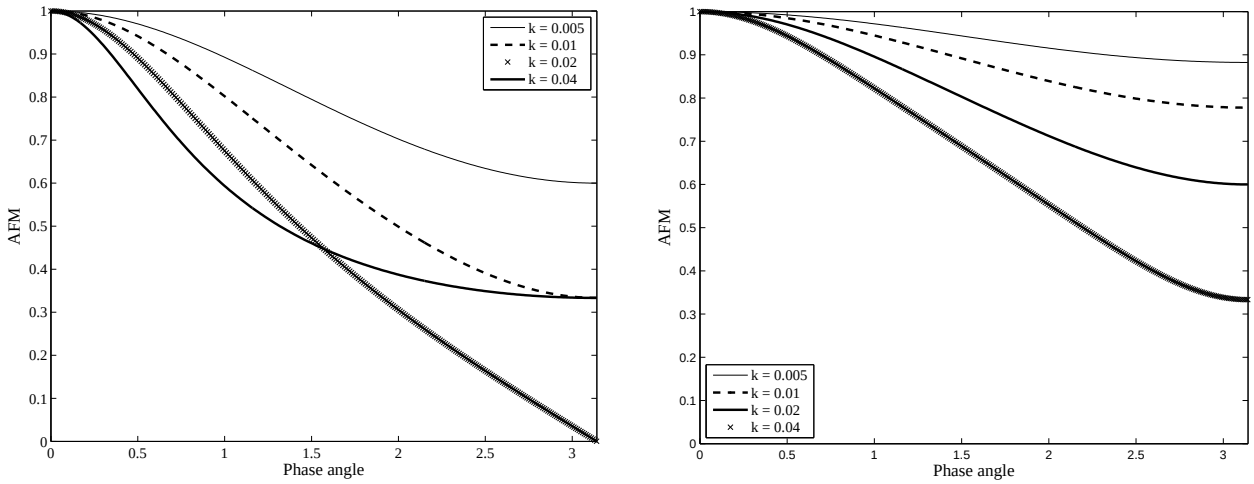
$$\xi = \Big(\frac{B_2\ D_2 - C_2^2}{B_2^2 + C_2^2}\Big) - I\ \Big(\frac{B_2 C_2 + C_2 D_2}{B_2^2 + C_2^2}\Big), \quad (43)$$

and the RPE is computed as

$$\frac{1}{cw}\tan^{-1}\Big(\frac{B_2 C_2 + C_2 D_2}{B_2 D_2 - C_2^2}\Big), \quad (44)$$

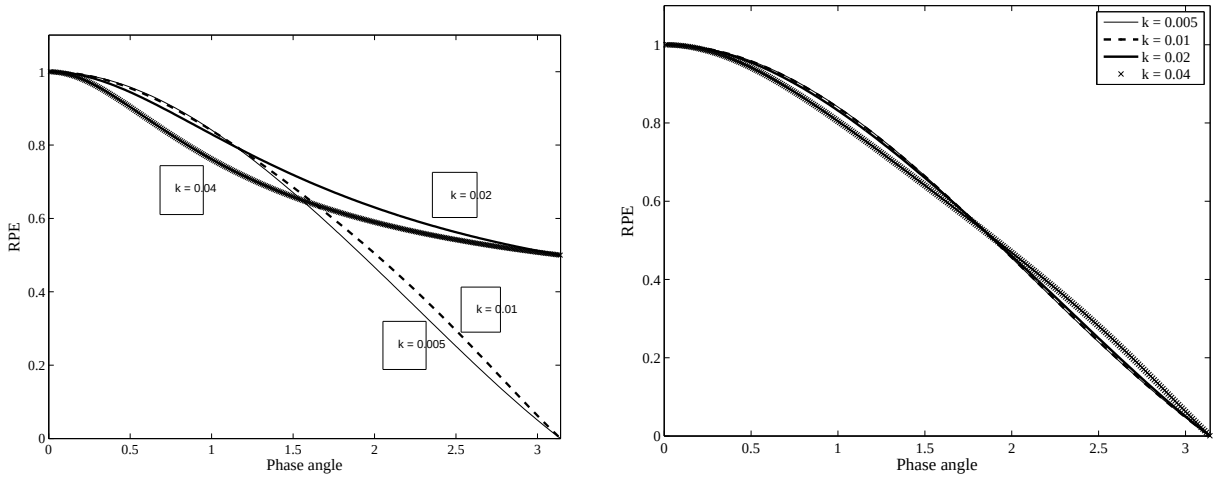
where $B_2 = 1 + s - s\cos(w)$, $C_2 = 2c\ \sin(w)$ and $D_2 = 4 + 4s\ \cos(w) - 4s$.

The scheme is unconditionally stable. We next plot the variation of the AFM vs phase angle for some values of k and h in Fig. (3(a)) and (3(b)). Plots of the RPE vs phase angle are depicted in Figs. (4(a)) and (4(b)).
In the case of Crank-Nicolson, the scheme is less dissipative at $h = 0.04$ as compared to $h = 0.02$ for all the four values of k namely; 0.005, 0.01, 0.02 and 0.04. The combination $h = 0.04$, $k = 0.005$ is the least dissipative one. Based on Fig. (4(b)), we can observe that dispersion character is slightly affected by the value of k used when $h = 0.04$. However, if we choose $h = 0.02$, the dispersion character is much affected by the value of k. In general for $h = 0.02$, the case $k = 0.02$ is in general the least dispersive one.
We tabulate the errors for the eight combinations of h and k in Table (2) and we observe that the errors are least when $k = 0.005$ and $h = 0.02$.



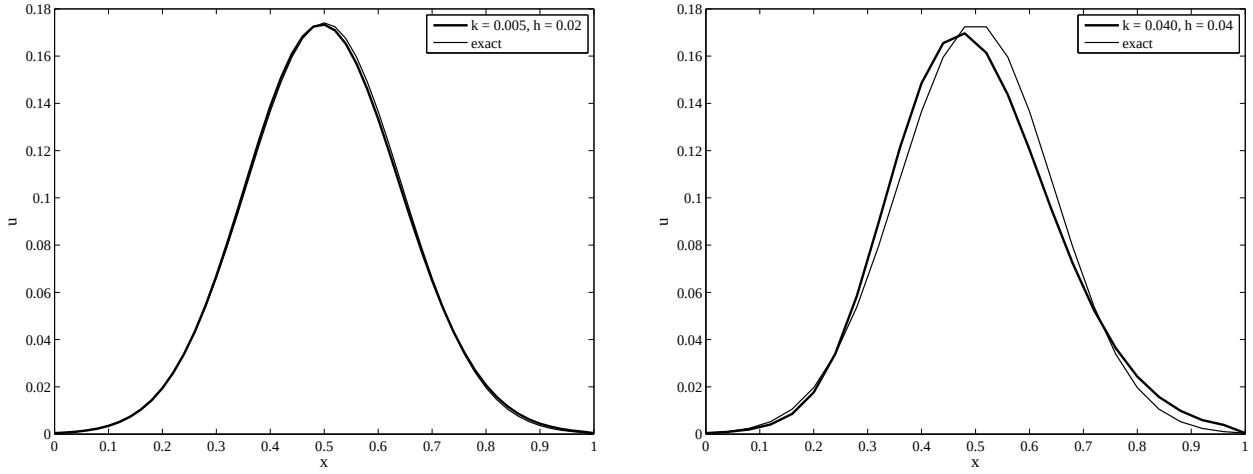
(a) $h = 0.02$ (b) $h = 0.04$

Figure 3: Plot of AFM vs phase angle for the Crank-Nicolson scheme.



(a) $h = 0.02$ (b) $h = 0.04$

Figure 4: Plot of RPE vs phase angle for the Crank-Nicolson scheme.



(a) (b)

Figure 5: Comparison of numerical results with exact results using Crank-Nicolson scheme at some values of k and h.

7 Non-Standard Finite Difference Scheme

In this section, we describe how a non-standard finite difference scheme (NSFD) is constructed [15] for the 1-D convection-diffusion equation.
The equation $u_t + u_x = \alpha\ u_{xx}$ has three sub-equations [14] which are given by

$$u_t + u_x = 0, \tag{45}$$

$$u_x = \alpha\ u_{xx}, \tag{46}$$

Table 2: Errors for Crank-Nicolson scheme

k	h	cfl	E_{num}	$max\ \lvert u_e - u_c \rvert$	Error at $(0.5, 1.0)$	Diss. error	Disp. Error
0.005	0.02	0.25	9.9859×10^{-4}	0.0032	7.3954×10^{-4}	1.4704×10^{-7}	1.6929×10^{-6}
0.01	0.02	0.50	0.0011	0.0035	7.3475×10^{-4}	1.6161×10^{-7}	2.0307×10^{-6}
0.02	0.02	1.0	0.0015	0.0046	7.4486×10^{-4}	2.2664×10^{-7}	3.7049×10^{-6}
0.04	0.02	2.0	0.0029	0.0092	0.0013	5.9447×10^{-7}	1.5389×10^{-5}
0.005	0.04	0.125	0.0037	0.0114	0.0020	2.2440×10^{-6}	2.3758×10^{-5}
0.01	0.04	0.25	0.0038	0.0116	0.0020	2.2981×10^{-6}	2.4852×10^{-5}
0.02	0.04	0.5	0.0042	0.0126	0.0021	2.5212×10^{-6}	2.9471×10^{-5}
0.04	0.04	1.0	0.0055	0.0162	0.0028	3.5178×10^{-6}	5.1581×10^{-5}

$$u_t = \alpha\ u_{xx}. \tag{47}$$

Eqs. (45) and (46) have known exact finite difference scheme which are

$$\frac{u_i^{n+1} - u_i^n}{k} + \frac{u_i^n - u_{i-1}^n}{h} = 0, \tag{48}$$

with $k = h$ and

$$\frac{u_i - u_{i-1}}{h} = \alpha\Big(\frac{u_{i+1} - 2\ u_i + u_{i-1}}{\alpha h(\exp(h/\alpha) - 1)}\Big), \tag{49}$$

respectively.

A finite difference scheme that englobes the features of the two equations namely (45) and (46) is

$$\frac{u_i^{n+1} - u_i^n}{k} + \frac{u_i^n - u_{i-1}^n}{h} = \alpha\Big(\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\alpha h(\exp(h/\alpha) - 1)}\Big). \tag{50}$$

On rearranging the terms in (50), we get the NSFD method which is [14, 15]

$$u_i^{n+1} = \beta\ u_{i+1}^n + (1 - \alpha_1 - 2\beta_1)\ u_i^n + (\alpha_1 + \beta_1)\ u_{i-1}^n, \tag{51}$$

where

$$\alpha_1 = \frac{k}{h}, \tag{52}$$

and

$$\beta_1 = \frac{\alpha_1}{\exp(h/\alpha) - 1}. \tag{53}$$

The square of the modulus of the amplification factor is given by

$$|\xi|^2 = \Big((1 - \alpha_1 - 2\beta_1) + (\alpha_1 + 2\ \beta_1)\ \cos(w)\Big)^2 + (\alpha_1 \sin(w))^2. \tag{54}$$

For stability, $0 < |\xi| \leq 1$ and this implies that $0 < |\xi|^2 \leq 1$. We now obtain the region of stability by using the approach used by Hindmarch et. al. [10] and Sousa [19].
We consider the case when $w = \pi$. The square of the modulus of the amplification factor is given by

$$|\xi|^2 = (1 - 2\ \alpha_1 - 4\ \beta_1)^2. \tag{55}$$

We thus need,

$$(1 - 2\ \alpha_1 - 4\ \beta_1)^2 \leq 1, \tag{56}$$

which implies that

$$|1 - 2\ \alpha_1 - 4\ \beta_1| \leq 1. \tag{57}$$

Thus, for stability, we have the following inequality

$$-1 \leq 1 - 2\ \alpha_1 - 4\ \beta_1 \leq 1, \tag{58}$$

which simplifies to

$$0 \leq \alpha_1 + 2\ \beta_1 \leq 1. \tag{59}$$

Since α_1 and β_1 are positive, $\alpha_1 + 2\ \beta_1 \geq 0$ is the trivial inequality. Hence, we consider the inequality

$$\alpha_1 + 2\ \beta_1 \leq 1. \tag{60}$$

Since, $\alpha_1 = \dfrac{k}{h}$ and $\beta_1 = \dfrac{\alpha_1}{\exp(h/\alpha) - 1}$, we have

$$\frac{k}{h} + \frac{2\ k}{h\ \Big(\exp(h/\alpha) - 1\Big)} \leq 1. \tag{61}$$

For stability, we need the following condition

$$k \leq \Big(\frac{\exp(h/\alpha) - 1}{\exp(h/\alpha) + 1}\Big)\ h. \tag{62}$$

We next consider the case when $w \to 0$. When $w \to 0$, $\cos(w) \approx 1 - \dfrac{1}{2}w^2$ and $\sin(w) \approx w$.
Thus, (54) reduces to

$$|\xi|^2 \approx 1 + (-2\ \beta_1 + \alpha_1^2 - \alpha_1)\ w^2. \tag{63}$$

We thus require

$$-2\ \beta_1 + \alpha_1^2 - \alpha_1 \leq 0. \tag{64}$$

Using (52) and (53), (64) becomes

$$\frac{-2k\ h + k\ (k - h)\ (\exp(h/\alpha) - 1)}{h^2\ (\exp(h/\alpha) - 1)} \leq 0. \tag{65}$$

From (65), we deduce $-2\ k\ h + (k^2 - k\ h)\ (\exp(h/\alpha) - 1) \leq 0$, which on expansion and simplification gives $(\exp(h/\alpha) - 1)\ (k - h) \leq 0$.
Since $\exp(h/\alpha) - 1 \geq 0$, therefore,

$$k \leq h. \tag{66}$$

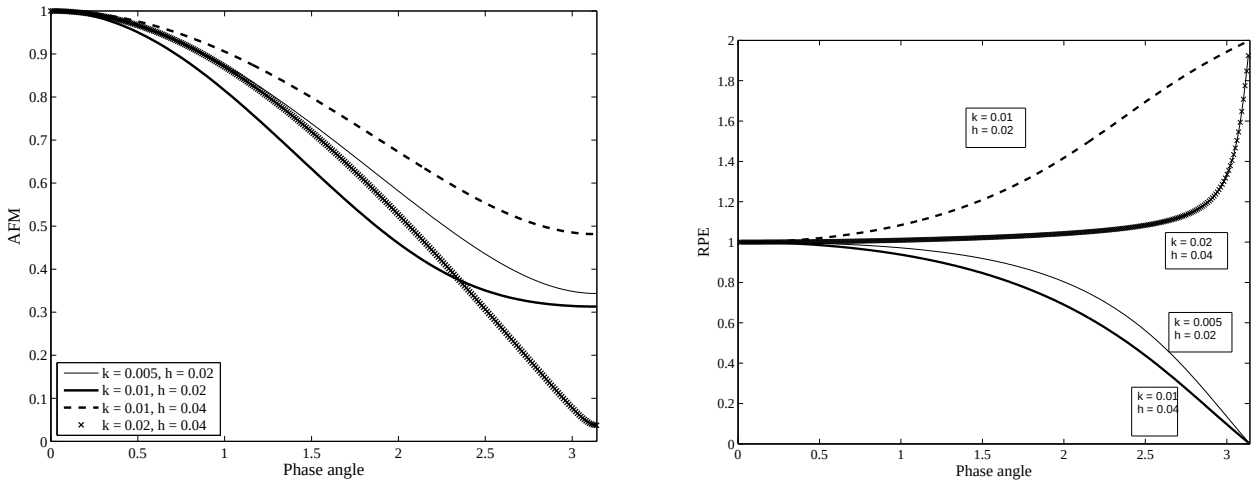
Combining (62) and (66), we obtain (62) and therefore the region of stability is decribed by

$$k \leq \frac{\exp(h/\alpha) - 1}{\exp(h/\alpha) + 1}\ h. \tag{67}$$

Case 1:
If $h = 0.02$, using (62), we have $k \leq 0.01523$. Hence, for $h = 0.02$ and $c = 0.25$, we have $k = 0.005$. Also, for $h = 0.02$ and $c = 0.5$, we have $k = 0.010$. However, if $h = 0.02$ and $c = 1.0$, we have $k = 0.020$ but this combination will give rise to an unstable method.

Case 2:
When $h = 0.04$, we require $k \leq 0.0386$ for stability. Therefore, for $h = 0.04$, we consider $k = 0.01$ and 0.02.

Plots of the AFM and RPE versus phase angle are shown in Figs. (6(a)) and (6(b)) respectively.



(a) AFM (b) RPE

Figure 6: Plot of AFM and RPE, vs phase angle

The NSFD scheme considered is an explicit one and we have four combinations of k and h namely;
(i) $k = 0.005$, $h = 0.02$
(ii) $k = 0.01$, $h = 0.02$.
(iii) $k = 0.01$, $h = 0.04$.
(iv) $k = 0.02$, $h = 0.04$.

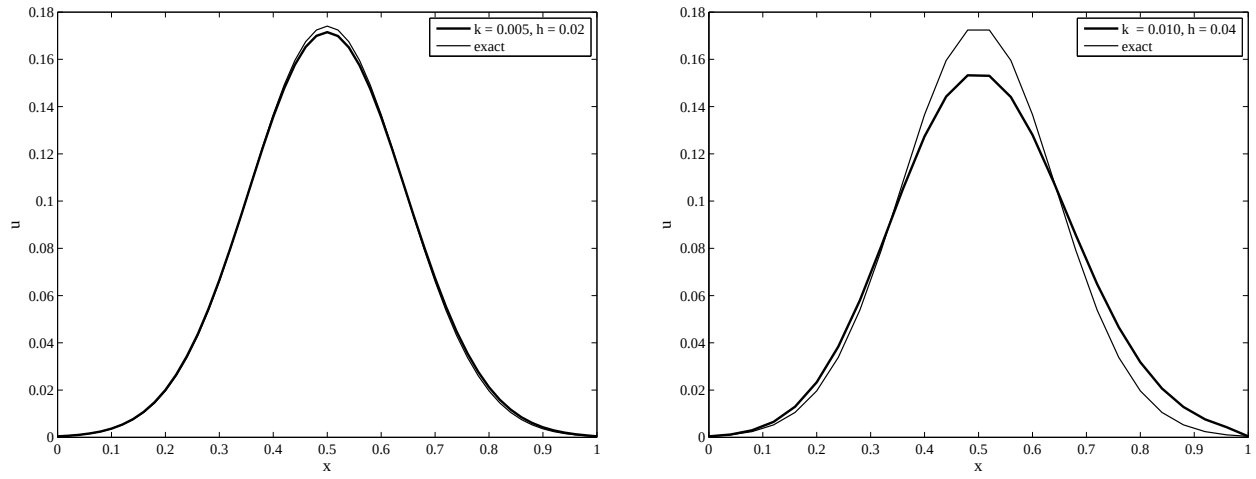
The scheme is least dissipative when $k = 0.01, h = 0.04$ and $k = 0.005, h = 0.02$. The scheme is least dispersive when $k = 0.02$, $h = 0.04$. The scheme experience both phase lead and phase lag behaviour, depending on the values of k and h.

The modified equation is given by

$$u_t + u_x + \frac{1}{2}\ h\ \left(ac - 1 - \frac{1}{\exp(h/\alpha) - 1}\right)\ u_{xx} + \frac{1}{6}\ h^2\ (1 - c^2 - 6s)\ u_{xxx} + ... = 0, \tag{68}$$

and this indicates that the leading error terms are dissipative. We tabulate the errors in Table (3) and we observe that the errors are least when $k = 0.005$ and $h = 0.02$ and greatest when $k = 0.02$ and

$h = 0.04$.



(a) (b)

Figure 7: Comparison of numerical results with exact results using NSFD scheme at some values of k and h.

Table 3: Errors for NSFD scheme

k	h	cfl	E_{num}	$max\|u_e - u_c\|$	Error at $(0.5, 1.0)$	Diss. Error	Disp. Error
0.005	0.02	0.25	8.7288×10^{-4}	0.0026	0.0026	8.0435×10^{-7}	5.5063×10^{-7}
0.01	0.02	0.50	0.0028	0.0085	-0.0084	8.3500×10^{-6}	5.8963×10^{-6}
0.01	0.04	0.25	0.0068	0.0194	0.0192	4.8616×10^{-5}	3.2639×10^{-5}
0.02	0.04	0.50	0.0010	0.0032	0.0032	8.7192×10^{-7}	1.0934×10^{-6}

Based on Tables (1), (2) and (3), we can see that the Lax-Wendroff and the NSFD schemes are most effective when $k = 0.005$ and $h = 0.02$. The errors are smaller for the Lax-Wendroff as compared to NSFD scheme when $k = 0.005$ and $h = 0.02$.

8 Optimising parameters in the Lax-Wendroff and NSFD scheme

Our aim in this section is to compute an optimal value of k for a given value of h, say $h = 0.02$. By optimal, we mean a value which reduces the errors. Since the partial differential equation considered is slightly dissipative and not dispersive, we aim to minimize the dispersion error of the scheme.

8.1 Proposed techniques of optimisation

Tam and Webb [21], Bogey and Bailly [5] among others have implemented techniques which enable coefficients to be determined in numerical schemes specifically designed for Computational Aeroacoustics. We develop these techniques into respective equivalent forms to determine the optimal value of k for the NSFD scheme [3].

We now describe briefly how Tam and Webb [21], Bogey and Bailly [5] define their measures and consequently their technique of optimisation in Computational Aeroacoustics.
The Dispersion-Relation-Preserving (DRP) scheme was designed so that the dispersion relation of the finite difference scheme is formally the same as that of the original partial differential equations. The integrated error is defined as

$$E = \int_{-\eta}^{\eta} |\theta^* h - \theta h|^2 \; d(\theta h),$$

where the quantities $\theta^* h$ and θh represent the numerical and exact wavenumbers respectively. The dispersion error and dissipation error are calculated as $|\Re(\theta^* h) - \theta h|$ and $|Im(\theta^* h)|$ respectively.

Tam and Shen [22] set η as 1.1 and optimise the coefficients in the numerical scheme such that the integrated error is minimised.
Bogey and Bailly [5] minimise the relative difference between the exact wavenumber, θh and the effective/numerical wavenumber, $\theta^* h$ and define their integrated errors as

$$E = \int_{(\theta h)_l}^{(\theta h)_h} \frac{|\theta^* h - \theta h|}{\theta h} \; d(\theta h), \tag{69}$$

or

$$E = \int_{\ln\ (\theta h)_l}^{\ln\ (\theta h)_h} |\theta^* h - \theta h| \; d(\ln\ (\theta h)). \tag{70}$$

In Computational Fluid Dynamics for a particular method under consideration, the dispersion error is calculated as

$$|1 - RPE|.$$

We have modified the measures used by Tam and Webb, Bogey and Bailly in a Computational Aeroacoustics framework to suit them in a Computational Fluid Dynamics framework [3] such that the optimal parameter can be obtained. Thus, we define the following integrals: Integrated Error from Tam and Webb, **(IETAM)**, Integrated Error from Bogey and Bailly **((IEBOGEY)** as follows:

$$\mathbf{IETAM} = \int_0^{w_1} |1 - RPE|^2 \; dw, \tag{71}$$

$$\mathbf{IEBOGEY} = \int_0^{w_1} |1 - RPE| \; dw, \tag{72}$$

8.2 Optimisation procedure

Lax-Wendroff
We consider the Lax-Wendroff scheme given by Eq. (37), with $h = 0.02$. The amplification factor of the resulting method is

$$\xi_{LW} = 1 - 50\ k - 2500\ k^2 + (50\ k + 2500\ k^2)\ \cos(w) - 50\ k\ \sin(w)\ I, \tag{73}$$

and thefore the RPE is computed as

$$RPE_{LW} = \frac{0.02}{k\ w} \tan^{-1}\Big(\frac{\Im(\xi_{LW})}{\Re(\xi_{LW})}\Big). \tag{74}$$

A plot of the exact RPE vs $w \in [0, \pi]$ is shown in Fig. (8) and we do not have phase wrapping phenomenon. We propose two measures, one adapted from Tam and Webb [21] and the other from Bogey and Bailly [5].

We compute the following

$$\textbf{IETAM} = \int_0^{1.1} (RPE_{LW} - 1)^2 \, dw, \tag{75}$$

and

$$\textbf{IEBOGEY} = \int_0^{1.1} |RPE_{LW} - 1| \, dw. \tag{76}$$

We plot the integrated errors vs k and obtain the optimal value of k. We can also use the function NLPSolve from Maple to determine the value of k which minimise each of these two integrals. In the case of **IETAM**, we obtain,

$$k = 0.00615029705055891978$$

while in the case of **IEBOGEY**, we are out with

$$k = 0.006112886302132816582.$$

We next validate whether this value of k computed does indeed minimise the errors by performing the numerical experiment using Lax-Wendroff with $h = 0.02$ at some different values of $k \in (0, 0.01236)$ and then compare the errors. The errors are tabulated in Table (4) and we can see that indeed for $k = 1/164 \approx 0.00601$, all the five types of errors are least.

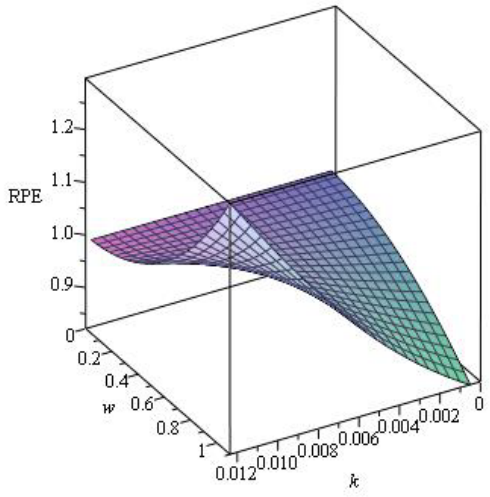
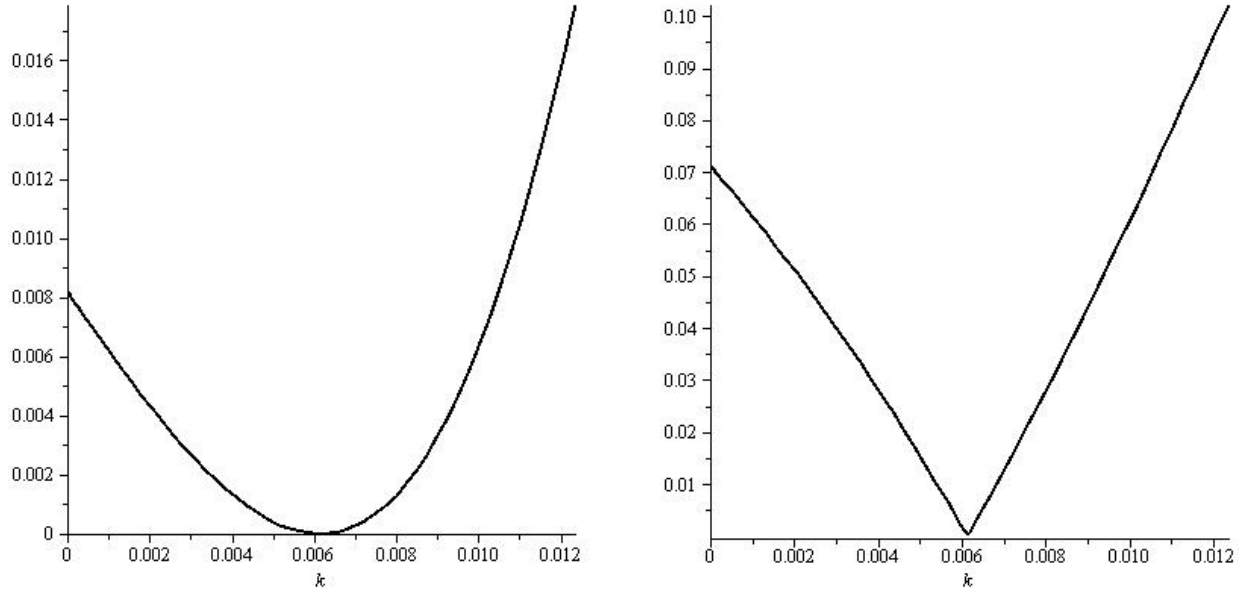


Figure 8: Plot of RPE vs k vs w for the Lax-Wendroff scheme at $h = 0.02$.



(a) IETAM (b) IEBOGEY

Figure 9: Plots of **IETAM** vs k and **EBOGEY** vs k for the Lax-Wendroff scheme when $h = 0.02$.

Table 4: Errors for the Lax-Wendroff scheme for $h = 0.02$

k	E_{num}	$max\|u_e - u_c\|$	Error at $(0.5, 1.0)$	Diss. Error	Disp. Error
0.001	8.2049×10^{-4}	0.0026	6.3090×10^{-4}	1.0506×10^{-7}	1.1375×10^{-6}
0.002	6.6803×10^{-4}	0.0021	5.1728×10^{-4}	7.1763×10^{-8}	7.5203×10^{-7}
1/333	5.1018×10^{-4}	0.0016	4.0089×10^{-4}	4.3376×10^{-8}	4.3728×10^{-7}
0.004	3.4840×10^{-4}	0.0011	2.8318×10^{-4}	2.1247×10^{-8}	2.0307×10^{-7}
0.005	1.8166×10^{-4}	5.8157×10^{-4}	1.6348×10^{-4}	6.3582×10^{-9}	5.4502×10^{-8}
1/164	1.3952×10^{-5}	4.3926×10^{-5}	3.0697×10^{-5}	1.1388×10^{-11}	3.6197×10^{-10}
1/143	1.6764×10^{-4}	5.3721×10^{-4}	-7.8352×10^{-5}	3.8582×10^{-9}	4.7968×10^{-8}
1/125	3.5162×10^{-4}	0.0011	-2.0134×10^{-4}	1.9362×10^{-8}	2.0827×10^{-7}
1/111	5.4133×10^{-4}	0.0017	-3.2451×10^{-4}	4.8426×10^{-8}	4.9113×10^{-7}
0.01	0.0011	0.0035	-6.5674×10^{-4}	2.1234×10^{-7}	1.9665×10^{-6}

NSFD

We consider the NSFD scheme given by Eq. (7(a)), with $h = 0.02$. The amplification factor of the resulting method is

$$\xi_{NSFD} = 1 + 65.65176427\ k\ (\cos(w) - 1) - 50\ (k\ \sin(w))\ I, \tag{77}$$

and thefore the RPE is computed as

$$RPE_{NSFD} = \frac{1}{\alpha_1\ w} \tan^{-1}\Big(\frac{\Im(\xi_{NSFD})}{\Re(\xi_{NSFD})}\Big), \tag{78}$$

where $\alpha_1 = \dfrac{k}{h}$.

A plot of the exact RPE vs $e \in [0, \pi]$ is shown in Fig. (10) and we do not have phase wrapping phenomenon. We propose two measures, one adapted from Tam and Webb [21] and the other from Bogey and Bailly [5].
We compute the following

$$\textbf{IETAM} = \int_0^{1.1} (RPE_{NSFD} - 1)^2 \, dw, \tag{79}$$

and

$$\textbf{IEBOGEY} = \int_0^{1.1} |RPE_{NSFD} - 1| \, dw. \tag{80}$$

We plot the integrated errors vs k and obtain the optimal value of k. We can also use the function NLPSolve from Maple to determine the value of k which minimise each of these two integrals. In the case of **IETAM**, we obtain,

$$k = 0.00611388415557632438$$

while in the case of **IEBOGEY**, we are out with

$$k = 0.00611348537281972832.$$

We next validate whether this value of k computed does indeed minimise the errors by performing the numerical axperiment using NSFD with $h = 0.02$ at some different values of $k \in (0, 0.01523)$ and then compare the errors. The errors are tabulated in Table (5) and we can see that indeed for $k = 1/164 \approx 0.00601$, all the five types of errors are least.

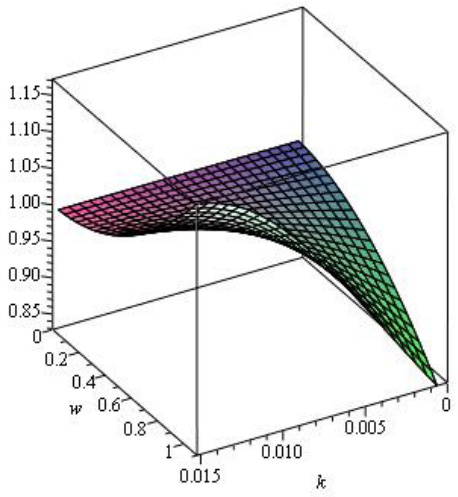
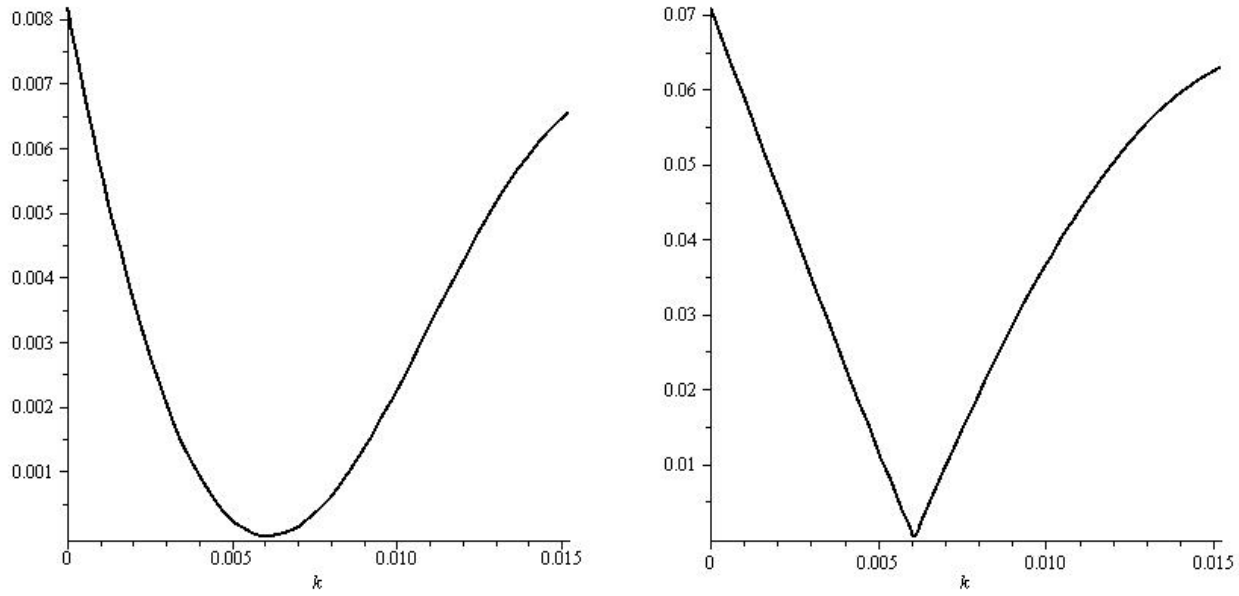


Figure 10: Plot of RPE vs k vs w for the NSFD scheme at $h = 0.02$.



(a) IETAM

(b) IEBOGEY

Figure 11: Plots of **IETAM** vs k and **EBOGEY** vs k

Table 5: Errors for NSFD scheme for $h = 0.02$

k	E_{num}	$max\|u_e - u_c\|$	Error at $(0.5, 1.0)$	Diss. Error	Disp. Error
0.001	0.0035	0.0100	0.0100	1.2802×10^{-5}	8.0987×10^{-6}
0.002	0.0028	0.0083	0.0083	8.6039×10^{-6}	5.5211×10^{-6}
1/333	0.0022	0.0064	0.0064	5.1527×10^{-6}	3.3593×10^{-6}
0.004	0.0015	0.0045	0.0045	2.5390×10^{-6}	1.6870×10^{-6}
0.005	8.7288×10^{-4}	0.0026	0.0026	8.0435×10^{-7}	5.5063×10^{-7}
1/164	1.1717×10^{-4}	3.5591×10^{-4}	3.4999×10^{-4}	1.2220×10^{-8}	1.2981×10^{-8}
1/143	5.2775×10^{-4}	0.001578	-0.001536	3.0107×10^{-7}	1.9762×10^{-7}
1/125	0.00126	0.003795	-0.00373	1.7163×10^{-6}	1.1639×10^{-6}
1/111	0.00201955	0.00610955	-0.0060209	4.3904×10^{-6}	3.0429×10^{-6}
0.01	0.002783	0.008479	-0.0083559	8.3500×10^{-6}	5.8963×10^{-6}

9 Conclusion

In this paper, three numerical methods have been used to solve a 1-D advection-diffusion equation with specified initial and boundary conditions. Both explicit and implicit finite difference methods as well as a non-standard finite difference scheme have been used. The results are much affected by the choice of k and h. In general, we observe that the Lax-Wendroff scheme is the most efficient method followed by the Non-Standard Finite Difference scheme. We perform two optimisation procedures by computing the optimal values of k when $h = 0.02$ for the Lax-Wendroff and NSFD schemes. We observe that when $k \approx 0.006$, the errors are reduced further for both methods.
This work can be extended to the case when α is large. Also, we can consider numerical solution of 1-D non-linear as well as 2-D linear and 2-D non-linear convection-diffusion problems and we can use appropriate optimisation techniques to choose parameters h and k for minimal numerical dispersion and numerical dissipation.

Nomenclature

$I = \sqrt{(-1)}$
k: time step
h: spatial step
n: time level
a: advection velocity
c: $cfl/Courant$ number
$c = \dfrac{ak}{h}$
$s = \dfrac{\alpha k}{h^2}$
w: phase angle in 1-D
$w = \theta h$
RPE: relative phase error per unit time step
AF: amplification factor
$AFM = |AF|$
Diss. Error:Dissipation Error
Disp. Error:Dispersion Error

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