Enhanced higher order unconditionally positive finite difference method for the advection-diffusion-reaction equations

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Introduction

Background

- Many problems in science and engineering are modeled by partial differential equations that are often difficult to solve for an exact solution and, in some cases, impossible.
- Numerical methods have proven a good alternative in providing approximate solutions close to the exact solution. As a result, several accurate numerical methods, such as the Crank-Nicolson method [7], finite element methods [4], finite volume methods [10], spectral methods [8] and nonstandard finite difference methods [2, 19], have been developed.
- Developing better numerical methods continues to stimulate a lot of interest amongst researchers.
- Motivated by the continued need for better performing numerical methods, in this work, we propose a hybrid method that is based on combining elements of the higher order unconditionally positive finite difference method (HUPFD) and the proper orthogonal decomposition method (POD).

Introduction

Background

- HUPFD is a finite difference-based method that guarantees the positivity of solutions, independent of the time step and mesh size. On the other hand, the POD is a powerful technique, widely used in statistics and image processing [21, 22], to reduce a large number of interdependent variables to a much smaller number of uncorrelated variables while retaining as much possible of the variation in the original variables.
- Numerical schemes that preserve the positivity of solutions are important in physical applications. To have significant meaning, quantities such as chemical species concentration, population sizes, neutron numbers, etc., require positive solutions.
- By utilizing the POD, the EHUPFD involves the extraction of a set of basis functions from the HUPFD solution called the snapshot matrix and then uses a small subset of leading basis functions to construct state variable approximations.

Introduction

Background

- We test the applicability of the EHUPFD on the ADR equations given below

$$\frac{\partial u}{\partial t} + U_a \frac{\partial u}{\partial x} - D \frac{\partial^2 u}{\partial x^2} = f(t, x, u), \tag{1}$$

$$u(0, x) = u_0(x) \geq 0, \tag{2}$$

$$u(a, t) = u_a(t) \qquad u(b, t) = u_b(t).$$

- The ADR equation is used to model exponential travelling waves, absorption of pollutants in soil, semiconductors, modelling of biological systems, and diffusion of neutrons [5, 11–13].

Literature Review

- The UPFD was developed by Chen-Charpentier & Kojouharov [6] for the advection-diffusion-reaction equation (ADR) and has since been used by several other researchers [3, 9, 20].
- The POD has been used to reduce the dimensions of numerical methods such as the Crank-Nicolson method [1, 14, 15, 17, 18, 23].
- The POD is useful when it is impossible to perform numerical simulations due to large scale computing requirements.

Research Aim and Objectives

Aim:

- The main contribution of this work is to extend the POD coupling by hybridising it with the HUPFD to obtain a novel numerical method that exhibits higher accuracy with less computing time, fewer degrees of freedom in numerical computations, and reduced truncation error, as well as ensuring positivity of the solutions.

Objectives:

The objectives of the study is to:

- Investigate the consistency and stability of the unconditionally positive finite difference methods.
- Compare the performance of the EHUPFD method to the Crank-Nicolson, NSFD methods in terms of computational time, error and convergence rate.

Problem formulation: UPFD

In this section, we present details of the UPFD schemes [6] as given below,

$$\frac{\partial u}{\partial x} \approx \begin{cases} \dfrac{u_i^n - u_{i-1}^{n+1}}{\Delta x} & (3a) \\[2ex] \dfrac{u_i^{n+1} - u_{i-1}^n}{\Delta x} & (3b) \end{cases}$$

$$\frac{\partial u}{\partial t} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t}, \quad (4)$$

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i+1}^n - 2u_i^{n+1} + u_{i-1}^n}{(\Delta x)^2}. \quad (5)$$

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Problem formulation: HUPFD 1

In this case, we consider the first-order formula for the first space derivative and the fourth order for the second space derivative approximations to obtain the higher order schemes as given below,

$$\frac{\partial u}{\partial x} \approx \begin{cases} \dfrac{u_i^n - u_{i-1}^{n+1}}{\Delta x} & (6a) \\[2ex] \dfrac{u_i^{n+1} - u_{i-1}^{n}}{\Delta x} & (6b) \end{cases}$$

$$\frac{\partial u}{\partial t} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t}, \quad (7)$$

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{-u_{i+2}^{n+1} + 16u_{i+1}^{n} - 30u_i^{n+1} + 16u_{i-1}^{n} - u_{i-2}^{n+1}}{12\Delta x^2}. \quad (8)$$

Problem formulation:HUPFD 2

In this case, the second order formula for first space derivative and fourth order for second space derivative is considered to obtain the HUPFD schemes as given below,

$$\frac{\partial u}{\partial x} \approx \begin{cases} \dfrac{u_{i+1}^{n+1} - u_{i-1}^{n}}{2\Delta x} & \text{(9a)} \\[2ex] \dfrac{u_{i+1}^{n} - u_{i-1}^{n+1}}{2\Delta x} & \text{(9b)} \end{cases}$$

$$\frac{\partial u}{\partial t} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t}, \tag{10}$$

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{-u_{i+2}^{n+1} + 16u_{i+1}^{n} - 30u_i^{n+1} + 16u_{i-1}^{n} - u_{i-2}^{n+1}}{12\Delta x^2}. \tag{11}$$

Problem formulation:HUPFD 3

In this case , the fourth order formula for first and second space derivatives is considered to obtain the HUPFD schemes as given below,

$$\frac{\partial u}{\partial x} \approx \begin{cases} \dfrac{-u_{i+2}^{n} + 8u_{i+1}^{n+1} - 8u_{i-1}^{n} + u_{i-2}^{n+1}}{12\Delta x} & (12a) \\ \\ \dfrac{-u_{i+2}^{n+1} + 8u_{i+1}^{n} - 8u_{i-1}^{n+1} + u_{i-2}^{n}}{12\Delta x} & (12b) \end{cases}$$

$$\frac{\partial u}{\partial t} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t} \tag{13}$$

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{-u_{i+2}^{n+1} + 16u_{i+1}^{n} - 30u_i^{n+1} + 16u_{i-1}^{n} + u_{i-2}^{n+1}}{12\Delta x^2} \tag{14}$$

Implementation of the higher order unconditionally positive finite difference schemes on the linear ADR equation

In this section, we set $f(t, x, u) = -u$, $U_a = 1$, and $D = 1$ in equation (1) to obtain the equation given below

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2} - u, \tag{15}$$

subject to the following initial and boundary conditions

$$\begin{cases} u(x,0) = e^{-x}, & 0 \leq x \leq 10 \\ u(0,t) = e^{t}, & 0 \leq t \leq 0.85 \\ u_x(10,t) = -u(10,t), & 0 \leq t \leq 0.85 \end{cases} \tag{16}$$

with the exact solution given by $u(x, t) = e^{(t-x)}$ [6].

Implementation of the higher order unconditionally positive finite difference schemes on the linear ADR equation.........

Solving the linear ADR equation using the HUPFD 1 scheme

Since the coefficient of $\frac{\partial u}{\partial x}$ in equation (15) is positive, we use equations (6b), (7), and (8) to find the UPFD scheme. Therefore, the HUPFD discretization of equation (15) is given by the equation below

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{u_i^{n+1} - u_{i-1}^n}{\Delta x} = \frac{-u_{i+2}^{n+1} + 16u_{i+1}^n - 30u_i^{n+1} + 16u_{i-1}^n - u_{i-2}^{n+1}}{12\Delta x^2} - u_i^{n+1}, (1$$

which simplifies to the following

$$\frac{1}{12\Delta x^2} u_{i-2}^{n+1} + \left(\frac{1}{\Delta t} + \frac{1}{\Delta x} + \frac{30}{12\Delta x^2} + 1 \right) u_i^{n+1} + \frac{1}{12\Delta x^2} u_{i+2}^{n+1} = \frac{1}{\Delta t} u_i^n + \left(\frac{1}{\Delta x} + \frac{16}{12Dx^2} \right) u_{i-1}^2 + \frac{16}{12\Delta x^2} u_{i+1}^n. \quad (18)$$

Consistency

We investigate the consistency by using the Taylor expansion on the point (m, n). The Taylor expansions of $u_i^{n+1}, u_i^{n-1}, u_{i-1}^n, u_{i+1}^n, u_{i-2}^{n+1}, u_{i+2}^{n+1}$ are as follows

$$
\begin{aligned}
u_i^{n+1} &\approx u_i^n + \Delta t\frac{\partial u}{\partial t} + \frac{(\Delta t)^2}{2}\frac{\partial^2 u}{\partial t^2} + \frac{(\Delta t)^3}{6}\frac{\partial^3 u}{\partial t^3} + \cdots \\
u_i^{n-1} &\approx u_i^n - \Delta t\frac{\partial u}{\partial t} + \frac{(\Delta t)^2}{2}\frac{\partial^2 u}{\partial t^2} - \frac{(\Delta t)^3}{6}\frac{\partial^3 u}{\partial t^3} + \cdots \\
u_{i-1}^n &\approx u_i^n - \Delta x\frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2}\frac{\partial^2 u}{\partial x^2} - \frac{(\Delta x)^3}{6}\frac{\partial^3 u}{\partial x^3} + \cdots \\
u_{i+1}^n &\approx u_i^n + \Delta x\frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2}\frac{\partial^2 u}{\partial x^2} + \frac{(\Delta x)^3}{6}\frac{\partial^3 u}{\partial x^3} + \cdots \\
u_{i-2}^{n+1} &\approx u_i^n + \Delta t\frac{\partial u}{\partial t} - 2\Delta x\frac{\partial u}{\partial x} + 2(\Delta x)^2\frac{\partial^2 u}{\partial x^2} - 2(\Delta t\Delta x)\frac{\partial^2 u}{\partial t\partial x} + \frac{(\Delta t)^2}{2}\frac{\partial^2 u}{\partial t^2} + \cdots \\
u_{i+2}^{n+1} &\approx u_i^n + \Delta t\frac{\partial u}{\partial t} + 2\Delta x\frac{\partial u}{\partial x} + 2(\Delta x)^2\frac{\partial^2 u}{\partial x^2} + 2(\Delta t\Delta x)\frac{\partial^2 u}{\partial t\partial x} + \frac{(\Delta t)^2}{2}\frac{\partial^2 u}{\partial t^2} + \cdots
\end{aligned}
\tag{20}
$$

Consistency................

By substituting equation (20) into the scheme (17) leads to the following equation

$$u_i^n + \left(\frac{\Delta t}{\Delta x} + \frac{32\Delta t}{12(\Delta x)^2} + \Delta t + 1\right)\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} - \left(1 + \frac{\Delta x}{2}\right)\frac{\partial^2 u}{\partial x^2}$$
$$+ \left(\frac{31}{12}\left(\frac{\Delta t}{\Delta x}\right)^2 + \frac{1}{2}\frac{(\Delta t)^2}{(\Delta x)} + \frac{(\Delta t)^2}{2} + \frac{(\Delta t)^2}{2}\right)\frac{\partial^2 u}{\partial t^2} = 0, \quad (21)$$

When $\Delta t \longrightarrow 0$ and $\Delta x \longrightarrow 0$, equation (21) is not consistent, hence we set $\Delta t = (\Delta x)^3$ to obtain the following equation

$$u_i^n + \left((\Delta x)^2 + \frac{32}{12}\Delta x + (\Delta x)^3 + 1\right)\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} - \left(1 + \frac{\Delta x}{2}\right)\frac{\partial^2 u}{\partial x^2}$$
$$+ \left(\frac{(\Delta t)^3}{2} + \frac{(\Delta x)^5}{2} + \frac{30(\Delta x)^4}{12} + \frac{(\Delta x)^6}{2} + \frac{(\Delta x)^2}{12}\right)\frac{\partial^2 u}{\partial t^2} = 0, \quad (22)$$

Consistency...............

When $\Delta x \longrightarrow 0$, equation (22) leads to the follow equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2} - u. \tag{23}$$

Thus, the original equation (15) is obtained, which implies the scheme is consistent when $\Delta t = (\Delta x)^3$.

Stability

The Von-Neumann stability analysis is used to investigate the stability region for the finite difference schemes. By applying Fourier series analyses to terms in equation (19), we obtain the following

$$\begin{cases} u_i^n & = \xi^n e^{j\Delta t i \Delta x} \\ u_{i-2}^{n+1} & = \xi^{n+1} e^{j\Delta t(i-2)\Delta x} \\ u_i^{n+1} & = \xi^{n+1} e^{j\Delta t(i)\Delta x} \\ u_{i+2}^{n+1} & = \xi^{n+1} e^{j\Delta t(i+2)\Delta x} \\ u_{i-1}^{n} & = \xi^{n} e^{j\Delta t(i-1)\Delta x} \\ u_{i-1}^{n-1} & = \xi^{n-1} e^{j\Delta t(i-1)\Delta x} \\ u_{i+1}^{n} & = \xi^{n} e^{j\Delta t(i+1)\Delta x} \\ u_i^{n-1} & = \xi^{n-1} e^{j\Delta t(i)\Delta x}, \end{cases} \tag{24}$$

Stability...........

The Von Neuman stability analyses is applied to terms in the dicritised equation, and we obtain the following

$$\xi^{n+1}\left(s_1 + s_2 e^{j\Delta t\Delta x} + s_3 e^{-2j\Delta\Delta x} + s_3 e^{2j\Delta t\Delta x}\right) = \xi^n\left((16s_3 + s_2)e^{-j\Delta t\Delta x} + 16s_3 e^{j\Delta t\Delta}\right.$$

Since $|\xi|^2 \leq 1$ from the Von Neuman stability analysis, we have the following

$$-1 + \frac{1}{3(\Delta x)^2 + 1} \leq \Delta t \tag{26}$$

The HUPFD scheme is stable, and that implies the scheme is convergence since is stable and consistent when $\Delta t = (\Delta x)^3$.

Numerical Results

We validate the results of the method by comparing them to the exact, Crank Nicolson, and NSFD solutions. The convergence rates, absolute errors, and computational time are calculated as to evaluate the methods' performance. The numerical and analytical solutions are denoted by $\bar{u}_{i,j}$ and $u_{i,j}$, respectively. The error is denoted by $e_{i,j}$, and its magnitude is measured by the L_∞-norm given by the formula below,

$$||e_{i,n}||_\infty = ||u_{i,n} - \bar{u}_{i,n}||_\infty = Max|u_{i,n} - \bar{u}_{i,n}| \tag{27}$$

The convergence rate is calculated by using the formula below,

$$q(\Delta t_k) = \frac{log_2\left(\frac{e_k}{e_{k+1}}\right)}{log_2\left(\frac{\Delta t}{\Delta t_{k+1}}\right)} \quad \text{or} \quad q(\Delta x_k) = \frac{log_2\left(\frac{e_k}{e_{k+1}}\right)}{log_2\left(\frac{\Delta x}{\Delta x_{k+1}}\right)} \tag{28}$$

Numerical Results...........

The accuracy of the EUPFD relies on the size of the snapshot, L. Therefore, finding the best snapshot size such that the accuracy is a maximum is paramount. To determine the best snapshot size, we first set $L = 1$ and find the solution. We then make increments of 1 on L until there is no significant change in the solution. To do this, we set up a tolerance as follows;

$$||u_{exact} - u_L||_\infty \leq \epsilon, \quad L = 1, 2, 3, \dots \tag{29}$$

where u_{exact} is the exact solution, and u_L is the solution at the specific value of L. The first value of L that satisfies (29) is the optimal value of L. In this work, we set ϵ to be 10^{-10}.

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Numerical Results....................

Numerical results for the linear advection-diffusion-reaction equation

Table: Convergence rates for the linear ADR equation by the UPFD,NSFD, Crank-Nicolson and HUPFD with respect to varying Δx and Δt.

		$q(\Delta t_k)$					
Δt_k	Δx_k	UPFD	EHUPFD 1	EHUPFD 2	EHUPFD 3	Crank-Nicolson	NSFD
0.00005	0.6667	2.1675	2.5233	1.6978	1.0006	2.5606	2.0579
0.0001	0.6667	0.9973	1.0054	1.1996	1.0212	1.0051	1.9427
0.0002	0.6667	1.8201	1.9990	1.5640	1.0023	2.7372	1.8871
0.0004	0.6667						

Numerical Results...........

Table: Infinity norm results of the linear ADR equation by using the exact, UPFD, Crank-Nicolson, NSFD and HUPFD solutions.

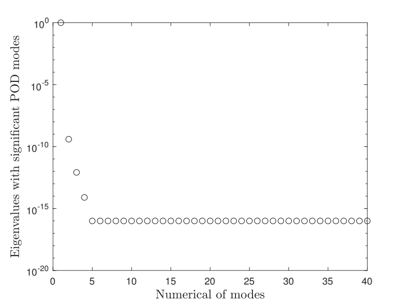
(t, x)	Exact	HUPFD	Error	First and Fourth order (HUPFD)	Error	Second and Fourth order (HUPFD)	Error	Fourth order (HUPFD)	Error	Enhanced Fourth order (HUPFD)	Error	Crank Nicolson	Error	NSFD	Error
$u(:, 0.0002)$	1.1654	1.1654	0.0025	1.1654	0.0025	1.1655	0.0025	1.1653	0.0025	1.1652	0.0047	1.1654	0.0025	1.1654	0.0025
$u(:, 0.0004)$	1.1657	1.1657	0.0025	1.1657	0.0025	1.1657	0.0025	1.1652	0.0027	1.1650	0.0059	1.1657	0.0025	1.1657	0.0025
$u(:, 0.0006)$	1.1659	1.1660	0.0025	1.1660	0.0025	1.1660	0.0025	1.1652	0.0030	1.1648	0.0077	1.1660	0.0025	1.1660	0.0025
Time		0.004230		0.002748		0.002717		0.003089		0.001396		0.002689		0.001033	

In this table we compare the infinity norms of the proposed HUPFD with the UPFD and the NSFD methods in solving the linear ADR equation. For this example, results show that HUPFD method preserve the accuracy.

Numerical Results....................

Numerical results for the linear advection-diffusion-reaction equation

(a)



(b)

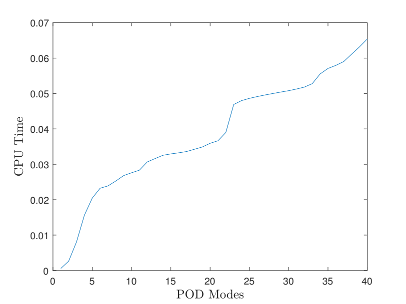


Figure: (**a**) POD modes for linear reaction diffusion equation. (**b**) Number of POD Modes vs CPU Time for the linear reaction diffussion equation.

Numerical Results....................

Numerical results for the linear advection-diffusion-reaction equation

(a)

(b)

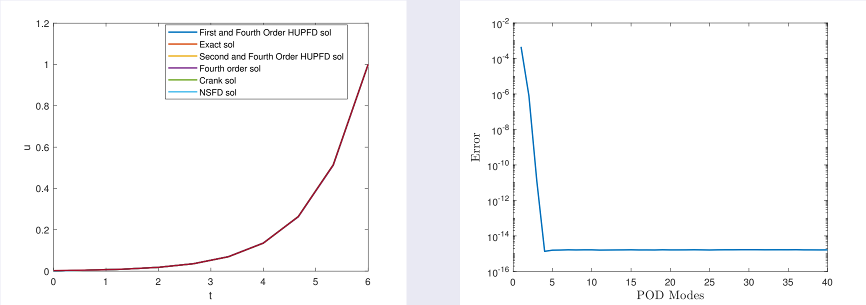


Figure: (**a**) Comparison of the exact and EHUPFD Solutions of the linear ADR equation. (**b**) Number of POD modes vs error.

Conclusion

- The results shows that the EHUPFD is a good approximation to the ADR problem.
- The EHUPFD saves computational time, reduces degrees of freedom in numerical computations, alleviates truncation error accumulation, and it preserves the positivity of the solution.
- We also observed that increasing the order of the UPFD scheme leads to the implicit scheme that is unconditionally stable with an increased order of accuracy in respect of time and space.

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