

HIGHER ORDER ACCURATE COMPACT SCHEMES FOR TIME DEPENDENT LINEAR AND NONLINEAR CONVECTION-DIFFUSION EQUATIONS

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ABSTRACT. The primary objective of this work is to study higher order compact finite difference schemes for finding the numerical solution of convection-diffusion equations which are widely used in engineering applications. The first part of this work is concerned with a higher order exponential scheme for solving unsteady one dimensional linear convection-diffusion equation. The scheme is set up with a fourth order compact exponential discretization for space and cubic C^1 -spline collocation method for time. The scheme achieves fourth order accuracy in both temporal and spatial variables and is proved to be unconditionally stable. The second part explores the utility of a sixth order compact finite difference scheme in space and Huta's improved sixth order Runge-Kutta scheme in time combined to find the numerical solution of one dimensional nonlinear convection-diffusion equations. Numerical experiments are carried out with Burgers' equation to demonstrate the accuracy of the new scheme which is sixth order in both space and time. Also a sixth order in space predictor-corrector method is proposed. A comparative study is performed of the proposed schemes with existing predictor-corrector method. The investigation of computational order of convergence is presented.

Key words and phrases: Convection-diffusion; Compact schemes; Cubic C^1 -spline; Stability; Predictor-corrector; Convergence; Computational order.

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1. INTRODUCTION

The major trials and tribulations in cracking numerical solutions for simulation models of real life problems in science is the lack of literature to felicitate analytical solutions of the governing partial differential equations. Hence, designing and analysis of innovative numerical techniques is one crucial far-reaching area of research. The convection-diffusion equation always attracts research interest for its academic significance and relevance to a broad range of practical applications that are more closely related to human activities. The behaviour of many parameters in fluid flow phenomena [1], the dispersion of dissolved material in estuaries and coastal seas [2], heat transfer in a draining film [3], thermal pollution in river system [4], dispersion of tracers in porous media [5], water transfer in soils [6], the spread of contaminants in rivers and streams [7] are some of the critical convection-diffusion models in science and engineering.

For the numerical solution of convection-diffusion equations, one of the familiar computational scheme is Crank-Nicolson scheme [8]. This scheme is unconditionally stable with second order accuracy in both space and time. In general, it has been observed that the numerical solution of initial-boundary value problems obtained with lower order schemes in space and time needs sufficiently refined meshes to attain higher accuracy. But higher order spatial discretizations are generally associated with large stencils [9] that increases the complexity of computations. The conventional higher accurate finite difference techniques use large stencil sizes that also make boundary treatment difficult to achieve the desired order of accuracy. In the context of higher order finite differences, compact finite difference methods are capable of producing higher order accuracy without any increase in the stencil size.

Based on the fourth order Padé-type schemes of first and second order spatial derivatives, Hirsh [10] developed a three-point fourth order compact finite difference method for the one dimensional convection-diffusion equations. Rigal [11] developed a scheme for unsteady convection-diffusion equations which is second order in time and fourth order in space. Also, it includes several schemes proposed by different authors. Ding and Zhang [12] used a semidiscrete and a Padé approximation method to present a new difference scheme for solving convection-diffusion problems. The scheme is fourth order in space and fifth order in time. Around the same time, Mohebbi and Dehghan [13] introduced a method by taking a compact finite difference approximation of fourth order for discretizing spatial derivatives and the cubic C^1 -spline collocation method for the time discretization. Recently, development of numerical methods like polynomial higher order compact schemes and exponential higher order compact schemes [14, 15, 16, 17] have generated significant interest because of the computational efficiency and higher accuracy. Tian and Yu [18] proposed a higher order exponential scheme for the unsteady convection-diffusion equations which is fourth order accurate in space and time. This scheme is proposed for the convection-diffusion equations with constant Dirichlet boundary conditions. Later, Fu, Tian and Liu [19] extended this scheme to Neumann boundary conditions and showed that order and stability do not change under the extended scheme.

Higher order accurate and efficient finite difference schemes are scarce in literature for solving nonlinear convection-diffusion equations. Burgers' equation is a quasilinear convectiondiffusion equation that arises in many physical phenomena such as one dimensional turbulence [20, 21], waves in fluid filled viscous elastic tubes [22], chemical reaction-diffusion model of Brusselator [23] etc. Due to the nonlinearity, the schemes mentioned above cannot be directly applied to the Burgers' equation. Most of the existing schemes in literature for Burgers' equation are based on reducing Burgers' equation to a linear heat equation and deriving finite difference approximations on the transformed heat equation. Such finite differences or compact finite differences can be found in [24, 25, 26]. There are finite difference schemes that can be directly implemented to the Burgers' equation. An implicit scheme introduced by Liao [27] and a predictor-corrector scheme by Zhand and Wang [28] are some of them. Also there are some special approaches for solving the Burgers equation like multiquadric quasi-interpolation by Hon and Mao [29], automatic differentiation by Asaithambi [30] etc.

In this work, we first propose a compact higher order scheme for solving transient linear one dimensional convection-diffusion equations. The unconditionally stable numerical scheme for 1D linear convection-diffusion equations is developed with fourth order exponential difference formula for the space discretization and a fourth order cubic C^1 -spline collocation method for time discretization. Next, we develop a scheme for one dimensional nonlinear convection-diffusion equations by replacing first and second order spatial derivatives with sixth order compact finite difference approximations and Huta's improved sixth order Runge-Kutta method for time discretization. The proposed sixth order scheme in space and time is applied to the Burgers' equation. We also performed numerical computations on Burgers' equation using predictor-corrector algorithm called MacCormack method. A comparative study of these methods is performed and finally the computational order of convergence is investigated. The structure of the paper is as follows: Section 1 gives the introduction. In Section 2, a fourth order scheme for the linear convection-diffusion equation is presented and it is proved that the method is unconditionally stable. Numerical results with the proposed scheme are presented. In Section 3, a sixth order scheme in space and time for the nonlinear convection-diffusion equation is summarized and applied to the Burgers' equation. In the same section, numerical results are presented and a comparative study is performed using CD4 predictor-corrector [28], CD6 predictor-corrector and CD6 Huta's improved RK6. Some concluding remarks are drawn in the last section.

2. LINEAR CONVECTION-DIFFUSION EQUATIONS

This section introduces a new higher order compact finite difference scheme for the linear 1D convection-diffusion equation with Dirichlet boundary conditions. Here we bring out the compact finite difference approximation to the governing equation by solving the steady linear 1D convection-diffusion equation using Green's function and the resulting solution is discretized by standard central difference operators. By this treatment, the unsteady linear 1D convection-diffusion equation is transformed into system of ordinary differential equations which are solved by C^1 -spline collocation method.

2.1. Governing Equation.

(2.1)
$$y_t + \alpha y_x = \nu y_{xx}, \ 0 < x < L, \ 0 < t \le T.$$

The initial condition is

$$y(x,0) = \psi(x), \ 0 \le x \le L,$$

and the Dirichlet boundary conditions are

$$y(0,t) = g_1(t), \ y(L,t) = g_2(t), \ 0 \le t \le T,$$

where y(x,t) represent a scalar variable with constant velocity $\alpha \neq 0$ and constant diffusivity $\nu > 0$.

2.2. Numerical scheme. Divide the spatial domain [0, L] into N + 1 grid points: $0 = x_0, x_1, x_2, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_N = L$, with mesh size $h = x_i - x_{i-1}$. Let Δt denote the time step size. Consider the steady 1D convection-diffusion equation

$$(2.2) \qquad \qquad -\nu y_{xx} + \alpha y_x = f, \ 0 < x < L,$$

where f is a sufficiently smooth function of x. First consider the following initial-boundary value problem in the sub domain $[x_{i-1}, x_{i+1}]$ (i = 1, 2, ..., N - 1):

(2.3)
$$\begin{aligned} -\nu y_{xx} + \alpha y_x &= f, \ x_{i-1} < x < x_{i+1}, \\ y(x_{i-1}) &= y_{i-1}, \ y(x_{i+1}) = y_{i+1}. \end{aligned}$$

Let $\psi_1(x)$ and $\psi_2(x)$ be the respective solutions of the following boundary value problems

(2.4)
$$\begin{aligned} -\nu\psi_{xx} + \alpha\psi_x &= 0, \ x_{i-1} < x < x_{i+1}, \\ \psi(x_{i-1}) &= 1, \ \psi(x_{i+1}) = 0, \end{aligned}$$

and

(2.5)
$$\begin{aligned} -\nu \psi_{xx} + \alpha \psi_x &= 0, \ x_{i-1} < x < x_{i+1} \\ \psi(x_{i-1}) &= 0, \ \psi(x_{i+1}) = 1. \end{aligned}$$

Then the solution of the problem (2.3) is

(2.6)
$$y(x) = \psi_1(x)y_{i-1} + \psi_2(x)y_{i+1} + \int_{x_{i-1}}^{x_{i+1}} G(x,\zeta)f(\zeta)d\zeta,$$

where $G(x, \zeta)$ is the Green's function of the following problem

(2.7)
$$\begin{cases} -\nu y_{xx} + \alpha y_x = 0, \quad x_{i-1} < x < x_{i+1} \\ y(x_{i-1}) = 0, \quad y(x_{i+1}) = 0. \end{cases}$$

By solving equations (2.4) and (2.5) we obtain,

(2.8)
$$\psi_1(x) = \frac{1 - e^{\frac{\alpha}{\nu}(x - x_{i+1})}}{1 - e^{-\frac{2\alpha}{\nu}h}} \text{ and } \psi_2(x) = \frac{e^{\frac{\alpha}{\nu}(x - x_{i-1})} - 1}{e^{\frac{2\alpha}{\nu}h} - 1}$$

Also,

(2.9)
$$G(x,\zeta) = \frac{1}{W(\zeta)} \begin{cases} \psi_1(x)\psi_2(\zeta), & x_{i-1} \le \zeta < x \\ \psi_1(\zeta)\psi_2(x), & x \le \zeta \le x_{i+1}. \end{cases}$$

By using Abel's formula we can find the Wronskian $W(\zeta)$ as,

(2.10)
$$W[\psi_1, \psi_2](\zeta) = W[\psi_1, \psi_2](x_{i-1})e^{-\int_{x_{i-1}}^{\zeta} -\frac{\alpha}{\nu}ds} = \frac{\alpha}{\nu} \frac{e^{\frac{\alpha}{\nu}(\zeta-x_i)}}{e^{\frac{\alpha}{\nu}h} - e^{-\frac{\alpha}{\nu}h}}.$$

Substituting (2.8), (2.9) and (2.10) in (2.6), we can obtain the solution of (2.2) as

(2.11)
$$y(x_{i}) = \psi_{1}(x_{i})y_{i-1} + \psi_{2}(x_{i})y_{i+1} + \frac{\nu}{\alpha}\psi_{1}(x_{i})\int_{x_{i-1}}^{x_{i}} \left(1 - e^{-\frac{\alpha}{\nu}(\zeta - x_{i-1})}\right)f(\zeta)d\zeta + \frac{\nu}{\alpha}\psi_{2}(x_{i})\int_{x_{i}}^{x_{i+1}} \left(e^{-\frac{\alpha}{\nu}(\zeta - x_{i+1})} - 1\right)f(\zeta)d\zeta.$$

Let the source term f(x) be expressed as

(2.12)
$$f(x) = f_i + (x - x_i)\delta_x f_i + \frac{(x - x_i)^2}{2!}\delta_x^2 f_i + \frac{(x - x_i)^3}{3!}f_{xxx}(\eta_i), \ \eta_i \in (x_{i-1}, x_{i+1}),$$

where δ_x and δ_x^2 are the standard second order central difference operators for $x \in (x_{i-1}, x_{i+1})$, i = 1, 2, ..., N - 1. Substituting (2.12) in (2.11) we obtain

(2.13)
$$-a\delta_x^2 y_i + \alpha \delta_x y_i = f_i + b\delta_x f_i + c\delta_x^2 f_i + O\left(h^4\right),$$

where

$$a = \frac{\alpha h}{2} \operatorname{coth}\left(\frac{\alpha h}{2\nu}\right), \quad b = \frac{\nu - a}{\alpha}, \quad c = \frac{\nu(\nu - a)}{\alpha^2} + \frac{h^2}{6}.$$

Omitting the truncation error in (2.13), a three-point fourth order compact finite difference scheme for (2.2) is obtained. Using this, a semi-discrete fourth order exponential approximation for the unsteady 1D convection-diffusion problem (2.1) is developed as follows,

(2.14)
$$\begin{pmatrix} \frac{c}{h^2} - \frac{b}{2h} \end{pmatrix} \left(\frac{\partial y}{\partial t} \right)_{i-1}^n + \left(1 - \frac{2c}{h^2} \right) \left(\frac{\partial y}{\partial t} \right)_i^n + \left(\frac{c}{h^2} + \frac{b}{2h} \right) \left(\frac{\partial y}{\partial t} \right)_{i+1}^n \\ = \left(\frac{a}{h^2} + \frac{\alpha}{2h} \right) y_{i-1}^n - \frac{2a}{h^2} y_i^n + \left(\frac{a}{h^2} - \frac{\alpha}{2h} \right) y_{i+1}^n.$$

This leads to a system of first order ordinary differential equations given by

(2.15)
$$A\frac{dY(t)}{dt} = BY(t) + G,$$
$$Y(0) = \Psi_0,$$

in which

$$\begin{split} Y(t) &= [y_1(t), y_2(t), \dots, y_{N-1}(t)]^T, \ \Psi_0 = [\psi_1, \psi_2, \dots, \psi_{N-1}]^T, \\ G &= \left[\left(\frac{a}{h^2} + \frac{\alpha}{2h} \right) g_1(t) - \left(\frac{c}{h^2} - \frac{b}{2h} \right) g_1'(t), 0, \dots, 0, \left(\frac{a}{h^2} - \frac{\alpha}{2h} \right) g_2(t) - \left(\frac{c}{h^2} + \frac{b}{2h} \right) g_2'(t) \right]^T, \\ A &= tri \left[\left(\frac{c}{h^2} - \frac{b}{2h} \right), \left(1 - \frac{2c}{h^2} \right), \left(\frac{c}{h^2} + \frac{b}{2h} \right) \right]_{N-1} \text{ and } B = tri \left[\left(\frac{a}{h^2} + \frac{\alpha}{2h} \right), -\frac{2a}{h^2}, \left(\frac{a}{h^2} - \frac{\alpha}{2h} \right) \right]_{N-1}. \\ \text{Since the matrix } A \text{ is tri-diagonal and strictly diagonally dominant, it is nonsingular. Therefore the system (2.15) can be written as \end{split}$$

(2.16)
$$\frac{dY(t)}{dt} = A^{-1}BY(t) + A^{-1}G,$$
$$Y(0) = \Psi_0.$$

This semi-discretized system of ordinary differential equations is solved by fourth order cubic C^1 -spline collocation method [31] given by

(2.17)
$$Y^{n} = Y^{n-1} + \frac{\Delta t}{6} \left((Y')^{n-1} + 4(Y')^{n-\frac{1}{2}} + (Y')^{n} \right),$$

(2.18)
$$Y^{n-\frac{1}{2}} = Y^{n-1} + \frac{\Delta t}{24} \left(5(Y')^{n-1} + 8(Y')^{n-\frac{1}{2}} - (Y')^n \right)$$

Let $M = A^{-1}B$, using (2.16), (2.17) and (2.18) we have

$$Y^{n} = Y^{n-1} + \frac{\Delta t}{6} \left(MY^{n-1} + A^{-1}G^{n-1} + 4MY^{n-\frac{1}{2}} + 4A^{-1}G^{n-\frac{1}{2}} + MY^{n} + A^{-1}G^{n} \right),$$
(2.20)

$$Y^{n-\frac{1}{2}} = Y^{n-1} + \frac{\Delta t}{24} \left(5MY^{n-1} + 5A^{-1}G^{n-1} + 8MY^{n-\frac{1}{2}} + 8A^{-1}G^{n-\frac{1}{2}} - MY^n - A^{-1}G^n \right).$$

On rearranging, (2.19) and (2.20) can be written as

$$(2.21) \left(I - \frac{\Delta t}{6}M\right)Y^{n} = \left(I + \frac{\Delta t}{6}M\right)Y^{n-1} + \frac{2\Delta t}{3}MY^{n-\frac{1}{2}} + \frac{\Delta t}{6}A^{-1}\left(G^{n-1} + 4G^{n-\frac{1}{2}} + G^{n}\right),$$

$$(2.22) \left(I - \frac{\Delta t}{3}M\right)Y^{n-\frac{1}{2}} = \left(I + \frac{5\Delta t}{24}M\right)Y^{n-1} - \frac{\Delta t}{24}MY^{n} + \frac{\Delta t}{24}A^{-1}\left(5G^{n-1} + 8G^{n-\frac{1}{2}} - G^{n}\right),$$

where I is the $(N-1) \times (N-1)$ identity matrix. Removing the term $Y^{n-\frac{1}{2}}$ from (2.21) and (2.22) we obtain the following proposed scheme, (2.23)

$$\begin{split} \left(I - \frac{\Delta t}{2}M + \frac{\Delta t^2}{12}M^2\right)Y^n &= \left(I + \frac{\Delta t}{2}M + \frac{\Delta t^2}{12}M^2\right)Y^{n-1} + \left(\frac{\Delta t}{6}A^{-1} + \frac{1}{12}\Delta t^2A^{-1}M\right)G^{n-1} \\ &+ \frac{2\Delta t}{3}A^{-1}G^{n-\frac{1}{2}} + \left(\frac{\Delta t}{6}A^{-1} - \frac{1}{12}\Delta t^2A^{-1}M\right)G^n \end{split}$$

Theorem 2.1. *The numerical scheme*(2.23) *is unconditionally stable.*

Proof. For a stable difference scheme, small errors in the initial condition only cause small errors in the solution. Let a small perturbation be introduced at t = 0 such that the initial vector Y_0 becomes Y_0^* . Denote $e^0 = Y_0 - Y_0^*$. Let

$$Q = \left(I - \frac{\Delta t}{2}M + \frac{\Delta t^2}{12}M^2\right)^{-1} \left(I + \frac{\Delta t}{2}M + \frac{\Delta t^2}{12}M^2\right).$$

We define error vector $\mathbf{e}^n = Y^n - Y^{*n}$, $n = 1, 2, \dots, \frac{T}{\Delta t}$. Thus,

(2.24)
$$\mathbf{e}^{n} = Y^{n} - Y^{*n} = Q(Y^{n-1} - Y^{*n-1}) = Q\mathbf{e}^{n-1}$$

Therefore from (2.24) we can say that $\mathbf{e}^n = Q\mathbf{e}^{n-1} = Q^2\mathbf{e}^{n-2} = Q^3\mathbf{e}^{n-3} = \ldots = Q^n\mathbf{e}^0$. Then we have $\|\mathbf{e}^n\|_2 \leq \|Q^n\|_2 \|\mathbf{e}^0\|_2$. Let λ_i be the eigenvalues of the matrix M, then the eigenvalues of matrix Q are

(2.25)
$$\frac{1 + \frac{1}{2}\Delta t\lambda_i + \frac{1}{12}(\Delta t\lambda_i)^2}{1 - \frac{1}{2}\Delta t\lambda_i + \frac{1}{12}(\Delta t\lambda_i)^2} \quad \text{for } i = 1, 2, \dots, N-1.$$

It is not difficult to show that the real part of the eigenvalues λ_i is nonpositive for every i = 1, 2, ..., N - 1. A straightforward calculation gives

(2.26)
$$\max_{i} \left[\frac{1 + \frac{1}{2} \Delta t \lambda_{i} + \frac{1}{12} (\Delta t \lambda_{i})^{2}}{1 - \frac{1}{2} \Delta t \lambda_{i} + \frac{1}{12} (\Delta t \lambda_{i})^{2}} \right] \leq 1 \quad \text{for every } i = 1, 2, \dots, N - 1.$$

Hence $||Q^n||_2 \longrightarrow 0$ as $n \longrightarrow \infty$. Since \mathbf{e}^0 is the initial error, $||\mathbf{e}^0||_2$ is finite. Therefore $||\mathbf{e}^n||_2 \longrightarrow 0$ as $n \longrightarrow \infty$. This completes the proof of the theorem (2.1).

2.3. Numerical observations. In this section, we present the numerical results of the proposed method on three test problems. The computational order of accuracy denoted by C-order is calculated with the formula $\log_2 \left(\frac{\mathbf{e_1}}{\mathbf{e_2}}\right)$ in which $\mathbf{e_1}$ and $\mathbf{e_2}$ are the errors corresponding to space steps h and $\frac{h}{2}$. The Péclet number is defined as $P_e = \left|\frac{\alpha}{\nu}\right|$ which determines whether the given equation is convection dominated or diffusion dominated.

2.3.1. *Problem 1.* Consider the convection-diffusion equation (2.1), with the initial condition (2.27) $y(x,0) = \sin(x), \quad 0 < x < 2,$

and the boundary conditions

(2.28)
$$y(0,t) = -e^{-\nu t}\sin(\alpha t), \ y(2,t) = e^{-\nu t}\sin(2-\alpha t).$$

The exact solution is given by $y(x,t) = e^{-\nu t} \sin(x - \alpha t)$. We take $\alpha = 1$ for the numerical computations using the proposed scheme given in Section 2.2. In Table 2.1, we show the absolute errors obtained for Problem 1 with various Péclet numbers P_e at final time T = 2 with h = 0.01. Fig. 1(a) shows the numerical solution of Problem 1 for several values of T with

$h = 0.01, \Delta t = 0.01$ and $P_e = 100$. Fig.	1(b) shows the s	space-time grap	ph of numerical	solution
with $h = 0.02$, $\Delta t = 0.05$ and $P_e = 100$.				

x	<i>P_e</i> =50	$P_{e} = 100$	$P_e = 1000$
	Absolute error	Absolute error	Absolute error
0.25	4.8446×10^{-8}	1.8349×10^{-7}	3.1187×10^{-6}
0.5	1.4795×10^{-8}	6.4951×10^{-8}	1.3160×10^{-6}
0.75	7.7077×10^{-8}	3.0928×10^{-7}	5.6685×10^{-6}
1	1.3437×10^{-7}	5.3406×10^{-7}	9.6672×10^{-6}
1.25	1.8234×10^{-7}	7.2503×10^{-7}	1.3062×10^{-5}
1.5	2.1187×10^{-7}	8.6508×10^{-7}	1.5642×10^{-5}
1.75	1.9999×10^{-7}	8.6441×10^{-7}	1.7245×10^{-5}

Table 2.1: Absolute error for Problem 1 with h = 0.01, $\Delta t = 0.005$ and T = 2.



Figure 1: (a) Numerical solution of Problem 1 for several values of T with h = 0.01, $\Delta t = 0.01$ and $P_e = 100$ (left). (b) Space-time graph of Problem 1 with h = 0.02, $\Delta t = 0.05$, $P_e = 100$ and T = 1 (right).

2.3.2. Problem 2. Consider the convection-diffusion equation (2.1), with $\alpha = 1, \nu = 0.1$ and the initial condition

(2.29)
$$y(x,0) = e^{5x} \left[\cos\left(\frac{\pi}{2}x\right) + 0.25 \sin\left(\frac{\pi}{2}x\right) \right], \ 0 \le x \le 1.$$

The exact solution is given by

(2.30)
$$y(x,t) = e^{5(x-\frac{t}{2})}e^{-\frac{\pi^2}{40}t} \left[\cos\left(\frac{\pi}{2}x\right) + 0.25\sin\left(\frac{\pi}{2}x\right)\right]$$

The boundary conditions are obtained from the exact solution. In Table 2.2, we show the absolute errors obtained for Problem 2 at final time T = 2 with several values of h. Fig. 2(a) presents the numerical solution of Problem 2 for various values of T with h = 0.02 and $\Delta t = 2h$. In Fig. 2(b) we show the space-time graph of Problem 2 with h = 0.02 and $\Delta t = 2h$.

x	h=0.1	h=0.05	h=0.01
	Absolute error	Absolute error	Absolute error
0.1	2.4415×10^{-6}	9.1067×10^{-8}	1.9957×10^{-9}
0.2	1.5594×10^{-5}	7.4122×10^{-7}	1.4759×10^{-9}
0.3	3.4709×10^{-5}	1.9498×10^{-6}	1.4046×10^{-10}
0.4	6.5946×10^{-5}	3.9224×10^{-6}	3.7904×10^{-9}
0.5	1.1024×10^{-4}	6.8973×10^{-6}	1.1037×10^{-8}
0.6	1.6797×10^{-4}	1.1053×10^{-5}	2.4446×10^{-8}
0.7	2.3460×10^{-4}	1.6354×10^{-5}	4.8187×10^{-8}
0.8	2.8296×10^{-4}	2.2225×10^{-5}	8.9010×10^{-8}
0.9	3.3511×10^{-4}	2.5916×10^{-5}	1.5787×10^{-8}

Table 2.2: Absolute error for Problem 2 with $\Delta t = 2h$ *and* T = 2*.*



Figure 2: (a) Numerical solution of Problem 2 for various values of T with h = 0.02 and $\Delta t = 2h$ (left). (b) Space-time graph of Problem 2 with h = 0.02, $\Delta t = 2h$ and T = 1 (right).

2.3.3. Problem 3. Consider the convection-diffusion equation (2.1), with the initial condition

(2.31)
$$y(x,0) = e^{-\frac{(x-\alpha)^2}{4\nu}}, \quad 0 < x < 2,$$

and the boundary conditions are

(2.32)
$$y(0,t) = \frac{1}{\sqrt{1+t}} e^{-\frac{(1+t)^2 \alpha^2}{4\nu(1+t)}}, \ y(2,t) = \frac{1}{\sqrt{1+t}} e^{-\frac{(2-(1+t)\alpha)^2}{4\nu(1+t)}}.$$

The exact solution is given by

(2.33)
$$y(x,t) = \frac{1}{\sqrt{1+t}} e^{-\frac{(x-(1+t)\alpha)^2}{4\nu(1+t)}}.$$

For this problem we take $\alpha = 0.25$ for the numerical computation. In Table 2.3, the numerical results obtained with different values of h and P_e at final time T = 2 are shown. Table 2.3 shows that the proposed scheme has achieved good accuracy and rate of convergence. In Fig.

3(a), numerical solution of Problem 3 for several values of T with h = 0.01, $\Delta t = 0.01$ and $P_e = 25$ is presented. Fig. 3(b) shows the space-time graph of Problem 3 with h = 0.01, $\Delta t = 0.01$, $P_e = 25$ and T = 1.

h	<i>P_e</i> =2	C-order	<i>P_e</i> =20	C-order	<i>P_e</i> =40	C-order
	Maximum error		Maximum error		Maximum error	
0.04	1.6900×10^{-7}		7.1007×10^{-5}		5.1492×10^{-4}	
0.02	1.0544×10^{-8}	4.0025	4.5219×10^{-6}	3.9730	3.3947×10^{-5}	3.9230
0.01	6.5253×10^{-10}	4.0142	2.8275×10^{-7}	3.9993	2.1416×10^{-6}	3.9865
0.005	1.9452×10^{-11}	5.0681	1.7526×10^{-8}	4.0120	1.3403×10^{-7}	3.9981

Table 2.3: Maximum error and convergence rate for Problem 3 with $\Delta t = 0.005$ *and* T = 2*.*



Figure 3: (a) Numerical solution of Problem 3 for several values of T with h = 0.01, $\Delta t = 0.01$ and $P_e = 25$ (left). (b) Space-time graph of Problem 3 with h = 0.01, $\Delta t = 0.01$, $P_e = 25$ and T = 1 (right).

It is clearly evident from the tables that the proposed scheme achieved high accuracy. Also the figures reveal the convective and diffusive nature of the given equations. Table (2.3) shows that the computational order of the proposed method is four, which agrees with the theoretical order. The numerical results obtained indicate that the combination of the exponential method for the space discretization and C^1 -spline collocation method for the time discretization is an effective tool for solving unsteady linear 1D convection-diffusion equations. However, the proposed unconditionally stable scheme described in this section is restricted to solving only linear unsteady 1D convection-diffusion problems.

3. NONLINEAR CONVECTION-DIFFUSION EQUATIONS

One of the basic approaches of higher order compact finite difference methods is to obtain all the numerical derivatives along a grid line using smaller stencils and solving the resulting linear system of ordinary differential equations. The present work also uses this approach in order to obtain the solution of nonlinear convection-diffusion equations with sixth order accuracy in both space and time. For the time discretization we presented Huta's improved RK6 method. Numerical experiments are conducted with Burgers' equation using CD6 Huta's improved RK6 method and also CD6 predictor-corrector method.

3.1. Numerical scheme-CD6. Consider the nonlinear convection-diffusion equation

(3.1)
$$y_t + f_1(x, t, y)y_x = f_2(x, t, y)y_{xx}, \quad c < x < d, \ t > 0,$$

with initial and boundary conditions. Divide the spatial domain [c, d] into N grid points: $c = x_1, x_2, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_N = d$ with mesh size $h = x_i - x_{i-1}$. Using the sixth order accurate compact difference scheme (CD6), see [32, 33], the spatial derivatives are calculated at each grid point. Let Δt denote the time step size. The first derivatives at interior nodes $3 \le i \le N - 2$ can be obtained as follows

(3.2)
$$\frac{1}{3}y'_{i-1} + y'_{i} + \frac{1}{3}y'_{i+1} = \frac{1}{9}\frac{(y_{i+2} - y_{i-2})}{4h} + \frac{14}{9}\frac{(y_{i+1} - y_{i-1})}{2h}.$$

For the nodes at the left boundary, i.e., at i = 1, 2, respectively, we have

$$(3.3) y'_{i} + 5y'_{i+1} = \frac{1}{h} \left(-\frac{197}{60}y_{i} - \frac{5}{122}y_{i+1} + 5y_{i+2} - \frac{5}{3}y_{i+3} + \frac{5}{12}y_{i+4} - \frac{1}{20}y_{i+5} \right),$$

$$(3.4) \\ \frac{2}{11}y'_{i-1} + y'_{i} + \frac{2}{11}y'_{i+1} = \frac{1}{h}\left(-\frac{20}{33}y_{i-1} - \frac{35}{132}y_{i} + \frac{34}{33}y_{i+1} - \frac{7}{33}y_{i+2} + \frac{2}{33}y_{i+3} - \frac{1}{132}y_{i+4}\right).$$

For the nodes at the right boundary, i.e., at i = N - 1, N, respectively, we have (3.5)

$$\frac{2}{11}y'_{i-1} + y'_{i} + \frac{2}{11}y'_{i+1} = \frac{1}{h}\left(\frac{20}{33}y_{i+1} + \frac{35}{132}y_{i} - \frac{34}{33}y_{i-1} + \frac{7}{33}y_{i-2} - \frac{2}{33}y_{i-3} + \frac{1}{132}y_{i-4}\right),$$

(3.6)
$$5y'_{i-1} + y'_{i} = \frac{1}{h} \left(\frac{197}{60} y_{i} + \frac{5}{122} y_{i-1} - 5y_{i-2} + \frac{5}{3} y_{i-3} - \frac{5}{12} y_{i-4} + \frac{1}{20} y_{i-5} \right).$$

The above equations (3.2-3.6) can be represented in the matrix form

(3.7)
$$BY' = AY$$
 where $Y = (y_1, y_2, ..., y_N),$

where the matrix B is

and the matrix A is

Applying the first order operator twice, we can obtain the second derivative terms i.e.,

$$BY'' = AY'.$$

Approximating the spatial derivatives in (3.1) at each grid point using (3.7) and (3.8) lead to a system of ordinary differential equations

(3.9)
$$\frac{dY}{dt} = LY,$$

where Ly_i denotes the residual at point *i*.

3.2. **Time discretization.** The semi-discrete equation (3.9) is solved using Huta's improved RK6 method [34] as follows,

$$\begin{split} Y^{(1)} &= Y^n + \frac{\Delta t}{9} L(Y^n), \\ Y^{(2)} &= Y^n + \frac{\Delta t}{24} \left(L(Y^n) + 3L(Y^{(1)}) \right), \\ Y^{(3)} &= Y^n + \frac{\Delta t}{6} \left(L(Y^n) - 3L(Y^{(1)}) + 4L(Y^{(2)}) \right), \\ Y^{(4)} &= Y^n + \frac{\Delta t}{8} \left(-5L(Y^n) + 27L(Y^{(1)}) - 24L(Y^{(2)}) + 6L(Y^{(3)}) \right), \\ Y^{(5)} &= Y^n + \frac{\Delta t}{9} \left(221L(Y^n) - 981L(Y^{(1)}) + 867L(Y^{(2)}) - 102L(Y^{(3)}) + L(Y^{(4)}) \right), \\ Y^{(6)} &= Y^n + \frac{\Delta t}{48} \left(-183L(Y^n) + 678L(Y^{(1)}) - 472L(Y^{(2)}) - 66L(Y^{(3)}) + 80L(Y^{(4)}) + 3L(Y^{(5)}) \right), \\ Y^{(7)} &= Y^n + \frac{\Delta t}{82} \left(716L(Y^n) - 2079L(Y^{(1)}) + 1002L(Y^{(2)}) + 834L(Y^{(3)}) - 454L(Y^{(4)}) - 9L(Y^{(5)}) + 72L(Y^{(6)}) \right). \\ (3.10) \\ Y^{n+1} &= Y^n + \frac{\Delta t}{840} \left[41 \left(L(Y^n) + L(Y^{(7)}) \right) + 216 \left(L(Y^{(2)}) + L(Y^{(6)}) \right) + 27 \left(L(Y^{(3)}) + L(Y^{(5)}) \right) + 272L(Y^{(4)}) \right]. \end{split}$$

3.3. Predictor-corrector method for Burgers' equation. Consider the Burgers' equation

(3.11)
$$\frac{\partial y}{\partial t} + y \frac{\partial y}{\partial x} = \nu \frac{\partial^2 y}{\partial x^2}, \ c < x < d, \ t > 0,$$

with respect to initial and boundary conditions. Here $\nu > 0$ is a small parameter known as the kinematics viscosity. We rewrite (3.11) as follows

(3.12)
$$\frac{\partial y}{\partial t} = -\frac{\partial f(y)}{\partial x} + \nu \frac{\partial^2 y}{\partial x^2},$$

where $f(y) = \frac{y^2}{2}$. The MacCormack method for solving equation (3.12) is given by

(3.13)
$$\bar{y}_{j}^{n+1} = y_{j}^{n} - \Delta t(f_{j}^{n})' + \nu \Delta t(y_{j}^{n})'',$$

(3.14)
$$y_j^{n+1} = \frac{1}{2} (y_j^n + \bar{y}_j^{n+1} - \Delta t(\bar{f}_j^n)' + \nu \Delta t(\bar{y}_j^n)'')$$

The derivatives in the MacCormack method are replaced by compact approximations (3.7) and (3.8).

3.4. Numerical observations.

3.4.1. *Problem 4.* Consider the equation (3.11) with the initial condition $y(x, 0) = \sin(\pi x)$,

0 < x < 1, and the boundary conditions y(0,t) = y(1,t) = 0. The exact solution is $y(x,t) = 2\pi \nu \frac{\sum_{n=1}^{\infty} a_n e^{-n^2 \pi^2 \nu t} n \sin(n\pi x)}{a_0 + \sum_{n=1}^{\infty} a_n e^{-n^2 \pi^2 \nu t} \cos(n\pi x)}$ with the Fourier coefficients

 $a_0 = \int_0^1 e^{\frac{\cos(\pi x) - 1}{2\pi\nu}} dx$ and $a_n = 2 \int_0^1 e^{\frac{\cos(\pi x) - 1}{2\pi\nu}} \cos(n\pi x) dx$, n = 1, 2, 3, ...

In Tables (3.1) and (3.2), we show the l_2 errors and average errors obtained for Problem 4 with various values of h at final time T = 0.2. Fig. (4)(a) shows the numerical solution with several values of T with $h = \frac{1}{30}$, $\Delta t = 0.00001$ and $\nu = 0.1$. In Fig. (4)(b) we plot the numerical solution with several values of T with $h = \frac{1}{30}$, $\Delta t = 0.00001$ and $\nu = 1$.

h	CD4 Predictor-Corrector		CD6 Predictor-Corrector		CD6-RK6 Huta	
	l_2 error	Average error	$l_2 \text{error}$ Average error		l_2 error	Average error
$\frac{1}{15}$	5.1211×10^{-04}	4.4152×10^{-05}	1.4546×10^{-04}	2.0211×10^{-05}	1.4518×10^{-04}	2.0181×10^{-05}
$\frac{1}{30}$	1.9812×10^{-05}	1.1010×10^{-06}	3.9653×10^{-06}	2.6521×10^{-07}	3.9437×10^{-06}	2.6381×10^{-07}
$\frac{1}{60}$	6.3522×10^{-07}	4.0822×10^{-08}	2.2119×10^{-08}	1.5450×10^{-09}	2.1321×10^{-08}	1.5108×10^{-09}
$\frac{1}{120}$	7.0524×10^{-08}	3.1637×10^{-09}	6.2751×10^{-10}	4.7686×10^{-11}	2.1016×10^{-10}	1.1783×10^{-11}

Table 3.1: l_2 -error and average error for Problem 4 with $\nu = 0.1, \Delta t = 0.00001$ and T = 0.2.

h	CD4 Predictor-Corrector		CD6 Predictor-Corrector		CD6-RK6 Huta	
	l_2 error	Average error	<i>l</i> ₂ error Average error		l_2 error	Average error
$\frac{1}{15}$	1.7374×10^{-06}	3.7098×10^{-07}	5.8862×10^{-07}	1.3084×10^{-07}	5.7635×10^{-07}	1.2810×10^{-07}
$\frac{1}{30}$	4.9613×10^{-07}	7.7575×10^{-08}	1.4039×10^{-09}	2.1757×10^{-10}	1.8894×10^{-09}	2.7520×10^{-10}
$\frac{1}{60}$	5.1135×10^{-08}	5.7826×10^{-09}	2.4253×10^{-09}	2.7664×10^{-10}	2.4495×10^{-11}	2.7740×10^{-12}
$\frac{1}{120}$	7.8064×10^{-09}	6.3341×10^{-10}	3.4598×10^{-09}	2.8184×10^{-10}	2.7290×10^{-13}	2.1513×10^{-14}

Table 3.2: l_2 -error and average error for Problem 4 with $\nu = 1, \Delta t = 0.00001$ and T = 0.2.



Figure 4: Numerical solution of Problem 4 at different times for (a) $h = \frac{1}{30}$, $\Delta t = 0.00001$ and $\nu = 0.1$ (left). (b) $h = \frac{1}{30}$, $\Delta t = 0.00001$ and $\nu = 1$ (right).

3.4.2. Problem 5. Consider the equation (3.11) in 0.5 < x < 1.5 with boundary conditions

$$y(0.5,t) = \frac{\nu}{1+\nu t} \left(0.5 + \tan\left(\frac{1}{4(1+\nu t)}\right) \right), \ y(1.5,t) = \frac{\nu}{1+\nu t} \left(1.5 + \tan\left(\frac{3}{4(1+\nu t)}\right) \right),$$

0 < t < T. The exact solution is given by $y(x,t) = \frac{\nu}{1+\nu t} \left(x + \tan\left(\frac{x}{2+2\nu t}\right) \right).$

The initial condition is obtained from the exact solution when t = 0. The problem is solved numerically at time T = 0.1 by predictor-corrector fourth order compact finite difference scheme, predictor-corrector sixth order compact finite difference scheme and Huta's improved Runge-Kutta sixth order compact finite difference scheme for $\nu = .001$ and $\nu = .00001$. The solution is obtained for different values of h, the l_2 errors and average errors of the solution by the three schemes are compared in Tables (3.3) and (3.4). Fig. (5)(a) and Fig. (5)(b) shows the numerical solution for $\nu = .0001$, $\nu = .00001$ at times T = 0.1 and T = 100 respectively.

h	CD4 Predictor-Corrector		CD6 Predictor-Corrector		CD6-RK6 Huta	
	l_2 error	Average error	<i>l</i> ₂ error Average error		l_2 error	Average error
$\frac{1}{15}$	4.6732×10^{-05}	3.9835×10^{-06}	3.9655×10^{-09}	3.0836×10^{-10}	3.9693×10^{-09}	3.0834×10^{-10}
$\frac{1}{30}$	1.7905×10^{-04}	7.5210×10^{-06}	3.9724×10^{-09}	1.6654×10^{-10}	3.9850×10^{-09}	1.6652×10^{-10}
$\frac{1}{60}$	6.1265×10^{-04}	1.3878×10^{-05}	4.0646×10^{-09}	9.9487×10^{-11}	4.0821×10^{-09}	9.9486×10^{-11}
$\frac{1}{120}$	1.5336×10^{-03}	2.3242×10^{-05}	4.6275×10^{-09}	7.5342×10^{-11}	4.6199×10^{-09}	7.5358×10^{-11}

Table 3.3: l_2 *-error and average error for Problem 5 with* $\nu = 0.001$, $\Delta t = 0.001$ and T = 0.1.

h	CD4 Predictor-Corrector		CD6 Predictor-Corrector		CD6-RK6 Huta	
	l_2 error	Average error	$l_2 \text{ error}$ Average error		l_2 error	Average error
$\frac{1}{15}$	4.7477×10^{-09}	4.1096×10^{-10}	3.9663×10^{-13}	3.0346×10^{-14}	3.9663×10^{-13}	3.0346×10^{-14}
$\frac{1}{30}$	1.8988×10^{-08}	8.4786×10^{-10}	3.9663×10^{-13}	1.5669×10^{-14}	3.9665×10^{-13}	1.5669×10^{-14}
$\frac{1}{60}$	7.5821×10^{-08}	1.7172×10^{-09}	3.9663×10^{-13}	7.9796×10^{-15}	3.9670×10^{-13}	7.9795×10^{-15}
$\frac{1}{120}$	3.0118×10^{-07}	3.4114×10^{-09}	3.9665×10^{-13}	4.0558×10^{-15}	3.9692×10^{-13}	4.0556×10^{-15}

Table 3.4: l_2 *-error and average error for Problem 5 with* $\nu = 0.00001$, $\Delta t = 0.001$ and T = 0.1.



Figure 5: Numerical solution of Problem 5 for (a) $h = \frac{1}{30}$, $\Delta t = 0.001$ and T = 0.1 (*left*). (*b*) $h = \frac{1}{30}$, $\Delta t = 0.001$ and T = 100 (*right*).

3.4.3. Problem 6. Consider the equation (3.11) in 0 < x < 1 with the boundary conditions y(0,t) = y(1,t) = 0, 0 < t < T, and with the initial condition $y(x,0) = \frac{2\nu\pi\sin(\pi x)}{a + \cos(\pi x)}$, where a > 1 is a parameter. The exact solution is given by $y(x,t) = \frac{2\nu\pi e^{-\pi^2\nu t}\sin(\pi x)}{a + e^{-\pi^2\nu t}\cos(\pi x)}$.

We take a = 2. In Table (3.5), we summarized the numerical results at T = 1 when $\nu = 10^{-4}$. The l_2 errors and average errors of the solution obtained by the three schemes with different space steps are presented in the Table (3.5). In Table (3.6), the numerical results obtained at T = 0.1 when $\nu = 0.01$ with different values of h are presented. Fig. (6)(a) shows the numerical solution with several values of ν with h = 0.05, $\Delta t = 0.0001$ and T = 0.1. In Fig. (6)(b) we plot the numerical solution with several values of ν with h = 0.05, $\Delta t = 0.001$ and T = 1.

h	CD4 Predictor-Corrector		CD6 Predictor-Corrector		CD6-RK6 Huta	
	l_2 error	Average error	$l_2 \text{ error}$ Average error		l_2 error	Average error
$\frac{1}{15}$	8.3553×10^{-09}	6.3854×10^{-10}	3.4878×10^{-09}	3.0920×10^{-10}	3.4874×10^{-09}	3.0917×10^{-10}
$\frac{1}{30}$	7.3481×10^{-10}	3.1517×10^{-11}	6.2117×10^{-11}	2.8977×10^{-12}	6.2094×10^{-11}	2.8969×10^{-12}
$\frac{1}{60}$	2.6786×10^{-11}	9.1923×10^{-13}	4.0143×10^{-12}	9.7291×10^{-14}	4.0043×10^{-12}	9.7108×10^{-14}
$\frac{1}{120}$	8.7270×10^{-13}	3.6763×10^{-14}	4.8640×10^{-14}	8.8030×10^{-16}	4.7893×10^{-14}	8.7054×10^{-16}

Table 3.5: l_2 *-error and average error for Problem 6 with* $\nu = 0.0001$, $\Delta t = 0.001$ and T = 1.

h	CD4 Predictor-Corrector		CD6 Predictor-Corrector		CD6-RK6 Huta	
	Average error	C-order	Average error	C-order	Average error	C-order
$\frac{1}{15}$	5.0592×10^{-07}		2.5452×10^{-07}		2.5427×10^{-07}	
$\frac{1}{30}$	2.1670×10^{-08}	4.5451	2.6227×10^{-09}	6.6006	2.6097×10^{-09}	6.6063
$\frac{1}{60}$	5.3203×10^{-10}	5.3480	2.8101×10^{-11}	6.5443	2.7273×10^{-11}	6.5803
$\frac{1}{120}$	2.8098×10^{-11}	4.2430	1.7235×10^{-13}	7.3491	1.7193×10^{-13}	7.3095

Table 3.6: Average error and convergence rate for Problem 6 with $\nu = 0.01, \Delta t = 0.0001$ and T = 0.1.

All the computations are performed in MATLAB version 9.9.0.1570001 (R2020b) update 4 on an AMD Ryzen 7 3700U 2.30 GHz CPU machine with 8 GB of memory. The results illustrated in the tables ensure that the computed solution is in good agreement with the exact



Figure 6: Numerical solution of Problem 6 for several values of ν with (a) h = 0.05, $\Delta t = 0.0001$ and T = 0.1 (left). (b) h = 0.05, $\Delta t = 0.001$ and T = 1 (right).

solution. Both the newly proposed schemes are better than the existing CD4 predictor-corrector scheme [28]. The proposed scheme CD6 predictor-corrector is only designed for Burgers' type of equations whereas CD6-RK6 Huta can be applied for nonlinear unsteady 1D convection diffusion equations. However, CD6 predictor-corrector needs less functional evaluations than the CD6-RK6 Huta. From the tables, it is clear that in most of the cases CD6-RK6 Huta gives better accuracy than the other two schemes. The newly proposed schemes achieved good computational order of accuracy which is compatible with the theoretical order.

4. CONCLUSIONS

We proposed new higher order accurate compact difference numerical schemes for solving unsteady linear and nonlinear 1D convection-diffusion equations. The work is divided into two parts. In the first part, a combined exponential fourth order compact finite difference scheme in space and fourth order C^1 -spline collocation method in time is introduced to solve the linear unsteady 1D convection-diffusion equations. This scheme is proved to be unconditionally stable and the numerical results obtained are in good agreement with the exact solution. In the second part, we introduced two numerical schemes for solving unsteady nonlinear 1D convection-diffusion equations. First scheme is a combined sixth order compact finite difference scheme for space and sixth order Huta's improved RK6 method for time and the second one is combined sixth order compact finite difference scheme in space and MacCormack predictorcorrector method for time. Numerical experiments are conducted on Burgers' equation. Both the proposed schemes achieved better accuracy than the existing CD4 predictor-corrector. The CD6 predictor-corrector scheme needs less evaluations than CD6-RK6 Huta, but it is restricted to Burgers' type equations. In most of the cases, the scheme CD6-RK6 Huta has better accuracy than CD6 predictor-corrector and is applicable to a large class of nonlinear unsteady 1D convection-diffusion problems. The computational order of accuracy agrees with the theoretical order.

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