Numerical Schemes for Partial Difference Equation in Physics

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Abstract. This paper examines various numerical schemes for 1-D and 2-D advection and diffusion equations using MATLAB, focusing on stability, accuracy, and performance under different boundary conditions [1]. For 1-D advection, methods such as the upwind, implicit upwind, Beam-Warming(B-W), Lax-Friedrichs(L-F), and Lax-Wendroff(L-W) schemes are evaluated. The implicit upwind scheme delivers consistent results, the Beam-Warming scheme works well under specific conditions, while the upwind scheme shows dissipation and dispersion. In 2-D advection, the upwind and Lax-Friedrichs schemes are tested, with the upwind scheme being more stable with discontinuities but less stable for smooth solutions. For diffusion, the Classical, Dufort-Frankel(D-F), and Crank-Nicolson(C-N) schemes are analyzed. The Crank-Nicolson scheme proves to be the most accurate, while the Classical scheme is fast but mesh-dependent, and the Dufort-Frankel scheme is stable but introduces minor fluctuations. The paper suggests using operator splitting to improve 2-D advection stability.

Keywords: Numerical Scheme, Diffusion Equation, Advection Equation, Partial Differential Equation

1 Introduction

1.1 Objectives

Our research aims to analyze the different numerical schemes used in various physical equations,and achieve the following three objectives: [2]
1.Analysis the stability of the numerical schemes.
2.Examine how changes in the advection speed a affect the numerical solution.
3.Investigate the impact of different initial conditions.

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1.2 Significance of the Study

For physical equations with extremely large computational demands or those without analytical solutions, directly seeking numerical solutions is impractical. [3] This research can be utilized to assist in selecting appropriate numerical schemes for numerical simulations of physical equations. Depending on the required resolution, boundary conditions, and initial conditions, different numerical models can be chosen accordingly.

2 Theoretical Background

2.1 Physical Significance of the Equations

2.1.1 1-Dimension Advection Equation

Here we present the 1-dimensional advection equation:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \tag{1}$$

Define $u(x,t)$ the quantity being transfered (e.g., temperature, concentration). t is time. x is the spatial coordinate. a is the advection speed, a constant representing the propagation speed of the substance in space.

This equation describes the propagation process of a substance in one direction. During this propagation, the concentration of the substance changes over time and space. If $a > 0$, it indicates that the substance propagates in the positive direction; if $a < 0$, it indicates that the substance propagates in the negative direction.

2.1.2 2-Dimension Advection Equation

Here we present the 2-dimensional advection equation:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} = 0 \tag{2}$$

It has the same physical significance as the one-dimensional case, but it needs to consider both directions in two dimensions.

2.1.3 Diffusion Equation

Similarly we present the diffusion equation:

$$\frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2} \tag{3}$$

We define u(x,t) is the quantity being diffused (e.g., temperature, concentration). t is time. x is the spatial coordinate. a is the diffusion coefficient, a positive constant that represents the rate at which diffusion occurs.

In various fields, the diffusion equation is applied to different aspects, such as studying how heat propagates through materials in thermodynamics and analyzing molecular motion in chemistry. However, their fundamental significance shares similarities.

The diffusion equation captures the essential idea that the change in the quantity at any point is proportional to the curvature of the distribution. High curvature (steep gradients) leads to rapid change, while low curvature leads to slower change.

2.2 Stability Analysis

To facilitate the discussion, we study the difference scheme within a relatively abstract framework. Consider the differential equation [4]:

$$Lu = 0$$

The corresponding difference scheme is:

$$L_h u_j^n = 0$$

2.2.1 Advection Equation

where L_h is a grid function mapping that depends on the spatial grid step h and the temporal grid step τ, known as the difference operator, and u_j^n is the grid function defined at (x_j, t_n). For example, for the problem where $Lu = u_t + au_x$, discretizing u_t with a first-order forward difference and u_x with a first-order backward difference, we obtain the following upwind scheme:

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_j^n - u_{j-1}^n}{h} = 0.$$

Direct computation shows that the truncation error of this scheme is $O(\tau + h)$ (Note: This paper focuses on the stability analysis of numerical schemes, so for certain numerical schemes, only the error order is provided without detailed computation and analysis). The growth factor is:

$$G(\tau, k) = a\lambda e^{-ikh} + (1 - a\lambda),$$

where $\lambda = \tau/h$ is the mesh ratio. The necessary and sufficient condition for the stability of the scheme is $a\lambda \leq 1$.

Let $u(x,t)$ be a sufficiently smooth solution of the differential equation (3.17). If $u_j^n = u(x_j, t_n)$, then we have:

$$L_h u_j^n = O(\tau^p + h^q).$$

Now, we present the method of undetermined coefficients for constructing difference schemes. Assume the desired scheme is a two-level difference scheme of the following form:

$$L_h u_j^n = u_j^{n+1} - \sum_{k=-1}^{1} \alpha_k u_{j+k}^n = 0. \tag{4}$$

The objective is to find the parameters α_k such that the above scheme has the highest possible truncation error order. Let u be a sufficiently smooth solution to the problem (). Denote $x = x_j, t = t_n$, and abbreviate $u(x,t)$ as u (partial derivatives of u are treated similarly). By the Taylor expansion, we have:

$$u(x_j, t_{n+1}) = u + u_t \tau + \frac{1}{2}\tau^2 u_{tt} + O(\tau^3),$$
$$u(x_j + lh, t_n) = u + u_x lh + \frac{1}{2} l^2 h^2 u_{xx} + O(h^3).$$

Substituting the grid function $u_j^n = u(x_j, t_n)$ into equation 4, and using the above expansions and the differential equation, we obtain:

$$\begin{aligned} L_h u_j^n &= \left(1 - \sum_{l=-1}^{1} \alpha_l\right) u + u_t \tau - \sum_{l=-1}^{1} \alpha_l l h u_x \\ &\quad + \frac{1}{2} u_{tt} \tau^2 - \sum_{l=-1}^{1} \frac{1}{2} (lh)^2 \alpha_l u_{xx} + O(h^3) \\ &= \left(1 - \sum_{l=-1}^{1} \alpha_l\right) u - \left(a\lambda + \sum_{l=-1}^{1} \alpha_l l\right) h u_x \\ &\quad + \frac{1}{2}\left(a^2\lambda^2 - \sum_{l=-1}^{1} \alpha_l l^2\right) h^2 u_{xx} + O(h^3). \end{aligned}$$

Setting the coefficients of the low-order terms in the above expansion to zero, we obtain:

$$\begin{cases} \alpha_{-1} + \alpha_0 + \alpha_1 = 1 \\ -\alpha_{-1} + \alpha_1 = -a\lambda \\ \alpha_{-1} + \alpha_1 = a^2\lambda^2 \end{cases}$$

Thus,

$$\begin{cases} \alpha_{-1} = \frac{1}{2}(a\lambda + a^2\lambda^2), \\ \alpha_0 = 1 - a^2\lambda^2, \\ \alpha_1 = \frac{1}{2}(a^2\lambda^2 - a\lambda). \end{cases}$$

Hence, we obtain the Lax-Wendroff scheme for solving the initial value problem (3.2) of the convection equation:

$$u_j^{n+1} = u_j^n - \frac{a\lambda}{2}(u_{j+1}^n - u_{j-1}^n) + \frac{a^2\lambda^2}{2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n).$$

From the construction of the algorithm, it is easy to see that the truncation error of this scheme is $O(\tau^2+h^2)$. Let $u_j^n = v^n e^{ijkh}$, substituting into equation (4.5) yields the growth factor:

$$G(\tau,k) = 1 - \frac{a\lambda}{2}(e^{ikh} - e^{-ikh}) + \frac{a^2\lambda^2}{2}(e^{ikh} - 2 + e^{-ikh})$$
$$= 1 - 2a^2\lambda^2 \sin^2\left(\frac{kh}{2}\right) - ia\lambda \sin(kh).$$

Thus,

$$|G(\tau,k)|^2 = 1 - 4a^2\lambda^2(1-a^2\lambda^2)\sin^4\left(\frac{kh}{2}\right),$$

Therefore, from $|G|^2 \leq 1$, we obtain the stability condition for the Lax-Wendroff scheme as $a\lambda \leq 1$.

For the equation (), discretizing u_t using a first-order forward difference and u_x using a first-order central difference, we obtain the following difference scheme:

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_{j+1}^n - u_{j-1}^n}{2h} = 0.$$

Using the Fourier stability criterion, it can be shown that this scheme is unstable. However, replacing u_j^n with $\frac{1}{2}(u_{j-1}^n + u_{j+1}^n)$ yields the following Lax-Friedrichs scheme:

$$\frac{u_j^{n+1} - \frac{1}{2}(u_{j-1}^n + u_{j+1}^n)}{\tau} + a\frac{u_{j+1}^n - u_{j-1}^n}{2h} = 0.$$

The truncation error of this scheme is:

$$\frac{\tau}{2}u_{tt} + \frac{h^2}{6}u_{xxx}.$$

From the stability condition of the Lax-Friedrichs scheme, we have $a\lambda \leq 1$.

Characteristics are an important tool in studying the qualitative theory of hyperbolic equations. In fact, they are also helpful in constructing difference schemes for hyperbolic equations. The characteristic line for the convection equation (4.1) is given by:

$$L: \frac{\mathrm{d}x}{\mathrm{d}t} = a,$$

that is,

$$x = at + x_0,$$

where x_0 is the x-coordinate of the intersection of the characteristic line with the x-axis. Along the characteristic line L, the solution u remains constant. Thus, determining the grid function value at the $n+1$-th time level translates to determining the value of the solution at the corresponding point on the n-th time level. If Q happens to be a grid node, the difference scheme is already obtained. If it is not a grid point, the value of u at point Q can be approximated using interpolation based on the grid function values given at the n-th time level, thereby obtaining the difference scheme.

If a quadratic interpolation is performed using the grid function values $u_j^n, u_{j-1}^n, u_{j-2}^n$, the following Beam-Warming scheme is obtained:

$$u_j^{n+1} = u_j^n - a\lambda(u_j^n - u_{j-1}^n) - \frac{a\lambda}{2}(1-a\lambda)(u_j^n - 2u_{j-1}^n + u_{j-2}^n).$$

This scheme is also known as the second-order upwind scheme. Through standard calculations, it is found that the growth factor of this scheme is:

$$G(\tau,k) = 1 - 2a\lambda\sin^2\left(\frac{kh}{2}\right) - a\lambda(1-a\lambda)\left(2\sin^4\left(\frac{kh}{2}\right) - \frac{1}{2}\sin^2(kh)\right)$$
$$-\mathrm{i}a\lambda\sin(kh)\left[1 + 2(1-a\lambda)\sin^2\left(\frac{kh}{2}\right)\right].$$

Thus,

$$|G|^2 = 1 - 4a\lambda(1-a\lambda)^2(2-a\lambda)\sin^4\left(\frac{kh}{2}\right).$$

Therefore, from $|G|^2 \le 1$, the stability condition is $a\lambda \le 2$.

This paper focuses on [5] [6]:

1. Upwind Scheme:

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_j^n - u_{j-1}^n}{h} = 0 \tag{5}$$

2. Lax-Friedrichs Scheme:

$$\frac{u_j^{n+1} - \frac{1}{2}(u_{j-1}^n + u_{j+1}^n)}{\tau} + a\frac{u_{j+1}^n - u_{j-1}^n}{2h} = 0 \tag{6}$$

3. Lax-Wendroff Scheme:

$$u_j^{n+1} = u_j^n - \frac{a\lambda}{2}(u_{j+1}^n - u_{j-1}^n) + \frac{a^2\lambda^2}{2}(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \tag{7}$$

4. Beam-Warming Scheme:

$$u_j^{n+1} = u_j^n - a\lambda(u_j^n - u_{j-1}^n) - \frac{a\lambda}{2}(1-a\lambda)(u_j^n - 2u_{j-1}^n + u_{j-2}^n) \tag{8}$$

For the two-dimensional wave equation, the above schemes can be easily generalized to obtain the corresponding numerical schemes and their stability conditions:

1. 2D Upwind Scheme:

$$\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\tau} + a\frac{u_{i,j}^n - u_{i-1,j}^n}{h} + b\frac{u_{i,j}^n - u_{i,j-1}^n}{h} = 0 \tag{9}$$

2. 2D Lax-Friedrichs Scheme:

$$\frac{u_{i,j}^{n+1} - \frac{1}{4}(u_{i-1,j}^n + u_{i+1,j}^n + u_{i,j-1}^n + u_{i,j+1}^n)}{\tau} + a\frac{u_{i+1,j}^n - u_{i-1,j}^n}{2h} + b\frac{u_{i,j+1}^n - u_{i,j-1}^n}{2h} = 0 \tag{10}$$

2.2.2 Diffusion Equation

For the heat (diffusion) equation:

$$u_t = a u_{xx}$$

we present several typical difference schemes [6] for the numerical solution of the initial value problem, where $a > 0$ is a given constant representing the thermal conductivity (diffusion) coefficient.

1. Classical Scheme: For equation (5.1), using a forward difference for u_t and a central difference for u_{xx}, we obtain the four-point explicit scheme:

$$\frac{u_j^{n+1} - u_j^n}{\tau} - a\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} = 0.$$

It is easy to see that the truncation error of this scheme is $O(\tau + h^2)$. Rewriting (5.2), we get:

$$u_j^{n+1} = u_j^n + a\lambda\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right),$$

where $\lambda = \tau/h^2$ is the grid ratio. Substituting $u_j^n = v^n e^{ijkh}$, $k \in \mathbb{R}$, into the above equation, we obtain $v^{n+1} = Gv^n$, where the growth factor G is:

$$G(\tau, k) = 1 - 4a\lambda \sin^2\left(\frac{kh}{2}\right).$$

According to the von Neumann condition, the necessary and sufficient condition for the stability of scheme (5.2) is $a\lambda \leq 1/2$.

If we perform differencing in the x-direction at time level t_{n+1}, we can obtain the implicit scheme for solving the advection equation:

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_j^{n+1} - u_{j-1}^{n+1}}{h} = 0$$

The amplification factor for this scheme is $G(\tau, k) = \frac{1}{1 + a\lambda - e^{-ikh}}$, which is unconditionally stable.

2. Weighted Implicit Scheme: [7] The difference equation for this scheme is:

$$\frac{u_j^n - u_j^{n-1}}{\tau} - a\left[\theta\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} + (1-\theta)\frac{u_{j+1}^{n-1} - 2u_j^{n-1} + u_{j-1}^{n-1}}{h^2}\right] = 0,$$

where $\theta \in [0, 1]$ is the weight. Equation (5.3) is:

$$\begin{aligned} &-a\lambda\theta u_{j+1}^n + (1 + 2a\lambda\theta)u_j^n - a\lambda\theta u_{j-1}^n \\ &= a\lambda(1-\theta)u_{j+1}^{n-1} - [1 + 2a\lambda(1-\theta)]u_j^{n-1} + a\lambda(1-\theta)u_{j-1}^{n-1}. \end{aligned}$$

Direct calculations show that the truncation error of the above scheme is:

$$E_h = L_h u_j^n = a\left(\frac{1}{2} - \theta\right)\tau\partial_{txx}u + O(\tau^2 + h^2).$$

Thus, when $\theta \neq \frac{1}{2}$, the truncation error is $O(\tau + h^2)$. When $\theta = \frac{1}{2}$, the truncation error is $O(\tau^2 + h^2)$, achieving second-order accuracy. In this case, the scheme is known as the Crank-Nicolson scheme:

$$\frac{u_j^n - u_j^{n-1}}{\tau} - a\left(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{2h^2} + \frac{u_{j+1}^{n-1} - 2u_j^{n-1} + u_{j-1}^{n-1}}{2h^2}\right) = 0.$$

Direct calculation shows that the growth factor of scheme (5.3) is:

$$G(\tau, k) = \frac{1 - 4(1-\theta)a\lambda\sin^2\left(\frac{kh}{2}\right)}{1 + 4\theta a\lambda\sin^2\left(\frac{kh}{2}\right)}.$$

From

$$|G(\tau, k)| \leq 1,$$

we get

$$4a\lambda(1-2\theta)\sin^2\left(\frac{kh}{2}\right) \leq 2.$$

3. Richardson Scheme:

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\tau} - a\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} = 0$$

is unstable. However, if u_j^n is replaced with $\frac{u_j^{n+1} + u_j^{n-1}}{2}$, we obtain the Dufort-Frankel scheme:

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\tau} - a\frac{u_{j+1}^n - \left(u_j^{n+1} + u_j^{n-1}\right) + u_{j-1}^n}{h^2} = 0.$$

This is a three-level explicit scheme [8], which is unconditionally stable.

This paper focuses on:

Classical explicit scheme

$$\frac{u_j^{n+1} - u_j^n}{\tau} - a\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} = 0 \tag{11}$$

Classical implicit scheme

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_j^{n+1} - u_{j-1}^{n+1}}{h} = 0 \tag{12}$$

Crank-Nicolson scheme:

$$\frac{u_j^n - u_j^{n-1}}{\tau} - a(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{2h^2} + \frac{u_{j+1}^{n-1} - 2u_j^{n-1} + u_{j-1}^{n-1}}{2h^2}) = 0 \tag{13}$$

Richardson Scheme

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\tau} - a\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} = 0 \tag{14}$$

Dufort-Frankel Scheme:

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\tau} - a\frac{u_{j+1}^n - (u_j^{n+1} + u_j^{n-1}) + u_{j-1}^n}{h^2} = 0 \tag{15}$$

3 Results

3.1 1-D Advection

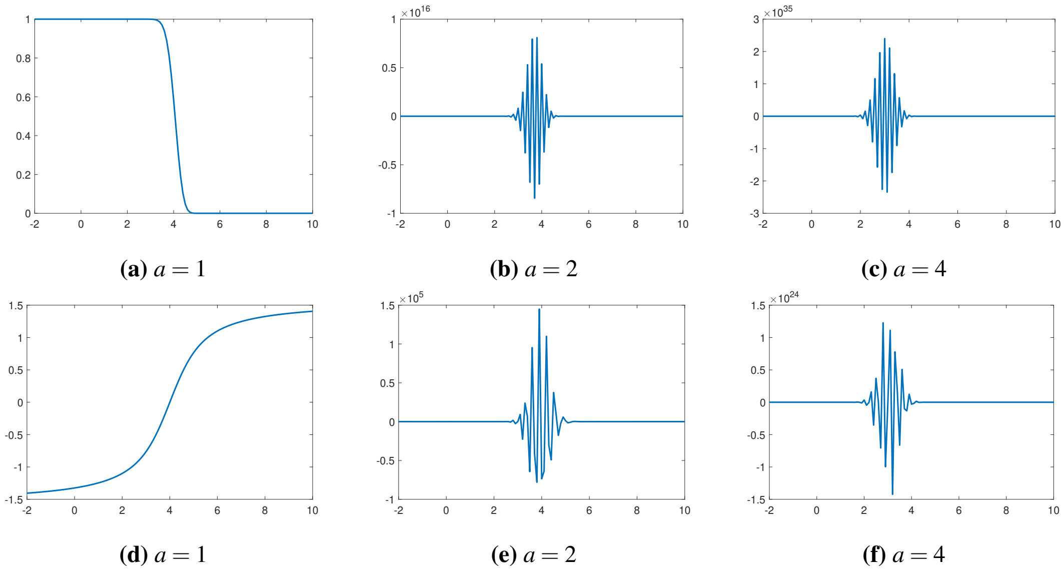
Assuming that a = 1, 2, 4, h = 0.1, τ = 0.08, this work applied upwind scheme, fully implicit scheme, Beam-Warming Scheme, Lax-Friedrichs Scheme, and Lax-Wendroff Scheme to solve 1-D advection numerically. The results when t = 4.0s and -2¡x¡10 are shown below. Based on equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \tag{16}$$

3.1.1 Upwind Scheme

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_j^n - u_{j-1}^n}{h} = 0 \tag{17}$$

From these figures, when the initial condition is a step function, it can be seen that when a = 1, the numerical solution obtained from the upwind scheme can approximate the analytical solution well, while when a = 2, 4, it cannot approximate the analytical solution. Also, when the initial condition is a continuous function, the situation is similar. However, we can tell from the amplitude of fluctuations of different initial conditions that continuous function works better.



(a) $a = 1$ **(b)** $a = 2$ **(c)** $a = 4$

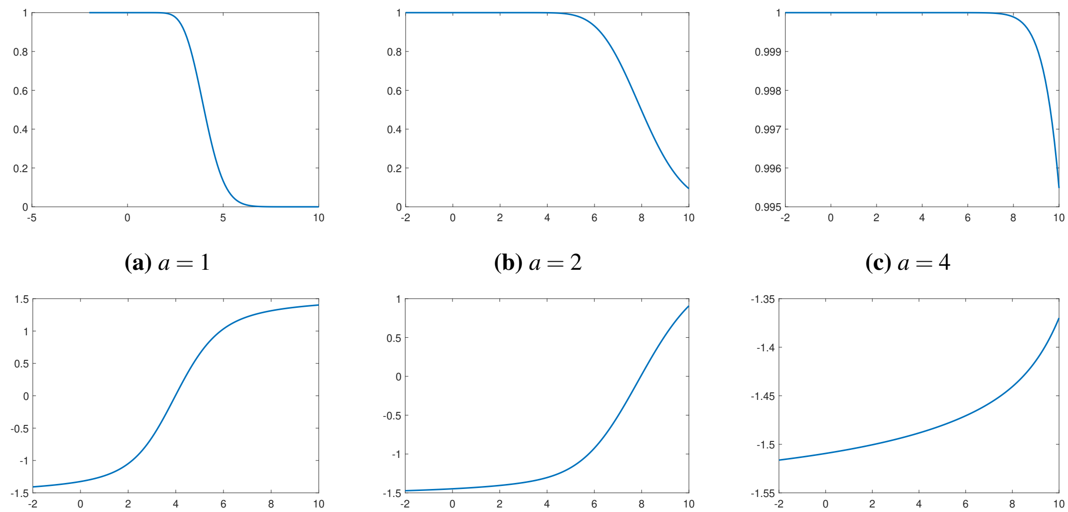
(d) $a = 1$ **(e)** $a = 2$ **(f)** $a = 4$

Fig. 1. Simulation results of 1-D advection in Upwind Scheme. The initial condition of (a)(b)(c) is a step function while the initial condition of (d)(e)(f) a continuous function.

3.1.2 Implicit Upwind Scheme

$$\frac{u_j^{n+1} - u_j^n}{\tau} + a\frac{u_j^{n+1} - u_{j-1}^{n+1}}{h} = 0 \tag{18}$$

In fully implicit scheme, the numerical solution can approximate the analytical solution well all the time, regardless of the initial condition and the value of a.



(a) $a = 1$ **(b)** $a = 2$ **(c)** $a = 4$

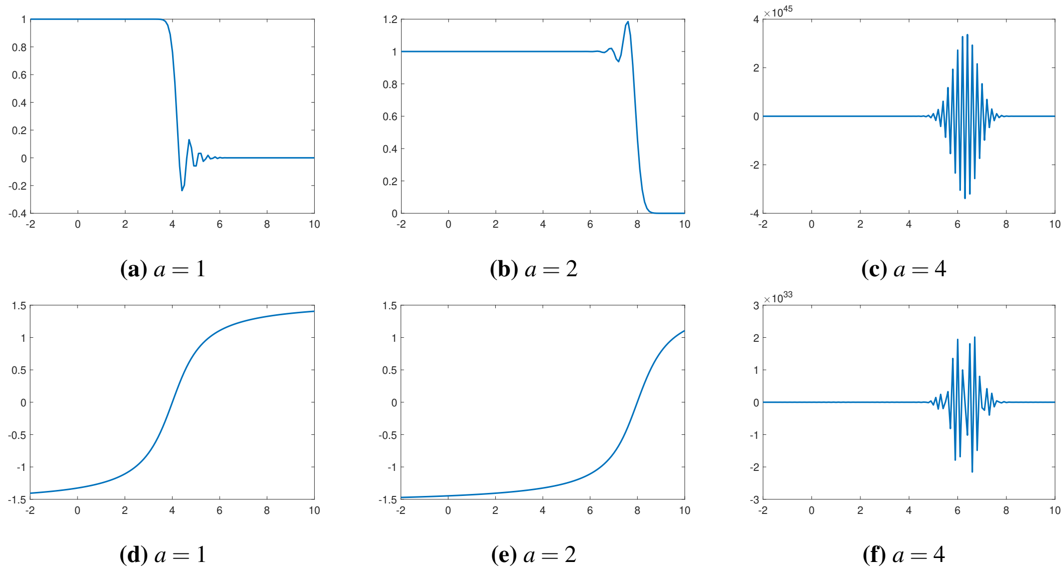
(d) $a = 1$ **(e)** $a = 2$ **(f)** $a = 4$

Fig. 2. Simulation results of 1-D advection in Fully Implicit Scheme. The initial condition of (a)(b)(c) is a step function while the initial condition of (d)(e)(f) a continuous function.

3.1.3 Beam-Warming Scheme

$$u_j^{n+1} = u_j^n - a\lambda(u_j^n - u_{j-1}^n) - \frac{a\lambda}{2}(1-a\lambda)(u_j^n - 2u_{j-1}^n + u_{j-2}^n) \tag{19}$$

From these figures, when the initial condition is a step function, it can be seen that when $a = 1$, 2, the numerical solution obtained from the Beam-Warming Scheme can approximate the analytical solution well, However, there are ringings resulting from discontinuity. When $a = 4$, it cannot approximate the analytical solution. When the initial condition is a continuous function and $a = 1$, 2, there is no fluctuation. When $a = 4$, the amplitude of fluctuations are smaller than the 1st condition. Beam-Warming Scheme works better under this initial condition



(a) $a = 1$ **(b)** $a = 2$ **(c)** $a = 4$

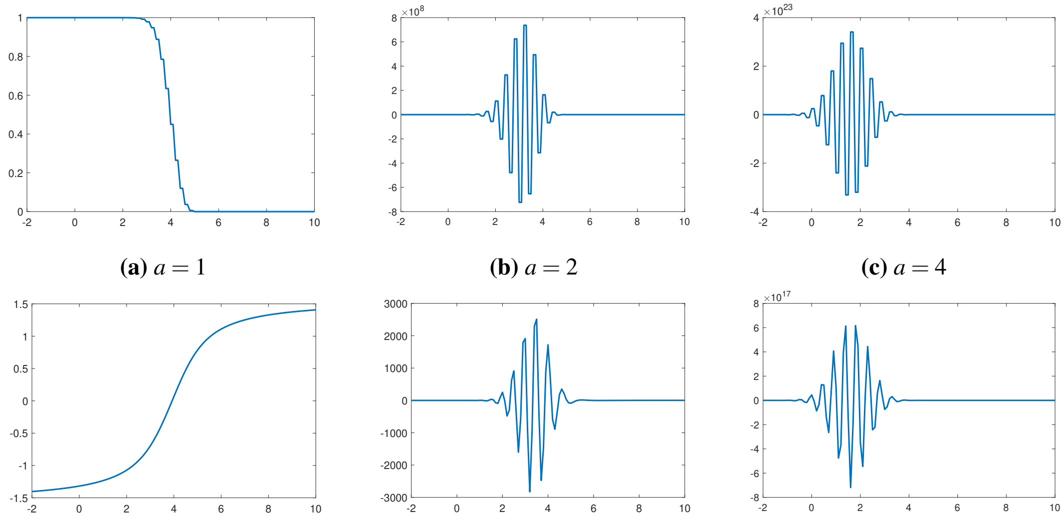
(d) $a = 1$ **(e)** $a = 2$ **(f)** $a = 4$

Fig. 3. Simulation results of 1-D advection in Beam-Warming Scheme. The initial condition of (a)(b)(c) is a step function while the initial condition of (d)(e)(f) a continuous function.

3.1.4 Lax-Friedrichs Scheme

$$\frac{u_j^{n+1} - \frac{1}{2}(u_{j-1}^n + u_{j+1}^n)}{\tau} + a\frac{u_{j+1}^n - u_{j-1}^n}{2h} = 0 \tag{20}$$

From these figures, when the initial condition is a step function, it can be seen that when a = 1, the numerical solution obtained from the Lax-Friedrichs Scheme can approximate the analytical solution well, However, the figure shows that it's a non-smooth line. When a = 2, 4, it cannot approximate the analytical solution.the analytical solution of the original equation cannot be approximated when a = 2, 4. When the initial condition is a continuous function and a = 1, the line is smooth, and there is no fluctuation. When a = 2, 4, the amplitude of fluctuations are smaller than that of the 1st condition. Lax-Friedrichs Scheme works better under smooth initial condition.



(a) $a = 1$ **(b)** $a = 2$ **(c)** $a = 4$

(d) $a = 1$ **(e)** $a = 2$ **(f)** $a = 4$

Fig. 4. Simulation results of 1-D advection in Lax-Friedrichs Scheme. The initial condition of (a)(b)(c) is a step function while the initial condition of (d)(e)(f) a continuous function.

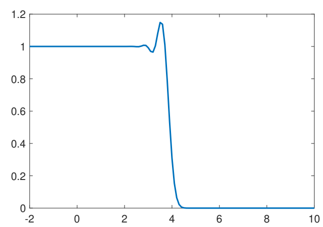
3.1.5 Lax-Wendroff Scheme

$$u_j^{n+1} = u_j^n - \frac{1}{2}a\lambda(u_{j+1}^n - u_{j-1}^n) - \frac{1}{2}a^2\lambda^2(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \tag{21}$$

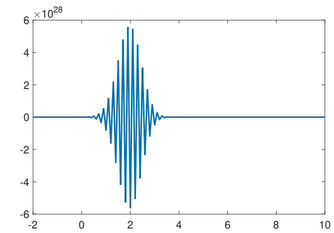
From these figures, when the initial condition is a step function, it can be seen that when a = 1, the numerical solution obtained from the Lax-Wendroff Scheme can approximate the analytical solution well. However, there are ringings resulting from discontinuity. When a = 2, 4, it cannot approximate the analytical solution. When the initial condition is a continuous function and a = 1,there is no fluctuation. When a = 2, 4, the amplitude of fluctuations are smaller than that of the 1st condition. Lax-Wendroff Scheme works better under smooth initial condition.

3.1.6 Conclusion

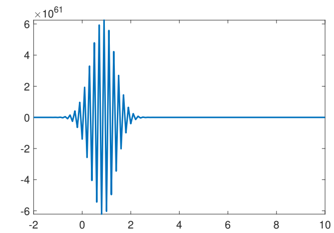
From the results, it can be seen that when initial condition is smooth, the computational results obtained from the above four difference numerical schemes can approximate the solution of the original equation.
When a = 2, only the Beam-Warming Scheme and implicit upwind Scheme approximates the solution of the original equation well, and in the rest of the cases, the numerical solutions cannot approximate the analytical solution of the original equation at all.



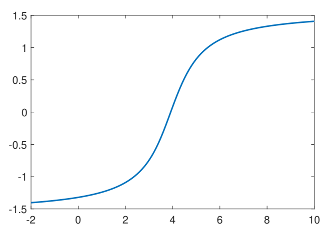
(a) $a = 1$



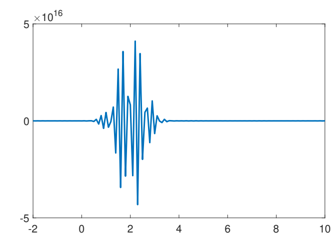
(b) $a = 2$



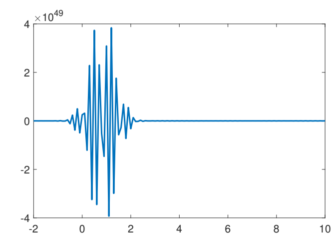
(c) $a = 4$



(d) $a = 1$



(e) $a = 2$



(f) $a = 4$

Fig. 5. Simulation results of 1-D advection in Lax-Wendroff Scheme. The initial condition of (a)(b)(c) is a step function while the initial condition of (d)(e)(f) a continuous function.

Upwind scheme has strong dissipation and dispersion for functions with discontinuities, and fully implicit scheme is stable all the time, while implicit upwind Scheme is stable all the time.
All the above results are consistent with the theoretical analysis.

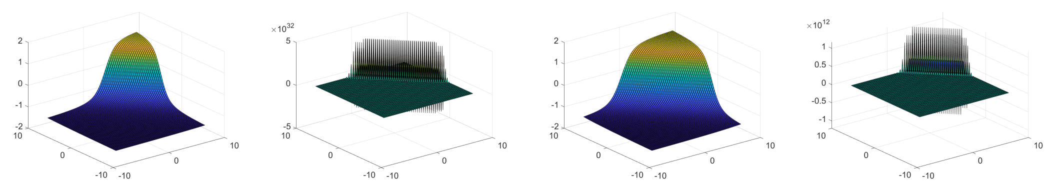
3.2 2-D Advection

Assuming that a = 0.01, b = 1.01; a = 0.1, b = 2.1; a = 0.4, b = 0.4; a = 0.8, b = 0.8, h = 0.2, τ = 0.16, this work applied upwind scheme and Lax-Friedrichs Scheme to solve 2-D advection numerically. The results when t = 4.0s and -10¡x¡10, -10¡y¡10 are shown below.

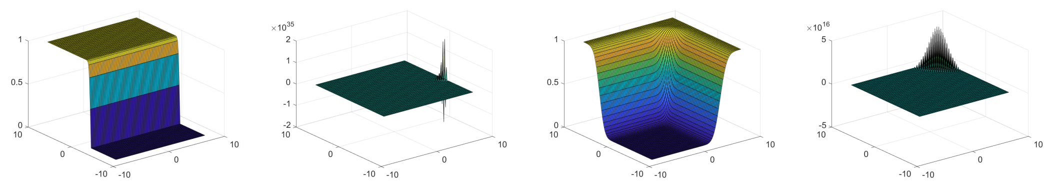
$$\frac{\partial u}{\partial t} + a(\frac{\partial u}{\partial x} + a\frac{\partial u}{\partial y}) = 0 \tag{22}$$

3.2.1 Upwind Scheme For Two Dimension

$$\frac{u_{j,l}^{n+1} - u_{j,l}^{n}}{\tau} + a\frac{u_{j,l}^{n} - u_{j-1,l}^{n}}{h} + b\frac{u_{j,l}^{n} - u_{j,l-1}^{n}}{h} = 0 \tag{23}$$



(a) $a = 0.01, b = 1.01$ **(b)** $a = 0.1, b = 2.1$ **(c)** $a = 0.4, b = 0.4$ **(d)** $a = 0.8, b = 0.8$



(e) $a = 0.01, b = 1.01$ **(f)** $a = 0.1, b = 2.1$ **(g)** $a = 0.4, b = 0.4$ **(h)** $a = 0.8, b = 0.8$

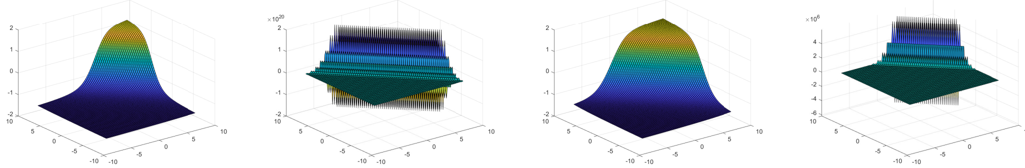
Fig. 6. Simulation results of 2-D advection equation in Upwind Scheme. The initial condition of (a)(b)(c)(d) is continuous function while the initial condition of (e)(f)(g)(h) is step function

From these figures, when a = 0.01, b = 1.01 and when a = 0.4, b = 0.4, upwind scheme for 2-D is stable, but when a = 0.1, b = 2.1 and when a = 0.8, b = 0.8, and we can tell from the amplitude of fluctuations of different initial conditions that continuous function works better.

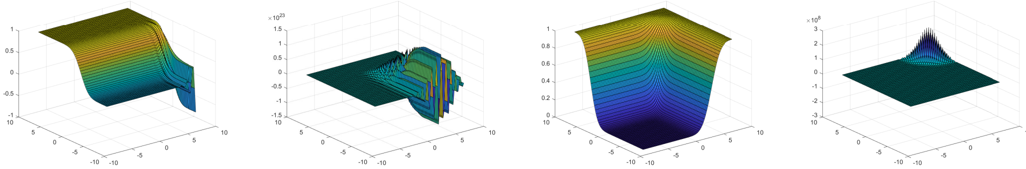
3.2.2 Lax-Friedrichs Scheme For Two Dimension

You can even break it up into smaller sections.

$$\frac{u_{j,l}^{n+1} - \frac{1}{4}(u_{j-1,l}^n + u_{j-1,l}^n + u_{j,l+1}^n + u_{j+1,l-1}^n)}{\tau} + a\frac{u_{j+1,l}^n - u_{j-1,l}^n}{2h} + b\frac{u_{j,l+1}^n - u_{j,l-1}^n}{2h} = 0 \qquad (24)$$



(a) $a = 0.01, b = 1.01$ **(b)** $a = 0.1, b = 2.1$ **(c)** $a = 0.4, b = 0.4$ **(d)** $a = 0.8, b = 0.8$



(e) $a = 0.01, b = 1.01$ **(f)** $a = 0.1, b = 2.1$ **(g)** $a = 0.4, b = 0.4$ **(h)** $a = 0.8, b = 0.8$

Fig. 7. Simulation results of 2-D advection equation in Lax-Fridrich Scheme. The initial condition of (a)(b)(c)(d) is continuous function while the initial condition of (e)(f)(g)(h) is step function

From these figures, when a = 0.01, b = 1.01 and when a = 0.4, b = 0.4, upwind scheme for 2-D is stable, but when a = 0.1, b = 2.1 and when a = 0.8, b = 0.8, and we can tell from the amplitude of fluctuations of different initial conditions that continuous function works better.

3.2.3 Conclusion

When dealing with discontinuity, upwind scheme performs better. For these two schemes, when a = 0.01, b = 1.01 and when a = 0.4, b = 0.4, upwind scheme for 2-D is stable, but when a = 0.1, b = 2.1 and when a = 0.8, b = 0.8. All the above results are consistent with the theoretical analysis.

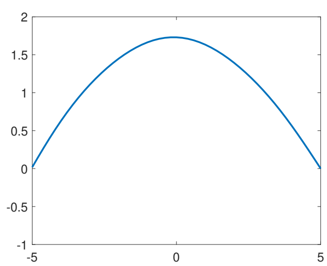
3.3 Diffusion

Assuming that $a = 0.4$, 0.8, 1.6, $h = 0.2$ diffusion equation, $\tau = 0.04$, this work applied Classical Scheme, Richardson Scheme, D-F Scheme and Crank-Nicolson Scheme to solve diffusion equation numerically. The results when t = 4.0s and -5¡x¡5 are shown below.

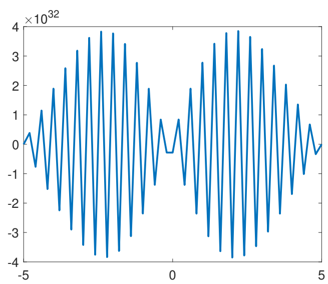
3.3.1 Classical

The classical scheme is expressed as follows:

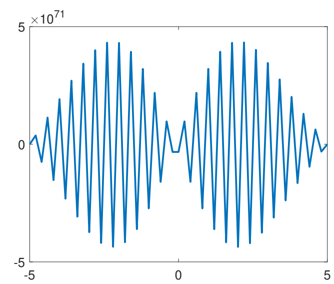
$$\frac{u_j^{n+1} - u_j^n}{\tau} - a\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} = 0, \text{where } \lambda = \frac{\tau}{h^2} \tag{25}$$



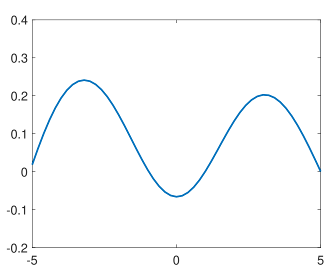
(a) $a = 0.4$



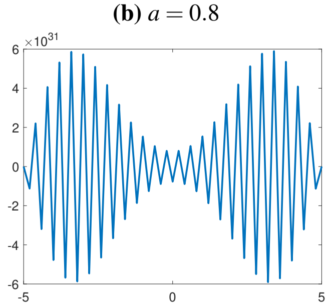
(b) $a = 0.8$



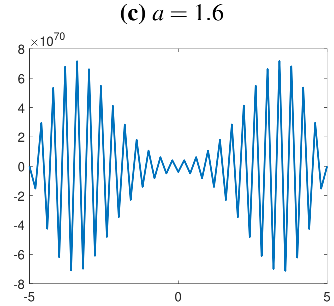
(c) $a = 1.6$



(d) $a = 0.4$



(e) $a = 0.8$



(f) $a = 1.6$

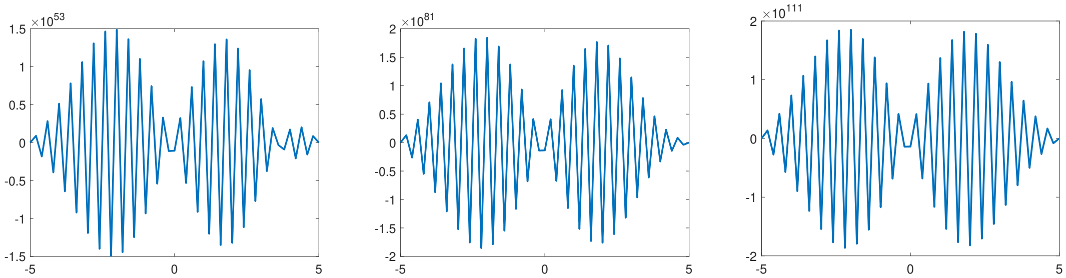
Fig. 8. Simulation results of the diffusion equation using the classical scheme. The initial condition of (a)(b)(c) is a step function while the initial condition of (d)(e)(f) a continuous function.

As the figures show, in Classical scheme, among the two BCs, only the results obtained with $a = 0.4$ were in a stable state. For a=0.8, the results reach an order of 10^{31} . Similarly, for a=1.6, the results diverged to the order of 10^{70}

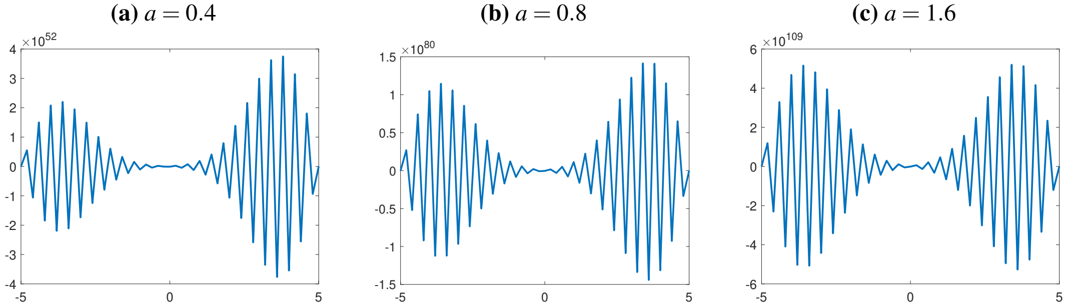
This result consists of the stability requirement of $a\lambda < 0.4$ (remind here $\lambda = \frac{0.04}{0.2^2} = 1$)

3.3.2 Richardson

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\tau} - a\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} = 0 \tag{26}$$



(a) $a = 0.4$ **(b)** $a = 0.8$ **(c)** $a = 1.6$



(d) $a = 0.4$ **(e)** $a = 0.8$ **(f)** $a = 1.6$

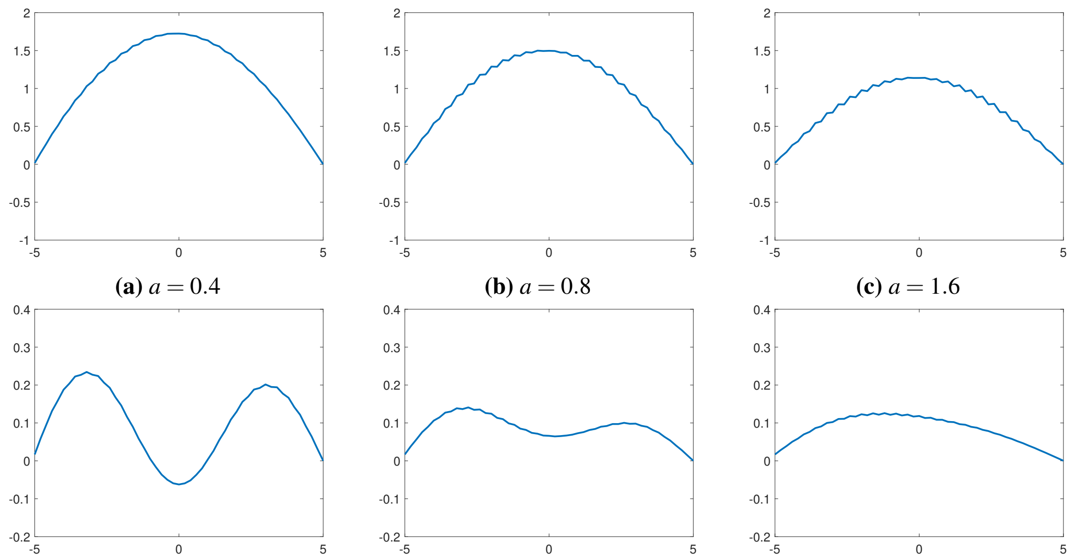
Fig. 9. Simulation results of diffusion equation in Richardson scheme. The initial condition of (a)(b)(c) is a step function while the initial condition of (d)(e)(f) a continuous function.

In Richardson scheme, all results are unstable. The values reach very large magnitudes from 10^{50} to 10^{110} in either step function or continues function with any values of a.

These results also consist with the prediction that Richardson scheme is unstable in any situation.

3.3.3 D-F

$$\frac{u_j^{n+1}-u_j^{n-1}}{2\tau}-a\frac{u_{j+1}^n-(u_j^{n+1}+u_j^{n-1})+u_{j-1}^n}{h^2}=0 \tag{27}$$



(a) $a = 0.4$ **(b)** $a = 0.8$ **(c)** $a = 1.6$

(d) $a = 0.4$ **(e)** $a = 0.8$ **(f)** $a = 1.6$

Fig. 10. Simulation results of diffusion equation in Dufort-Frankel scheme. The initial condition of (a)(b)(c) is a step function while the initial condition of (d)(e)(f) a continuous function.

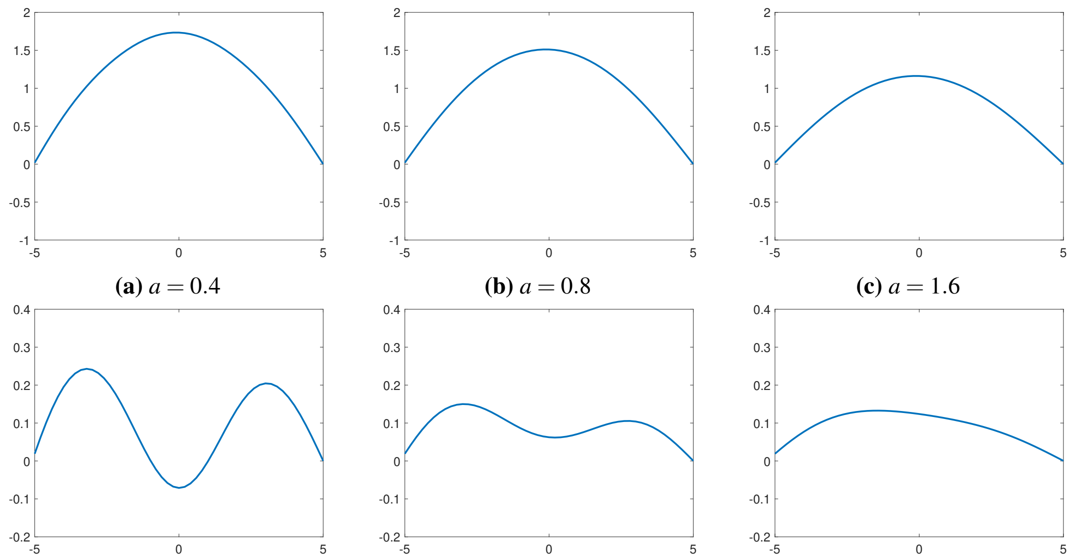
From the figures above, all results from Dufort-Frankel scheme show their stability in all situations. with the increase of a, the results goes more flat in either BC. which are caused by the ”faster” diffusion rate.

In this scheme, it is noticeable that some fluctuations occurs, this is caused by discretization of time and space. These errors accumulate during the iterative process. Improvement can be done by providing more precise grids.

The overall stability consist with the prediction that Dufort-Frankel scheme is stable under all circumstances.

3.3.4 C-N

$$\frac{u_j^{n+1} - u_j^n}{2\tau} - \frac{1}{2}a(\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} + \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{h^2}) = 0 \tag{28}$$



(a) $a = 0.4$ (b) $a = 0.8$ (c) $a = 1.6$

(d) $a = 0.4$ (e) $a = 0.8$ (f) $a = 1.6$

Fig. 11. Simulation results of diffusion equation in Crank-Nicolson scheme. The initial condition of (a)(b)(c) is a step function while the initial condition of (d)(e)(f) a continuous function

Similar to Dufort-Frankel scheme, as predicted, Crank-Nicolson scheme provides a general stable results. The values of the functions are very similar to the previous scheme. The repeatability shows that both D-F and C-N schemes run reliably in this simulation.

However, the ”fluctuations” not exists any more. Which shows that Crank-Nicolson scheme provides better simulations.

3.3.5 Conclusion of the Diffusion schemes

From the results above, the Classical scheme shows a quick and convenient way to simulate the Diffusion equation but with a restriction of MESH ratio provided.

The Richardson scheme is not acceptable since it is not stable in any situations.

The Dufort-Frankel scheme and the Crank-Nicolson scheme both provide universally stability under arbitrary conditions. The Dufort-Frankel scheme have some errors from the fluctuations of its results, while if better accuracy is required, the Crank-Nicolson scheme can provide more accurate results in simulations.

4 Conclusion

4.1 Advection equation

From the results, it can be seen that when initial condition is smooth, the computational results obtained from the above four difference numerical schemes can approximate the solution of the original equation.

The implicit upwind scheme performs stable in all cases. When a = 2, expect for implicit upwind scheme, the beam-warming scheme approximates the solution of the original equation well, and in the rest of the cases, the numerical solutions cannot approximate the analytical solution of the original equation at all. Upwind scheme has strong dissipation and dispersion for functions with discontinuities. All the above results are consistent with the theoretical analysis.

4.2 2-Dimension Advection equation

In the 2-dimensional space, the behavior of the advection equation is similar to that in the 1-dimensional space. When dealing with discontinuity, upwind scheme is better, but when the solution is unstable, we can see from the amplitude that upwind scheme is less stable, because errors travel faster. All the above results are consistent with the theoretical analysis.

4.3 Diffusion equation

From the results above, the Classical scheme shows a quick and convenient way to simulate the Diffusion equation but with a restriction of mesh ratio provided. The Richardson scheme is not acceptable since it is not stable in any situations. The Dufort-Frankel scheme and the Crank-Nicolson scheme both provide universally stability under arbitrary conditions. The Dufort-Frankel scheme have some errors from the fluctuations of its results, while if better accuracy is required, the Crank-Nicolson scheme can provide more accurate results in simulations.

4.4 further improvement

1. For the two-dimensional advection equation, the operator splitting method can be used to construct schemes with stronger stability.
2. Since it is inherently unreasonable to use difference quotients at discontinuities of a function, the error produced by difference schemes at these points still needs to be

Acknowledge

These three authors contributed equally to this work

References

[1] Reguly, I.Z.; Mudalige, G.R. (2020). Productivity, performance, and portability for computational fluid dynamics applications. *Computers & Fluids*, **199**, 104425.

[2] Verma, A.K.; Kayenat, S. (2020). An efficient Mickens' type NSFD scheme for the generalized Burgers Huxley equation. *Journal of Difference Equations and Applications*, **26**, 1213–1246.

[3] Gagliardi, F.; Moreto, M.; Olivieri, M.; Valero, M. (2019). The international race towards Exascale in Europe. *CCF Transactions on High Performance Computing*, **1**, 3–13.

[4] Appadu, A.R. (2017). Performance of UPFD scheme under some different regimes of advection, diffusion, and reaction. *International Journal of Numerical Methods for Heat & Fluid Flow*, **27**, 1412–1429.

[5] Kovács, E.; Nagy, Á.; Saleh, M. (2021). A set of new stable, explicit, second-order schemes for the non-stationary heat conduction equation. *Mathematics*, **9**, 2284.

[6] Sanjaya, F.; Mungkasi, S. (2017). A simple but accurate explicit finite difference method for the advection-diffusion equation. *Journal of Physics: Conference Series*, **909**, 12038.

[7] Karahan, H. (2007). Unconditional stable explicit finite difference technique for the advection–diffusion equation using spreadsheets. *Advances in Engineering Software*, **38**, 80–86.

[8] Pourghanbar, S.; Manafian, J.; Ranjbar, M.; Aliyeva, A.; Gasimov, Y.S. (2020). An efficient alternating direction explicit method for solving a nonlinear partial differential equation. *Mathematical Problems in Engineering*, **2020**, 9647416.