Second or fourth-order finite difference operators, which one is most effective?

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This paper presents higher-order finite difference (FD) formulas for the spatial approximation of the time-dependent reaction-diffusion problems with a clear justification through examples, “why fourth-order FD formula is preferred to its second-order counterpart” that has been widely used in literature. As a consequence, methods for the solution of initial and boundary value PDEs, such as the method of lines (MOL), is of broad interest in science and engineering. This procedure begins with discretizing the spatial derivatives in the PDE with algebraic approximations. The key idea of MOL is to replace the spatial derivatives in the PDE with the algebraic approximations. Once this procedure is done, the spatial derivatives are no longer stated explicitly in terms of the spatial independent variables. In other words, only one independent variable is remaining, the resulting semi-discrete problem has now become a system of coupled ordinary differential equations (ODEs) in time. Thus, we can apply any integration algorithm for the initial value ODEs to compute an approximate numerical solution to the PDE. Analysis of the basic properties of these schemes such as the order of accuracy, convergence, consistency, stability and symmetry are well examined.

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Keywords: Consistency, Finite difference, PDEs, Reaction-diffusion, Stability, Symmetry.

INTRODUCTION

Reaction-diffusion equations are classified as a special class of parabolic time-dependent partial differential equations. The major way of solving the class of these equations is through discretization. A well-known approach to solve time-dependent partial differential equation, with solutions varying in both time and space, is the method of lines (MOL), see Ascher et al. (1995), Schisser and Griffits (2009), Holden and Karlsen (2012) and Strikwerda (2004) for details. Application of this method requires to first constructing a semi-discrete approximation to the problem by setting up a regular grid in space, this is achieved by discretising the spatial independent variables with boundary constraints. Hence, a couple systems of ordinary differential equations are generated in time, which is associated with the initial value. Once that is done, we numerically approximate the solutions to the original time-dependent partial differential equation by marching forward in time on this grid. Conveniently, we can now apply any existing, and generally well established, time-stepping numerical methods such as the implicit-explicit (IMEX) schemes, Runge-Kutta methods or exponential time differencing (ETD) schemes among many others.

In this paper, for the spatial discretisation, we are primarily concerned with the use of higher-order finite difference method. The discrete approximation to the derivatives will be converted into Toeplitz matrices. The discretisation in time uses majorly the exponential time differencing schemes, other time-stepping methods include but not limited to the fourth-order Runge-Kutta (RK4) method and implicit-explicit schemes. A brief of each of these methods will be
discussed later in this paper. In the title I propose second or fourth-order operators which one is more effective? Once computational experiments are conducted, there are some important issues such as consistency, stability and convergence that are required to be investigated, once these issues as pointed out are addressed, the question posed by the title of this paper is answered. We can now proceed to solve numerically the class of reaction-diffusion problems to be considered.

The rest of this paper is structured into 5 sections. Higher order finite difference approximations are discussed in Section 2. Section 3 gives a detail report on error analysis and order of accuracy of the schemes. Stability analysis, convergence and symmetric properties are presented in Section 4 with numerical results on reaction-diffusion problems. Conclusions are drawn in Section 5.

**Finite Difference Approximations**

The finite difference methods have gained its dominance in the various fields of computational science since its inception as the major method of choice back to 1960s. Other methods such as finite element and boundary element methods enjoyed recent popularity, finite difference methods are still well utilized for a wide array of computational engineering and science problems.

A finite difference scheme is produced when the partial derivatives in the partial differential equation(s) governing a physical phenomenon are replaced by a finite difference approximation. The result is a single algebraic equation or a system of algebraic equations which, when solved, provide an approximation to the solution of the original partial differential equation at selected points of a solution grid. The solution grid (also referred to as computational grid or numerical grid) is originated by dividing the axes representing the independent variables in the solution domain into a number of intervals. The two extreme points of the interval are replaced by the boundary conditions in the given problem. If we draw lines perpendicular to a given axes passing through the extreme points of the intervals, the resulting grid is the computational grid.

**Higher order finite difference approximations**

Higher order finite difference approximations can be obtained by taking more terms in Taylor series expansion. The Taylor expansion provides a very useful tool for the derivation of higher order approximation to derivatives of any order. Our interest in this work is to use higher order finite difference formula for the spatial discretization of the problems to be considered later in this work, so we need to create an estimate based on step size $2\Delta x$ through the Taylor series expansion

\[
u(x_j + 2\Delta x) = \sum_{k=0}^{\infty} \frac{(2\Delta x)^k}{k!} u^{(k)}(x_j)\] (2.1)

\[
u(x_j - 2\Delta x) = \sum_{k=0}^{\infty} (-1)^k \frac{(2\Delta x)^k}{k!} u^{(k)}(x_j)\] (2.2)

Better approximation is obtained by combining these two estimates through the process called Richardson extrapolation. For instance, we present the fourth-order centred finite difference schemes for the first and second derivatives as

\[
u'(x_j) = \frac{u(x_j - 2\Delta x) - 8u(x_j + \Delta x) + 8u(x_j + 2\Delta x) - u(x_j + 2\Delta x)}{12\Delta x} + O(\Delta x^4)\] (2.3)

and

\[
u''(x_j) = \frac{-u(x_j - 2\Delta x) + 16u(x_j - \Delta x) - 30u(x_j) + 16u(x_j + \Delta x) - u(x_j + 2\Delta x)}{12\Delta x^2} + O(\Delta x^4)\] (2.4)

respectively. For the purpose of comparison, we present the conventional second order FD scheme as

\[
u''(x_j) = \frac{u(x_j - \Delta x) + 2u(x_j) + u(x_j + \Delta x)}{\Delta x^2} + O(\Delta x^2)\] (2.5)

Some of the important features to notice about centred finite difference schemes, they are symmetric in nature and posses an even-order of accuracy. The weights of some of the central finite difference formulas are presented in the Tables 1 and 2 for the approximations of first and second derivatives respectively.

Second or fourth-order finite difference operators, which one is most effective?
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Table 1. Weights of some higher order centered finite difference approximation for the first derivatives on equi-spaced grids

<table>
<thead>
<tr>
<th>Order of accuracy</th>
<th>$u_{-4}$</th>
<th>$u_{-3}$</th>
<th>$u_{-2}$</th>
<th>$u_{-1}$</th>
<th>$u_{0}$</th>
<th>$u_{1}$</th>
<th>$u_{2}$</th>
<th>$u_{3}$</th>
<th>$u_{4}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td></td>
<td></td>
<td>$-\frac{1}{2}$</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$\frac{1}{12}$</td>
<td></td>
<td>$\frac{8}{12}$</td>
<td>0</td>
<td>$\frac{8}{12}$</td>
<td>$-\frac{1}{12}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$-\frac{1}{60}$</td>
<td>$\frac{9}{60}$</td>
<td>$\frac{45}{60}$</td>
<td>0</td>
<td>$\frac{45}{60}$</td>
<td>$\frac{9}{60}$</td>
<td>$\frac{1}{60}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>$\frac{3}{840}$</td>
<td>$-\frac{32}{840}$</td>
<td>$168$</td>
<td>$-\frac{672}{840}$</td>
<td>0</td>
<td>$\frac{672}{840}$</td>
<td>$-\frac{168}{840}$</td>
<td>$\frac{32}{840}$</td>
<td>$-\frac{3}{840}$</td>
</tr>
</tbody>
</table>

Table 2. Weights of some higher order centered finite difference approximation for the second derivatives on equi-spaced grids

<table>
<thead>
<tr>
<th>Order of accuracy</th>
<th>$u_{-4}$</th>
<th>$u_{-3}$</th>
<th>$u_{-2}$</th>
<th>$u_{-1}$</th>
<th>$u_{0}$</th>
<th>$u_{1}$</th>
<th>$u_{2}$</th>
<th>$u_{3}$</th>
<th>$u_{4}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-2</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$\frac{1}{12}$</td>
<td></td>
<td>$\frac{16}{12}$</td>
<td>$-\frac{30}{12}$</td>
<td>$\frac{16}{12}$</td>
<td>$-\frac{1}{12}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$\frac{3}{180}$</td>
<td>$\frac{27}{180}$</td>
<td>$\frac{270}{180}$</td>
<td>$-\frac{490}{180}$</td>
<td>$\frac{27}{180}$</td>
<td>$-\frac{27}{180}$</td>
<td>$\frac{3}{180}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>$-\frac{1}{560}$</td>
<td>$\frac{8}{315}$</td>
<td>$-\frac{1}{5}$</td>
<td>$\frac{8}{5}$</td>
<td>$-\frac{205}{72}$</td>
<td>$\frac{8}{5}$</td>
<td>$-\frac{1}{5}$</td>
<td>$\frac{8}{315}$</td>
<td>$-\frac{1}{560}$</td>
</tr>
</tbody>
</table>

where $u_i$ for $i = 1, 2, 3, 4$ has the equivalence $u_{-4} = u(x_j - 4\Delta x), \ldots, u_{4}(x_j + 4\Delta x)$ in the tables. In general, schemes for any given derivatives of any chosen order can be derived from Taylor expansions as long as sufficient number of sample points is used. These approximations are much more difficult far beyond the simple cases shown, most especially, the higher order formulas. Readers are referred to the books by Fornberg (1995, 1998), Fornberg and Driscoll (1999) where schematic illustration of how to generate the weights of higher order centered and one-side finite differences formulas for approximating derivatives up to fourth-order equi-spaced grids with order of accuracy up to eighth can be found.

For more general finite difference approximations, we follow the description given by Fornberg (2011) and present briefly the short code that can be used to generate weights of any order approximation schemes on equi-spaced grids. The program only requires Mathematica package (version seven and above) that contains pre-loaded Pade' package. The complete code is

```mathematica
m = PadeApproximation[x^((Log[x]/h))", {x, 1, {n, m}}] ;
CoefficientList[Denominator[m], {x, n}]
```

The numbers d, m, n and s describe the shape of the stencil, where d is the number of grid intervals in between the left- and right most derivative entries, m indicates the number of derivatives to be approximated, n stands for the number of grid intervals in between the left- and rightmost function entries, and s the number of grid intervals in between the leftmost derivative and function entries.

**Error Analyses**

Next, we need to ask ourselves why using fourth-order approximation scheme instead of the commonly used second-order scheme approximation? To answer this question, let us quickly consider an example (Mathews and
Fink 1999). Given \( u(x) = \cos(x) \), we use formulas (2.5) and (2.4) with \( \Delta x = 0.1, 0.01 \) and 0.001 to find approximations to \( u''(0.8) \). The true value here is taken to be \( u''(0.8) = -\cos(0.8) \). For instance, the calculation for \( \Delta x = 0.1 \) with methods (2.5) is

\[
u''(0.8) \cong u(0.81) - 2u(0.8) + u(0.79) \approx -0.696690000.
\]

By subtracting the computed value from the true value, we found the error in this approximation to be 1.0671e-005. The remaining calculations are summarized in the Table 3

<table>
<thead>
<tr>
<th>Step size (( \Delta x ))</th>
<th>Approximation</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta x = 1.0 )</td>
<td>-0.640548935</td>
<td>-0.056157774</td>
</tr>
<tr>
<td>( \Delta x = 0.1 )</td>
<td>-0.696126300</td>
<td>-0.000580409</td>
</tr>
<tr>
<td>( \Delta x = 0.01 )</td>
<td>-0.696600000</td>
<td>-0.000016709</td>
</tr>
<tr>
<td>( \Delta x = 0.001 )</td>
<td>-0.696600000</td>
<td>-0.000070679</td>
</tr>
</tbody>
</table>

In the same manner, for the fourth-order formula, we obtain

<table>
<thead>
<tr>
<th>Step size (( \Delta x ))</th>
<th>Approximation</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta x = 1.0 )</td>
<td>-0.689625413</td>
<td>-0.007081296</td>
</tr>
<tr>
<td>( \Delta x = 0.1 )</td>
<td>-0.696705958</td>
<td>-0.000000751</td>
</tr>
<tr>
<td>( \Delta x = 0.01 )</td>
<td>-0.696000000</td>
<td>-0.000016709</td>
</tr>
<tr>
<td>( \Delta x = 0.001 )</td>
<td>-0.697500000</td>
<td>-0.000031709</td>
</tr>
</tbody>
</table>

The results obtained in the Tables 3 and 4 have shown that the fourth-order scheme produces a better approximation when compared to its second-order counterpart. The optimal step-size for the formula (2.5) is at when \( \Delta x = 0.01 \) as shown in Table 3 and the optimal step-size to be used for equation (2.4) is when \( \Delta x = 0.1 \). We can see here that the fourth-order allows large step-size.

Next, we analyze briefly the two approximation methods of orders \( O(\Delta x^2) \) and \( O(\Delta x^4) \) that are paramount to our discussion in this paper. Let \( u_k = \xi_k + \epsilon_k \), where \( \epsilon_k \) is the error in computing \( u(x_k) \), then (2.5) can be written in the form

\[
u''(x) = \frac{u(x + \Delta x) - 2u(x) + u(x - \Delta x)}{\Delta x^2} + E(u, \Delta x).
\]

The error term \( E(u, \Delta x) \) consists of both the truncation and the round-off errors. That is,

\[
E(u, \Delta x) = E_{\text{round}}(u, \Delta x) + E_{\text{trunc}}(u, \Delta x)
\]

\[
= \frac{\epsilon(x - \Delta x) - 2\epsilon(x) + \epsilon(x + \Delta x)}{\Delta x^2} - \frac{\Delta x^2 u^{(4)}(c)}{12}
\]

where \( |u^{(4)}(c)| \) is assumed to be bounded for \( c = c(x) \in [x - \Delta x, x + \Delta x] \), then the truncation error in (3.7) goes to zero in the same manner with \( O(\Delta x^2) \). Since one can assume that each error \( \epsilon_i \) has magnitude \( \xi \), and that \( |u^{(4)}(x)| \leq M \), then we can obtain the error bound, if \( |\epsilon_i| \leq \xi \) and \( M = \max[x - \Delta x, x + \Delta x][u^{(4)}(x)] \), then \( |E(u, \Delta x)| \leq 4\xi / \Delta x^2 + M\Delta x^2 / 12 \). On simplifying further, the optimum step size is obtained as \( \Delta x = (48\xi / M)^{1/4} \) and that \( M = |u^{(4)}(x)| \leq \cos(x) \leq 1 \).

It is clear that the portion of the error due to round off is inversely proportional to the square of $\Delta x$, this particular term grows when $\Delta x$ gets small, and it is referred to as the step-size dilemma in most cases. The only way out of this problem is to use a higher order method that would accommodate a larger value of $\Delta x$ to yield the desired accuracy. This assertion actually prompts us to seek higher order approximation method. Similarly, we define the bound for the error term in (2.4) as $|E(u, \Delta x)| \leq 16\xi / 3\Delta x^2 + M\Delta x^4 / 90$ with an optimal step size value given as $\Delta x = (240\xi / M)^{1/6}$, in such that $M = |u^{(6)}(x)| \leq \cos(x) \leq 1$. Convergence of the second- and fourth-order finite difference approximations are shown in Tables 1 and 2 respectively.

Illustrative Example

Most physical applications encountered in the various fields of science and engineering are described in term of dimensions (space and time). Most mathematical description exists in terms of partial differential equations.
explaining the concept of physical space-time. As a result of this fact, methods for the solution of partial differential equations, such as the method of lines by Hamdi et al. (2010) and Strikwerda (2004) are still active in the current field of research. As a basic illustrative example of a PDE, let us consider the diffusion equation

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}, \quad t > 0$$  \hspace{1cm} (3.8)

where \( u(x,t) \) is the population density in biological or ecological processes or the concentration in the chemical or physical contexts. \( D \) is regarded as the diffusion. Equation (3.8) also governs unsteady heat transfer in a solid medium and one-dimensional Stokes flow.

Solution of equation of the form (3.8) is subjected to some auxiliary conditions that can be determined by the highest order of the derivatives in each of the independent variables present (see Powers (2006), Meyer (1973), Kreiss and Lorenz (1989)). To illustrate the method of lines procedure to solve diffusion equation (3.8), suppose that \( u(x,t) \) is discretized in space with \( N + 1 \) points, of which \( N - 1 \) are the interior points, on a uniform grid with step size \( \Delta x \), we have

$$u(x_j,t) \approx u_j(t), \quad 0 \leq j \leq N,$$

(3.9)

where the index \( j \) indicating a position along the grid in \( x \) and \( \Delta x \) is the spacing in \( x \) along the grid, assumed to be constant. To find an algebraic approximation to the spatial derivative \( \partial^2 u / \partial x^2 \) in (3.8). For instance, the fourth-order centered finite difference approximation, yields the following ODEs

$$\begin{align*}
\frac{du_0(t)}{dt} &= D \left[ -u_4(t) + 16u_3(t) - 30u_2(t) + 16u_1(t) - u_0(t) \right] / 12\Delta x^2 \\
\vdots & \quad \vdots \\
\frac{du_{N-1}(t)}{dt} &= D \left[ -u_{N-4}(t) + 16u_{N-3}(t) - 30u_{N-2}(t) + 16u_{N-1}(t) - u_N(t) \right] / 12\Delta x^2 \\
u_N(t) &= f_N(t),
\end{align*}$$

(3.10)

subject to the initial condition

$$u_j(x,t = 0) = u_0(x_j), \quad 0 \leq j \leq N,$$  \hspace{1cm} (3.11)

where \( f_a(t) \) and \( f_N(t) \) are the left and right boundaries of \( u \) for all \( t \). Equations (3.10) and (3.11) constitute the complete MOL approximations of (3.8).

**Order of Accuracy and Consistency**

With the second order schemes and by means of the Taylors expansion, Eq. (3.8) becomes

$$\begin{align*}
\frac{u(x_0,t_0 + \Delta t) - u(x_0,t_0)}{\Delta t} &= D \frac{u(x_0 + \Delta x,t_0) - 2u(x_0,t_0) + u(x_0 - \Delta x,t_0)}{\Delta x^2} \\
+ \frac{\partial}{\partial x}u(x_0,t_0) - D \frac{\partial^2}{\partial x^2}u(x_0,t_0) 
\end{align*}$$

= $$-\frac{\Delta t^2}{2} \frac{\partial}{\partial x}u(x_0,t_0) + D \frac{\Delta x^2}{24} \frac{\partial^3}{\partial x^3}u(x_0,t_0)$$

$$-\frac{\Delta t^2}{6} \frac{\partial}{\partial x}u(x_0,t_0) + D \frac{\Delta x^4}{320} \frac{\partial^5}{\partial x^5}u(x_0,t_0) + \cdots$$

(3.12)

The right hand side of (3.12) is the so-called truncation error, and the lowest powers of \( \Delta t \) and \( \Delta x \) in the truncation error are the respective order of accuracies of the finite difference approximations in time and space. Thus, the finite difference scheme in (3.12) is consistent with the diffusion equation (3.8) to first-order accuracy in time and second-order accuracy in space.

In the same way, when fourth-order schemes are applied to (3.8), we obtain
\[
-\frac{u(x_0, t_0 + 2\Delta t) + 8u(x_0, t_0 + \Delta t) - 8u(x_0, t_0 + \Delta t) + u(x_0, t_0 - 2\Delta t)}{12\Delta t}
\]
\[
D - \frac{u(x_0, 2\Delta x, t_0) + 16u(x_0 + \Delta x, t_0) - 30u(x_0 + 2\Delta x, t_0) + 16u(x_0 + \Delta x, t_0) - u(x_0 - 2\Delta x, t_0)}{12\Delta x^2}
\]
\[
+ \partial_t u(x_0, t_0) + D\partial_x u(x_0, t_0)
\]
\[
= \frac{\Delta t^4}{30} \partial_{xxxx} u(x_0, t_0) + D \frac{\Delta x^4}{90} \partial_{xxxx} u(x_0, t_0) + \cdots
\]

The truncation error is defined as \(T_j^n = u(x_j, t_n) - u^n_j\). Hence, \(|T_j^n| \leq \beta_1 \Delta t^4 + \beta_2 \Delta x^4\), where \(\beta_1\) and \(\beta_2\) denote two constants that depend on some norms of the derivatives of \(u\). As a result, this scheme is consistent with order of accuracy 4 in both space and time. Generally, if the truncation error is \(O(\Delta x^p, \Delta t^q)\), the method is \(p^{th}\) order accurate in \(x\) and \(q^{th}\) order accurate in \(t\). If the truncation error tends to zero as \(\Delta x, \Delta t \to 0\), the scheme is said to be consistent.

A finite difference scheme is convergent to \(p^{th}\) order in \(x\) and \(q^{th}\) in \(t\) if
\[
\|u - u^n\| = \left( \sum_{j=1}^{N} |u_j^n|^{\frac{1}{H}} \right)^H,
\]
where \(H = 2\) corresponds to the Euclidean norm and \(H = \infty\) is the maximum norm. By Lax Equivalence Theorem (Lax and Richtmyer 1956), the importance of the concepts of consistency and stability is seen in the Lax-Richtmyer equivalence theorem, which is the fundamental theorem in the theory of finite difference schemes for initial value problem. It states that, if a finite difference method for a given partial differential equation for which initial value problem is well-posed and that the scheme is linear, stable and accurate of order \(O(\Delta x^p, \Delta t^q)\), it is convergent.

**Definition of Illustrative Example**

A numerical scheme that is symmetric is consistent (see Fatunla (1988), Lambert and Watson (1976)) if
(i) it has order \((p, q) \geq 1\).
(ii) the sum of its first characteristic polynomial is zero., that is
\[
\sum_{j=0}^{N} \alpha_j = 0.
\]
Hence the schemes are consistent.

**The matrix notation**

The easiest way of representing the approximation to the differential operator is by the use of the differentiation matrix, Trefethen (1996, 2000). The matrix operator forms a Toeplitz matrix in which the order of the approximation determines the sparsity of the matrix.

**Definition Order of Accuracy and Consistency**

A Toeplitz matrix, is a matrix in which each ascending diagonal from left to right has constant entries, that is, a matrix of the form
\[
L = \begin{bmatrix}
I_0 & I_1 & I_2 & \cdots & I_{N-1} \\
I_{-1} & I_0 & I_1 & \cdots & \vdots \\
I_{-2} & I_{-1} & I_0 & I_1 & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots \\
I_{N+1} & I_{N} & I_{N-1} & \cdots & I_0
\end{bmatrix}
\]

where the entries of \(L\) satisfy the property \(L_{ij} = I_{j-i}\), then \(L\) is said to be a circulant matrix with eigenvalues given by
\[
\lambda_n = \sum_{j=1}^{N} I_j e^{2\pi i (j-1) \frac{n}{N}}, \text{ for } n = 0, 1, \ldots, N-1.
\]

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Considering the sequence  
\[ s = \{l_k : k = -p, \ldots, -1, 0, \ldots, q\}, \]
where \( p \) and \( q \) are positive integers. A square Toeplitz matrix \( L \) of order \( N \) is of the bandwidth \((p + q + 1) \leq N\), if its entry \( l_{ij} \) is a member of the sequence \( s \) and zero otherwise. For instance, if \( p = q = 2 \), then \( L \) is a pentadiagonal Toeplitz matrix.

The present paper is primarily concerned with the eigenvalues of Toeplitz matrices obtained from the finite difference schemes. It will also be of paramount importance for determining the linear stability of our problems. The eigenvalues of a tridiagonal Toeplitz matrix of arbitrary order \( N \) are well understood Mitchell (1980). The major challenge rest upon the Toeplitz matrix with higher bandwidth, the eigenvalue problems become intractable, see for instance the work of Sogabe (2004, 2008), although some algorithms have been derived for pentadiagonal matrices, see Cinkir (2012), Hoffman (2001), Leveque (2007), Durran (2010), Kilic and El-Milakkawy (2008) and El-Milakkawy (2004) for details. An attempt to circumvent the difficulty in finding the eigenvalues of higher bandwidth Toeplitz matrices, we shall concentrate basically on the eigenvalues of the circulant Toeplitz matrices, which is more importantly related to our assumption of periodic boundary conditions.

**Stability Analysis**

Let us consider the parabolic partial differential equation with one spatial independent variable

\[ \frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + \nu(1 - \frac{u}{\kappa}), \]  

(4.15)

known as the Fisher equation, where \( \alpha, \tau \) and \( \kappa \) are positive parameters. Using second order schemes, the Von Neumann’s stability of the Eq. (4.15) can be verified as

\[ 1 - 4\omega \sin^2 \left( \frac{k_m \Delta x}{2} \right) \leq 1, \]

where \( k_m \) is the wave number, \( \omega = \alpha \Delta t / \Delta x^2 \) called the Courant number (Courant et al. (1967)) and we also let \( \tau = \kappa = 1 \), for simplicity. The maximum value of the sine function is considered so that \( 1 - 4\omega \geq 1 \) and \( \omega \geq 0 \). For \( \omega = 0 \), it implies that \( \Delta t = 0 \), which is impractical. Thus, we have \( 0 < \omega \leq 1/2 \). In order to ensure a stable solution or reduce errors, maximum care must be exercised in selecting the value of \( \omega \). It further implies that for a given \( \Delta x \), the allowed value of \( \Delta t \) must be small enough to satisfy \( \omega \leq 1/2 \). We conclude by saying that a finite difference equation is stable if it produces a bounded solution when the exact solution is bounded, and is unstable if it produces an unbounded solution when the exact solution is bounded.

Similarly, when the fourth order scheme is applied to (4.15), we obtain the amplification polynomial

\[ \xi^4 - 8\xi^3 - \sigma \xi^2 + 8\xi - 1 = 0, \]

where \( G = -2 \cos 2\theta + 32 \cos \theta - 3\theta \). By Intermediate Value Theorem, we let

\[ g(\xi) = \xi^4 - 8\xi^3 - \sigma \xi^2 + 8\xi - 1, \]

which is a continuous function. We want to show that there exists a root \( \xi \leq 1 \) for \( g(x) = 0 \) on \([0, 1]\). Observe that \( g(0) = -1 < 0 \) and \( g(1) = -\sigma G \) with possibility of cases (i) \( \sigma G > 0 \) (ii) \( \sigma G = 0 \) and (iii) \( \sigma G < 0 \). It is obvious that the method is stable if \( \| \xi G \| \leq 1 \), so the scheme is conditionally stable.

Linear stability analysis can also be verified by setting \( \tau = 0 \), reaction-diffusion Eq.(4.15) reduces to a standard diffusion equation (3.8) , its two level difference is presented as

\[ L_0 u^{n+1} = L_0 u^n + b^n, \quad n = 0, 1, 2, \ldots \]  

(4.16)

where \( b^n \) is expected to have contained the boundary conditions and \( L_0 \neq 0 \). For \( L_0 = I \), the difference scheme (4.16) is explicit otherwise it is an implicit method. In the stability analysis of the matrix method, we determine the conditions under which the error norm

\[ \| Er^{n+1} \| = \| u^n - u^r \| \]

where \( \| \cdot \| \) indicates the stable norm, is bounded as \( n \to \infty \). Again, we can rewrite (4.16) in the form

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\[ E^{n+1} = \xi E^n, \quad n = 0, 1, 2, \ldots \]

where \( \xi = L_0^{-1} L_1 \) and \( \xi \) is called the amplification matrix. With \( n = 1, 2, \ldots \), we have

\[ \| E^{n+1} \| \leq \| \xi \| \| E^n \| . \]

Therefore, for the stability we require that \( \| \xi \| \leq 1 \). In this paper, our particular case is when \( \xi \) is symmetric matrix, then \( \| \xi \| = \rho(\xi) \) in such a way that it equivalence form \( \rho(\xi) \leq 1 \). Hence, von Neumann necessary condition is satisfied.

**Convergence**

On applying the second order scheme to the diffusion equation (3.8) and let \( \Delta t \to k \) and \( \Delta x \to h \), and expand each terms in Taylors series, we obtain the truncation error formula

\[ E_{\text{trunc}} = u(x_j, t_{n+1}) - u(x_j, t_n) - \lambda [u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)] \]

\[ = \left[\left(ku_t + \frac{k^2}{2} u_{tt} + \cdots\right) - \frac{k}{h^2} \left(h^2 u_t^2 + \frac{h^4}{12} u_t^4\right)\right] \]

\[ = \frac{k^2}{2} u_{tt} - \frac{kh^2}{12} u_t^4 u + O(k + h^2) \]

where \( u_t = \partial / \partial t \) and \( u_x = \partial / \partial x \). The \( E_{\text{trunc}} \) of the method is of order \( O(k^2 + kh^2) \). The order of the method is given as

\[ \frac{1}{k} (E_{\text{trunc}}) = O(k + h^2) \]

If the solution of the difference equation tends to the solution of the differential equation as \( h \to 0 \) and \( k \to 0 \), then the difference equation is said to be convergent. The same process can be repeated for the fourth-order scheme. Hence, we conclude with the definition of convergence.

**Definition Convergence**

Gedney (2011) that says; A finite difference equation (FDE) is consistent with a partial differential equation (PDE) if the difference between the FDE and the PDE (i.e., the truncation error) vanishes as the sizes of the time step \( k \) or \( \Delta t \) and spatial grid spacing \( h \) or \( \Delta x \) go to zero independently, is satisfied.

In addition, the Lax-Richtmyer (1956) equivalence theorem states that a consistent finite-difference scheme for a partial differential equation for which the initial-value problem is well posed is convergent if and only if it is stable, for a proof, readers are referred to Strikwerda (2004), Thomas (1995, 1999) and Sewel (1991). Finally, by Dahlquist equivalence theorem, a linear multistep formula is convergent if and only if it is consistent and stable.

**Symmetry**

According to Fatunla (1988), Jain (1984) and Lambert and Watson (1976), the fourth-order schemes (2.3-2.4) is said to be symmetric if when the values of \( \alpha_j^s \) and \( \beta_j^s \) are interchanged, the function is the same or is multiplied by minus one.

\[ \alpha_j = \alpha J^{-j}, \quad \beta_j = \beta J^{-j}, \quad j = 0(1)J \]  \hspace{1cm} (4.18)

where \( \alpha_j \) and \( \beta_j \) correspond to the coefficients of the first and second characteristic polynomial when applied to (3.8). It follows that

\begin{align*}
\alpha_0 &= -\alpha_4 = -1 \\
\alpha_1 &= -\alpha_3 = -8 \\
\alpha_2 &= -\alpha_2 = 0 \\
\beta_0 &= \beta_4 = -1 \\
\beta_1 &= \beta_3 = -16 \\
\beta_2 &= \beta_2 = 30
\end{align*}

Hence, the method is symmetric.

Second or fourth-order finite difference operators, which one is most effective?
Numerical results

Numerical method of solution discussed earlier is applied to solve both the diffusion equation (3.8) and the reaction-diffusion equation (4.15), subject to the initial condition
\[ u(x,0) = \frac{1}{\cosh(\delta x)}, \quad x \in [a,b] \] (4.19)

and homogeneous Dirichlet boundary conditions
\[ u(a,t) = u(b,t) = 0, \quad t > 0 \] (4.20)

The choices of parameters \(a\) and \(b\) determines how well the waves propagate. When both equations (3.8) and (4.15) are discretized in space with the fourth-order central difference scheme (2.4), it results to the ordinary differential equations in time. The resulting ODEs is advanced with the MATLAB ode15s solver.

Figure 3. Solution of the reaction-diffusion equation (4.15) at parameters values \(D = 0.5, \delta = 1/2, t = 0.001, N = 200\) for \(x \in [-15,15]\).
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To this end, we have dealt with spatial discretization method using finite difference (FD) schemes of higher orders. A less rigorous method of derivation of higher-order FD schemes has been reported with the aid of a Mathematica program that contains the pre-loaded Pad'e package, with a view of circumventing the difficulty associated with the derivation of FD formula with order greater than two, see Tables 1 and 2 for details. Also in this paper, the question of "why using fourth-order FD schemes against the commonly used second-order scheme" is well-answered. A proof to this assertion is clearly shown in the results presented in Tables 3 and 4 for the second- and fourth-order FD schemes respectively for different values of $\Delta x$. It is evident from the results presented that the fourth-order scheme yields a better approximation in comparison to the second-order scheme, as it permits the use of higher step-size. More importantly, the convergence test results presented in Figures 1 and 2 further justify the supremacy of fourth-order scheme (2.4) over its second-order counterpart (2.5) by error factor of about $10^{-14}$ against $10^{-7}$ respectively.

Accuracy and suitability of our schemes was ascertained via the analysis of their basic properties such as order of accuracy, consistency, convergence, stability and symmetry.

REFERENCES

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