A stability preserved time-integration method for nonlinear advection–diffusion-reaction processes

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Abstract
A new implicit-explicit local differential transform method (IELDTM) is derived here for time integration of the nonlinear (2 + 1)-dimensional advection–diffusion-reaction (ADR) equations. The IELDTM is adaptively constructed as a stability preserved and high order time integrator for spatially discretized ADR equations. For spatial discretization of the model equation, the Chebyshev spectral collocation method (ChCM) is utilized. A robust stability analysis and global error analysis of the IELDTM are presented with respect to the direction parameter $\theta$. With the help of the global error analysis, adaptivity equations are derived to minimize the computational costs of the algorithms. The produced method is shown to eliminate the accuracy disadvantage of the classical $\theta$-method and the stability disadvantages of the existing differential transform-based methods. Two examples of the Burgers equation in one and two space dimensions and the Chapman oxygen-ozone ADR model are solved via the ChCM-IELDTM hybridization. The present time integrator is proven to provide more efficient numerical characteristics than the various multi-step and multi-stage time integration methods. The IELDTM is extensively compared with the widely used MATLAB solvers, ode45 and ode15s. The adaptive IELDTM has been proven to integrate the stiff Chapman ADR equations with optimum costs over relatively long-time intervals.

Keywords Chapman model · Advection–diffusion-reaction processes · Stability analysis · Taylor series · Time-integration

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1 Introduction

Time integrations of the reduced space–time partial differential equations are of great importance. Various versions of both explicit and implicit time integrators are always under development to create both accurate and stable numerical solvers. For higher dimensional parabolic PDEs, the computational efficiency of the time integrator becomes more critical due to the large ODE systems obtained after spatial discretization. In such cases, performance of the effective explicit ODE solvers such as Taylor series methods or explicit Runge–Kutta methods is weakened due to instability [1–3]. Implicit time integration schemes are the best options in such situations, but require more computational effort, especially for nonlinear problems [1–3].

Time integration methods are mainly divided into two subgroups, such as multi-point [4–9] and multi-derivative methods [10–18]. The multi-point methods are based on interpolation, such as finite element and spectral methods. Even if this group of methods is widely used for the spatial parts of PDEs, it is possible to solve also IVPs effectively with these methods. The multipoint methods are stability preserved and even capable of solving stiff IVPs. Despite all these flexibilities, this group of methods leads to a large degrees of freedom and a large system of linear/nonlinear algebraic equations for solving ODEs due to their non-iterative nature. This is an essential drawback due to both computational cost and loss of accuracy over large time scales. The multi-derivative methods such as Runge–Kutta methods [10–12], Rosenbrock methods [13–15], Taylor series methods [16–18] have been used extensively to observe the behavior of stiff IVPs. As for this group of methods, they are iterative in nature and have both explicit and implicit forms of their own. The Runge–Kutta and Rosenbrock methods are derived from the Taylor series expansions by introducing interior ghost nodes to get higher-order approximations. The Taylor series methods directly use the higher-order derivatives of given implicit/explicit functions by the procedure known as automatic differentiation or differential transformation [16–23]. The idea of differential transformation leads us to a useful procedure for recursively evaluating higher-order Taylor coefficients [19–23]. With the work of Tunc and Sari [24], a significant progress was made to solve stiff IVPs with the idea of differential transformation. The derived method is called the implicit/explicit local differential transformation method (IELDTM).

Numerous numerical methods have been proposed in the literature when dealing with the time integration of advection–diffusion-reaction processes [25–36]. Explicit Runge–Kutta schemes are more common in applications [25–29] due to their efficient computational structures. It is well known that this group of time-integrators has a lack of stability preserving properties. The second-order and unconditionally stable Crank-Nicolson method (CNM) is another widely used time integrator in advection–diffusion processes, and the CNM is a special case of the well-known θ-method [30–34]. Even if the stability properties of the CNM was found to be excellent, the method is second order and needs small time increments to get higher accuracy. Here the CNM has proven to be a special case of the
current IELDTM and therefore, the restriction of the Crank-Nicolson approach has been overcome by the IELDTM by increasing its order. Another time-integration technique for solving reduced ODEs is the backward differentiation method (BDM), in which stability is preserved and has higher-order formulae [35, 36]. The BDM has \( A^- \) stable formulae up to the second-order accuracy, while the present IELDTM has \( A^- \) stable formulae up to the fourth-order accuracy [24].

Here we have derived an implicit-explicit local differential transform method for time integration of the (2+1)-dimensional ADR equations. The Chebyshev spectral collocation method (ChCM) has been used for the spatial discretization of considered PDEs, due to the important interpolation characteristics of the method [27]. The flexibility, stability characteristics, adaptivity and computational efficiency of the IELDTM [24] led us to improve our work in solving nonlinear advection–diffusion–reaction equations with the ChCM-IELDTM hybridization. It has been shown that the current hybrid approach destroys the disadvantages of the existing numerical methods such as \( \theta^- \) methods and DTM-based methods. A priori error analysis has been done, and convergence rates are determined according to the direction parameter \( \theta \). Numerical properties of the current hybrid approach have been compared with the literature and MATLAB solvers, \textit{ode15s} and \textit{ode45}. It has been shown that the present approach offers numerically better performance than the previously produced methods, and the IELDTM is found to be a great option for time integrations of the PDEs. In order to fully demonstrate the capabilities of the proposed method, a Chapman oxygen-ozone-linked coupled ADR system, which emerged as an important application of chemistry, has been solved with the time-adaptive ChCM-IELDTM, and numerical observations have been discussed in detail.

2 ChCM-IELDTM hybridization

In this section, we introduce the implementation procedure of the IELDTM-ChCM hybridization to the following 2D advection–diffusion–reaction equation

\[
 u_t + u(u_x + u_y) = \varepsilon (u_{xx} + u_{yy}) + w(u), (x, y) \in D, t > 0
\]  

(2.1)

with the boundary conditions

\[
 u(a, y, t) = f_1(y, t), u(b, y, t) = f_2(y, t)
\]  

(2.2)

\[
 u(x, c, t) = h_1(x, t), u(x, d, t) = h_2(x, t)
\]  

(2.3)

and initial condition

\[
 u(x, y, 0) = g(x, y)
\]  

(2.4)

where \( D = \{(x, y)|a \leq x \leq b, c \leq y \leq d\} \), \( \varepsilon \) is the kinematic viscosity constant for \( \varepsilon > 0 \), \( w(u) \) represents the nonlinear reaction term and \( f_1, f_2, h_1, h_2, \) and \( g \) are known as smooth functions. The subscripts \( x, y \) and \( t \) represent differentiations with respect to spaces \( x, y \) and time \( t \), respectively. Note that taking \( w(u) = 0 \) in Eq. (2.1) yields
the well-known Burgers equation, which has two space dimensions and represents only the advection–diffusion mechanism.

Let us approximate the solution \( u(x, y, t) \) with \((N, M)\) order Chebyshev polynomials as follows [27]

\[
u(x, y, t) = \sum_{n=0}^{N} \sum_{m=0}^{M} \alpha_{nm} \beta_{nm}(t) \overline{T}_n(x) \overline{T}_m(y) \tag{2.5}
\]

where \( \beta_{nm}(t) \) are time dependent parts of the representation, \( \alpha_{nn} = 1 \) for interior points and \( \alpha_{nm} = 1/2 \) for any boundary point. In Eq. (2.5), \( \overline{T}_n(x) \) and \( \overline{T}_m(y) \) are defined in terms of the first kind Chebyshev polynomials \( T_n(x) \) and \( T_m(y) \) as

\[
\overline{T}_n(x) = T_n \left( \frac{2x - (a + b)}{b - a} \right) = \cos \left( n \arccos \left( \frac{2x - (a + b)}{b - a} \right) \right) \tag{2.6}
\]

\[
\overline{T}_m(y) = T_m \left( \frac{2y - (c + d)}{d - c} \right) = \cos \left( m \arccos \left( \frac{2y - (c + d)}{d - c} \right) \right) \tag{2.7}
\]

We define the following restricted collocation points on \([-1, 1]\) as

\[
x_n = \frac{1}{2} \left( (a + b) - (b - a) \cos \left( \frac{\pi n}{N} \right) \right), \quad n = 0, 1, 2, \ldots, N, \tag{2.8}
\]

\[
y_m = \frac{1}{2} \left( (c + d) - (d - c) \cos \left( \frac{\pi m}{M} \right) \right), \quad m = 0, 1, 2, \ldots, M. \tag{2.9}
\]

The discrete orthogonality relation is vital for the ChCM defined as

\[
\sum_{n=0}^{N} \alpha_n \overline{T}_i(x_n) \overline{T}_j(x_n) = \gamma_i \delta_{ij} \tag{2.10}
\]

\[
\sum_{m=0}^{M} \alpha_m \overline{T}_i(y_m) \overline{T}_j(y_m) = \omega_i \delta_{ij} \tag{2.11}
\]

with

\[
\gamma_i = \begin{cases} 
\frac{N}{2}, & i \neq 0, N \\
N, & i = 0, N,
\end{cases} \tag{2.12}
\]

\[
\omega_i = \begin{cases} 
\frac{M}{2}, & i \neq 0, M \\
M, & i = 0, M.
\end{cases} \tag{2.13}
\]

Thus, we reach the required derivatives at predetermined collocation points in Eq. (2.1) as follows:
\[ u_x(x_i, y_j, t) = \sum_{n=0}^{N} [A_x]_{in} u_{nj}(t), \quad (2.14) \]

\[ u_{xx}(x_i, y_j, t) = \sum_{n=0}^{N} [B_x]_{in} u_{nj}(t), \quad (2.15) \]

\[ u_y(x_i, y_j, t) = \sum_{m=0}^{M} [A_y]_{jm} u_{im}(t), \quad (2.16) \]

\[ u_{yy}(x_i, y_j, t) = \sum_{m=0}^{M} [B_y]_{jm} u_{im}(t), \quad (2.17) \]

where \( i = 0, 1, 2, \ldots, N, \ j = 0, 1, 2, \ldots, M, u_{nm}(t) = u(x_i, y_j, t), B_x = A^2_x, B_y = A^2_y, A_x \)
and \( A_y \) are \((N \times N)\) and \((M \times M)\) matrices are defined by

\[
[A_x]_{in} = \begin{cases} 
\mu_1 \sum_{j=0}^{N} (-1)^j j^2 \cos \left( j \left( \pi - \frac{(N+1-1)n}{N} \right) \right), & i = 0 \\
\mu_1 \sum_{j=0}^{N} \frac{j \sin \left( j \left( \pi - \frac{(N+1-1)n}{N} \right) \right) \left( \cos j \left( \pi - \frac{(N+1-1)n}{N} \right) \right)}{\sqrt{1 - \cos^2 \left( \pi - \frac{(N+1-1)n}{N} \right)}}, & i = 1, 2, \ldots, N - 1 \\
\mu_1 \sum_{j=0}^{N} (-1)^j j^2 \cos \left( j \left( \pi - \frac{(1-1)n}{N} \right) \right), & i = N, 
\end{cases}
\]

\[
[A_y]_{im} = \begin{cases} 
\mu_2 \sum_{j=0}^{M} (-1)^j j^2 \cos \left( j \left( \pi - \frac{(M+1-1)n}{M} \right) \right), & i = 0 \\
\mu_2 \sum_{j=0}^{M} \frac{j \sin \left( j \left( \pi - \frac{(M+1-1)n}{M} \right) \right) \left( \cos j \left( \pi - \frac{(M+1-1)n}{M} \right) \right)}{\sqrt{1 - \cos^2 \left( \pi - \frac{(M+1-1)n}{M} \right)}}, & i = 1, 2, \ldots, M - 1 \\
\mu_2 \sum_{j=0}^{M} (-1)^j j^2 \cos \left( j \left( \pi - \frac{(1-1)n}{M} \right) \right), & i = M
\end{cases}
\]

where \( \mu_1 = \frac{2}{b-a}, \mu_2 = \frac{2}{d-c}, [A_x]_{in} \) and \([A_y]_{jm}\) are called the Chebyshev differentiation matrices. Writing Eqs. (2.14)–(2.17) into Eq. (2.1) and imposing the boundary conditions leads to the following nonlinear ODE system,

\[
\frac{d\beta}{dt} = \varepsilon \left( \vec{B}_y \beta + \beta \vec{B}_y^T \right) - \langle \beta, \left( \vec{A}_y \beta + \beta \vec{A}_y^T \right) \rangle + W(\beta) + F(t) \quad (2.20)
\]

where \( \langle ., . \rangle \) is the standard elementwise product, \( \beta(t) = [\beta(t)]_{nm} \) is \((N - 1) \times (M - 1)\) is matrix of time variable, \((W(\beta))_{ij} = w(\beta_{ij}) \) and \( F(t) = [F(t)]_{nm} \) is \((N - 1) \times (M - 1)\) matrix of time variable related to boundary conditions (2.2)-(2.3). After applying the boundary conditions to the matrices \( A_x, A_y, B_x \) and \( B_y \),
respectively, \( \overline{A}_x, \overline{A}_y, \overline{B}_x, \) and \( \overline{B}_y \) are obtained. Note that the initial condition of the nonlinear ODE system is defined by

\[
\beta(0) = [\beta(0)]_{nm} = g(x_n, y_m). \tag{2.21}
\]

Now, we construct the IELDTM to solve IVP stated in (2.20)-(2.21). Detailed description of the IELDTM for the solution of IVPs for ODEs can be found in the literature [24]. For simplicity, we omit the differential transform properties here. Let us divide the time interval \([0,t_f]\) into at most \(P\) time elements with \(\Delta t_i = t_{i+1} - t_i\) and the partition of the interval as \(\omega = \{0 = t_0 < t_1 < \cdots < t_{P^*} = t_f\}\). Let us then consider the convergent Taylor series representation of the function \(\beta(t)\) of order \(K\) about \(t = t_i\) as

\[
\beta_i(t) = \sum_{k=0}^{K} \overline{\beta}_i(k)(t - t_i)^k + O((t - t_i)^{K+1}), \quad t_i - \rho^i \leq t \leq t_i + \rho^i \tag{2.22}
\]

where \(i = 0,1,\ldots,P^*\), \(\overline{\beta}_i(k)\) is the local differential transformation of \(\beta_i(t)\) and \(\rho^i\) is the radius of convergence of the representation. Taking differential transform of Eq. (2.20) leads to,

\[
\overline{\beta}_{i+1}(k) + 1 = \frac{1}{k + 1} \left[ \epsilon \left( \overline{B}_x \overline{\beta}_i(k) + \overline{B}_y \overline{\beta}_i(k) \right) - \sum_{s=0}^{k} \overline{\beta}_i(s) \left( \overline{A}_x \overline{\beta}_i(k - s) + \overline{\beta}_i(k - s) \overline{A}_y \right) \right] + \overline{W}(\overline{\beta}_i(k)) + \overline{F}_i(k) \tag{2.23}
\]

where \(\overline{W}\) is the local transformation operator related to the function \(w\) and \(\overline{F}_i(k)\) is the local differential transformation of \(F(t)\). By defining the parameter \(\theta \in [0,1]\) as a direction parameter, the continuity requirement of the two consecutive solutions yields the following equation system,

\[
\sum_{k=0}^{K} \overline{\beta}_{i+1}(k) (-\theta \Delta t_i)^k = \sum_{k=0}^{K} \overline{\beta}_i(k) \left( (1 - \theta) \Delta t_i \right)^k + O( (\Delta t_i)^{K+1}, \theta) \tag{2.24}
\]

where \(O((\Delta t_i)^{K+1}, \theta)\) represents the dependency of the local truncation error to time increment, transformation order and direction parameter. By defining \(\overline{\beta}_i(0) = \beta(0)\), the rest of \(\overline{\beta}_i(k)\) can be calculated from the recursive relation (2.23). Since \(\overline{\beta}_i(0)\) is known from the previous step, Eq. (2.24) is an implicit/explicit algebraic equation system of \(\overline{\beta}_{i+1}(0)\). This numerical algorithm finds all local solutions \(\beta_i(t)\) by solving Eq. (2.24) at each time step. Finally, by obtaining all local solutions \(\beta_i(t)\), we reach

\[
u^i(x,y,t) = \sum_{n=0}^{N} \sum_{m=0}^{M} \alpha_{nm} (\beta_{nm})_i(t) \overline{T}_n(x) \overline{T}_m(y) \tag{2.25}
\]

where \(i = 0,1,\ldots,P^*\).
3 Error analysis

In this section, priori error estimation of the IELDTM for solving the nonlinear ODE system (2.20) will be presented. Let us first define the map \( \phi: \mathbb{R}^{(N-1)\times(M-1)} \to \mathbb{R}^{(N-1)(M-1)\times1} \) as

\[
\phi(\vec{p}_j(k)) = \begin{bmatrix}
(\vec{p}_j(k))_{11}, (\vec{p}_j(k))_{12}, \ldots, (\vec{p}_j(k))_{21}, \ldots, (\vec{p}_j(k))_{(N-1)(M-1)}
\end{bmatrix}^T = \vec{q}_j(k)
\]

(3.1)

The map \( \phi \) reshapes the matrix \( \vec{p}_j(k) \) as a related vector \( \vec{q}_j(k) \) for further analysis. The exact form of the continuity Eq. (2.24) can be written as

\[
\vec{q}_{i+1}(0) = \vec{q}_i(0) + \sum_{k=1}^{K} \vec{q}_i(k)((1 - \theta)\Delta t)^k - \sum_{k=1}^{K} \vec{q}_{i+1}(k)(-\theta \Delta t)^k + \Delta t \rho_i
\]

(3.2)

where \( \vec{q} \) is the exact form of \( \vec{p} \) and then the local truncation error \( \rho_i \) takes the following form

\[
\rho_i = \left[ \vec{q}_{i+1}(K + 1)(1 - \theta)^{K+1} - \vec{q}_i(K + 1)(-\theta)^{K+1} \right] \Delta t^K.
\]

(3.3)

Here \( \vec{q}_{i+1} \) defines the local transform at the local point \( t_i \in [t_{i-1}, t_{i+1}] \) for all \( i = 0, 1, 2, \ldots, P - 1 \). With the use of recursive relation (2.23), Eq. (3.2) can be rewritten as

\[
\vec{q}_{i+1}(0) = \vec{q}_i(0) + (1 - \theta)\Delta t H_1(\vec{q}_i(0), \theta, \Delta t) + \theta \Delta t H_2(\vec{q}_{i+1}(0), \theta, \Delta t) + \Delta t \rho_i
\]

(3.4)

where \( H_1: \mathbb{R}^{(N-1)(M-1)\times1} \times [0,1] \times \mathbb{R}^+ \to \mathbb{R}^{(N-1)(M-1)\times1} \) and \( H_2: \mathbb{R}^{(N-1)(M-1)\times1} \times [0,1] \times \mathbb{R}^+ \to \mathbb{R}^{(N-1)(M-1)\times1} \) are defined by

\[
H_1(\vec{q}_i(0), \theta, \Delta t) = \sum_{k=1}^{K} \vec{q}_i(k)((1 - \theta)\Delta t)^{k-1},
\]

(3.5)

\[
H_2(\vec{q}_{i+1}(0), \theta, \Delta t) = \sum_{k=1}^{K} \vec{q}_{i+1}(k)(-\theta \Delta t)^{k-1}.
\]

(3.6)

The IELDTM form of the continuity Eq. (2.24) takes the form

\[
\vec{q}_{i+1}(0) = \vec{q}_i(0) + (1 - \theta)\Delta t H_1(\vec{q}_i(0), \theta, \Delta t) + \theta \Delta t H_2(\vec{q}_{i+1}(0), \theta, \Delta t).
\]

(3.7)

Let us define the following Jacobian matrices

\[
J_1(\vec{q}, \theta, \Delta t) = \frac{\partial(H_1)}{\partial \vec{q}}.
\]

(3.8)
\[
J_2(\varphi, \theta, \Delta t) = \frac{\partial (H_2)}{\partial \varphi_j}.
\]

(3.9)

Assume that the conditions

\[
\mu(J_1(\varphi, \theta, \Delta t)) \leq 0 \text{ and } \mu(J_2(\varphi, \theta, \Delta t)) \leq 0
\]

(3.10)

hold for all \((\varphi, \theta, \Delta t) \in \mathbb{R}^{(N-1)(M-1) \times 1} \times [0,1] \times \mathbb{R}^+\) and \(\mu(A) = \lim_{\tau \to 0} \frac{|I+\tau A|^{-1}}{\tau}\) is the logarithmic norm \cite{[39]}. Let \(Z^1_i \in \mathbb{R}^{(N-1)(M-1) \times (N-1)(M-1)}\) and \(Z^2_i \in \mathbb{R}^{(N-1)(M-1) \times (N-1)(M-1)}\) be defined for \(i \geq 0\) with

\[
Z^1_i = \int_0^1 \Delta t J_1(\varphi(\varphi_i(0), (1 - \sigma)\varphi_i(0), \theta, \Delta t) d\sigma,
\]

(3.11)

\[
Z^2_{i+1} = \int_0^1 \Delta t J_2(\varphi(\varphi_{i+1}(0), (1 - \sigma)\varphi_{i+1}(0), \theta, \Delta t) d\sigma.
\]

(3.12)

Applying the mean value theorem to vector-valued functions \(H_1\) and \(H_2\) yields

\[
\Delta t H_1(\bar{\varphi}_i(0), \theta, \Delta t) - \Delta t H_1(\bar{\varphi}_i(0), \theta, \Delta t) = Z^1_i(\bar{\varphi}_i(0) - \bar{\varphi}_i(0)),
\]

(3.13)

\[
\Delta t H_2(\bar{\varphi}_{i+1}(0), \theta, \Delta t) - \Delta t H_2(\bar{\varphi}_{i+1}(0), \theta, \Delta t) = Z^2_{i+1}(\bar{\varphi}_{i+1}(0) - \bar{\varphi}_{i+1}(0)).
\]

(3.14)

Defining global discretization error \(\varepsilon_i = \varphi(t_i) - \bar{\varphi}_i(0) = \bar{\varphi}_i(0) - \bar{\varphi}_i(0)\) and subtracting Eq. (3.7) from Eq. (3.4) give rise to

\[
\varepsilon_{i+1} = \varepsilon_i + (1 - \theta)Z^1_i\varepsilon_i + \theta Z^2_{i+1}\varepsilon_{i+1} + \Delta t \rho_i.
\]

(3.15)

From (3.11), (3.12) and Lemma 2.6 in literature \cite{[39]}, the following inequalities hold

\[
\mu(Z^1_i) \leq 0 \text{ and } \mu(Z^2_i) \leq 0.
\]

(3.16)

The analysis is considered in two main cases as follows:

**Case 1** Assume that \(\theta = 1\), i.e. a backward local differential transform method is obtained. Equation (3.15) gives

\[
\varepsilon_{i+1} = (I - Z^2_{i+1})^{-1}(\varepsilon_i + \Delta t \rho_i).
\]

(3.17)

Since \(\|I - Z^2_{i+1}\|^{-1} \leq 1\) according to Eq. (3.16) and the Theorem 2.13 of literature \cite{[39]}, we find
\[ \| \varepsilon_i \| \leq \| \varepsilon_0 \| + \sum_{j=0}^{i-1} \Delta t \| \rho_j \| \leq \| \varepsilon_0 \| + t_i \max_{0 \leq j \leq i-1} \| \rho_j \|. \tag{3.18} \]

Assumption of \( \varepsilon_0 \to 0 \) leads to the following global error estimate
\[ \| \Phi(t_i) - \bar{\Phi}_i(0) \|_\infty = \| \beta(t_i) - \bar{\beta}_i(0) \|_\infty \leq t_i \omega \Delta t^K. \tag{3.19} \]

where
\[
\omega = \left| \frac{1}{(K+1)!} \max_{t \in [0,T]} \left( \frac{d \Phi^{K+1}}{dt^{K+1}} \right) \right|.
\]

Case 2 Let us now consider the rest of the implicit cases for \( \theta \geq 1/2 \). The transformed errors are defined as
\[ \bar{\varepsilon}_i = (I - \theta Z_i^2) \varepsilon_i \tag{3.20} \]

where \( i = 0, 1, \ldots, P \). Then the following recursive relation can be obtained from Eq. (3.15)
\[ \bar{\varepsilon}_{i+1} = (I + (1 - \theta) Z_i^1) (I - \theta Z_i^2)^{-1} \bar{\varepsilon}_i + \Delta t \rho_i = R(Z_i^1, Z_i^2) \bar{\varepsilon}_i + \Delta t \rho_i. \tag{3.21} \]

Assume also that the following stability condition holds
\[ \| R(Z_i^1, Z_i^2) \| = \| (I + (1 - \theta) Z_i^1) (I - \theta Z_i^2)^{-1} \| \leq 1. \tag{3.22} \]

Thus, Eq. (3.21) becomes
\[ \| \bar{\varepsilon}_i \| \leq \| \bar{\varepsilon}_0 \| + \sum_{j=0}^{i-1} \Delta t \| \rho_j \| \leq \| \bar{\varepsilon}_0 \| + t_i \max_{0 \leq j \leq i-1} \| \rho_j \|. \tag{3.23} \]

Since \( \| (I - \theta Z_{i+1}^2)^{-1} \| \leq 1 \) according to Eq. (3.16) and the Theorem 2.13 of literature [39] for \( \theta \geq 1/2 \), we have \( \| \varepsilon_i \| \leq \| \bar{\varepsilon}_i \| \). Thus, the main global error estimate can be constructed from Eq. (3.23) as
\[ \| \varepsilon_i \| \leq \| \varepsilon_0 \| + t_i \max_{0 \leq j \leq i-1} \| \rho_j \|. \tag{3.24} \]

Assumption of \( \varepsilon_0 \to 0 \) leads to the following global error estimate
\[ \| \Phi(t_i) - \bar{\Phi}_i(0) \|_\infty = \| \beta(t_i) - \bar{\beta}_i(0) \|_\infty \leq \begin{cases} t_i \omega \Delta t^{K+1}, & \text{if } \theta = 1/2 \text{ and } K \text{ is odd} \\ t_i \omega \Delta t^K, & \text{otherwise} \end{cases} \tag{3.25} \]
where

\[
\omega = \begin{cases}
    \frac{1}{(K+2)!} \max_{t \in [0,T]} \left( \frac{d\varphi^{K+2}}{dt^{K+2}} \right) \left( \left( \frac{1}{2} \right)^{K+1} (K+1) \right), & \text{if } \theta = \frac{1}{2} \text{ and } K \text{ is odd} \\
    \frac{1}{(K+1)!} \max_{t \in [0,T]} \left( \frac{d\varphi^{K+1}}{dt^{K+1}} \right) \left[ (1 - \theta)^K - (-\theta)^K \right], & \text{if } \theta \neq \frac{1}{2} \text{ and } K \text{ is arbitrary.}
\end{cases}
\]

(3.26)

Adaptive construction of the step-sizes is important to estimate the accuracy of the solution and to reduce the computational cost. With the help of the local truncation error defined in Eq. (3.25), adaptive step-sizes of the algorithm can be determined with the following inequalities

\[
\Delta t_i < \begin{cases}
    \frac{tol}{\left( \left( \frac{1}{2} \right)^{K+1} (K+1) \right) \| \tilde{p}_i(K+2) \|_{\infty}}, & \text{if } \theta = 0.5 \text{ and } K \text{ is odd} \\
    \frac{tol}{\left[ (1 - \theta)^K - (-\theta)^K \right] \| \tilde{p}_i(K+1) \|_{\infty}}, & \text{otherwise}
\end{cases}
\]

(3.27)

(3.28)

where \( K \) is the order of local polynomial approximation (2.22), \( tol \) is the predetermined tolerance and \( \tilde{p}_i(K+1) \) or \( \tilde{p}_i(K+2) \) can be obtained from the recursive relation (2.23).

4 Numerical experiments

In this section, we have numerically analyzed the present ChCM-IELDTM approach over the 1D-2D Burgers equations. The exponential convergence of the IELDTM has been proven for various values of the direction parameter \( \theta \). The computational efficiency of the adaptive IELDTM has been shown in comparison with the literature and MATLAB solvers, \textit{ode}15\textit{s} and \textit{ode}45. The performance of the currently produced time integration algorithm has also been compared with the widely used multi-step and multi-stage time integration algorithms. To measure the accuracy of the current numerical method, we prefer to use the maximum error norm as follows:

\[
\| E \|_{\infty} = \max_i | u_i^{\text{exact}} - u_i^{\text{numerical}} |.
\]
Problem 1 Sari [31] Consider the one-dimensional form of main Eq. (2.1) with \( w(u) = 0 \), representing the nonlinear advection–diffusion process, and the initial condition.

\[
u(x, 0) = \sin \pi x, 0 < x < \quad (4.1)
\]

and the homogenous Dirichlet boundary conditions

\[
u(0, t) = u(1, t) = 0, t > 0. \quad (4.2)
\]

The exact solution of one-dimensional behaviour of the advection–diffusion equation with conditions (4.1), (4.2) is given by [31]

\[
u(x, t) = 2\pi \frac{\sum_{n=1}^{\infty} a_n \exp(-n^2 \pi^2 \varepsilon t) \sin(n\pi x)}{a_0 + \sum_{n=1}^{\infty} a_n \exp(-n^2 \pi^2 \varepsilon t) \cos(n\pi x)} \quad (4.3)
\]

with the Fourier coefficients

\[
a_0 = \int_0^1 \exp\left\{-(2\pi \varepsilon)^{-1} [1 - \cos(n\pi)]\right\} dx, \quad (4.4)
\]

\[
a_n = 2 \int_0^1 \exp\left\{-(2\pi \varepsilon)^{-1} [1 - \cos(n\pi)]\right\} \cos(n\pi x) dx. \quad (4.5)
\]

Implicit time-integration methods are the best options for solving stiff initial value problems [2], even though they are computationally costly, especially for solving large nonlinear systems such as the reduced system of IVPs like Eq. (2.20). Therefore, an implicit algorithm must be optimized in terms of the local degrees of freedom of the algebraic system of equations. The multi-stage implicit algorithms such as the Norsett’s diagonally implicit Runge–Kutta method (NDIRKM), implicit Lobatto methods (LBM) or implicit Radau methods (RDM) [2] have more degrees of freedom than the linear multi-step methods. The implicit linear multi-step methods such as the backward differentiation formulae (BDF) and the Adams–Moulton methods (AMM) take advantage of the optimized degrees of freedom. In Fig. 1, the current group of multi-derivative time-integration algorithms (IELDTM) are compared with the well-known implicit multi-stage and multi-step time integration methods (NDIRKM4, RDM4, LBM4, BDF4, BDF3, BDF2 and AMM4). The illustrated step-sizes are the threshold values to get \( \|E\|_\infty = 10^{-6} \) accuracy for solving the Burgers equation with the parameter values \( \varepsilon = 0.001 \) and \( N = 40 \). The spatial discretization of the corresponding PDE is carried out with the ChCM, and then the reduced ODE system (like Eq. (2.20)) is solved by various implicit time integration methods to produce Fig. 1. As seen from the figure, the implicit multi-step algorithms lack order-preservation property for solving the stiff ODE system as opposed to the current IELDTM and the implicit multi-stage methods. Here we show that multi-step methods require generally fewer time-steps than the multi-stage methods to obtain the same accuracy for the solution of relatively large stiff IVPs. Even if the implicit multi-stage methods provide order-preservation property, those methods
need far more local degrees of freedom than the current IELDTM and the implicit multi-step methods. As a multi-derivative method, the IELDTM has been proven to provide both optimized degrees of freedom and order-preservation property, as seen in Fig. 1. Both the central and backward IELDTMs provide the same accuracy with larger step sizes than the rival algorithms.

The performance of the current ChCM-IELDTM is shown by comparing the maximum errors depending on the varying values of the direction parameter \( \theta \) (see Fig. 2). As theoretically expected, the maximum errors are reduced exponentially by increasing the order of the method. It can be observed from Fig. 2 that choosing \( \theta = 0.5 \) with odd number \( K \) values leads to the numerical method of \( K + 1 \) order. Note that the exponential convergence is verified for both \( \varepsilon = 1 \) and \( \varepsilon = 0.1 \) selections. The advection-dominated cases of the present example exhibit challenging behavior as has been widely discussed in the literature [25, 31, 33]. The ChCM-IELDTM hybridization produces non-oscillatory solutions in such stiff cases as shown in Fig. 3. The sharp behaviors are demonstrated by choosing the kinematic viscosity constants as \( \varepsilon = 0.001 \) and \( \varepsilon = 0.0005 \). Using the current central time integration method and high-degree spectral approach, challenging numerical solutions have been captured for both cases. The performance of time adaptive ChCM-IELDTM hybridization have been illustrated based on the error norms and the required step sizes as seen in Table 1. It is obvious from the table that the IELDTM time-integration is more preferable than the \textit{ode45-ode15s} of MATLAB. The overall performance of the current approach is compared with finite element-based techniques such as the weak Galerkin finite element method (WFEM) [37] and the strong Galerkin finite element method (GFEM) [38] as shown in Table 2.
temporal part of FEM based algorithms, the Crank-Nicolson method (a special case of IELDTM; \( \theta = 0.5 \) and \( K = 1 \)) has been used as a time integration technique. The current approach, ChCM-IELDTM, produces more reliable results than the FEM-based techniques, even if their degrees of freedom are lower than the literature [37, 38]. The effect of the IELDTM is easily seen from the results in the table, i.e. the case of \( K = 3 \) and \( \theta = 0.5 \) (fourth order in time) reduces the maximum error from \( 5.57E - 07 \) to \( 8.97E - 10 \).

Fig. 2 Order refinement results of the ChCM-IELDTM at \( t_f = 0.5 \) for various values of the direction parameter \( \theta \) with the parameter values a \( \epsilon = 1, N = 10 \) and \( dt = 0.0025 \) b \( \epsilon = 0.1, N = 40 \) and \( dt = 0.0025 \)

Fig. 3 The ChCM-IELDTM solutions of Problem 1 at various times for the parameter values a \( \epsilon = 0.001, N = 80, \theta = 0.5, K = 4 \) and \( dt = 0.001 \) b \( \epsilon = 0.0005, N = 120, \theta = 0.5, K = 4 \) and \( dt = 0.001 \)
Problem 2 Zhao [28] Consider the two-dimensional form of advection–diffusion Eq. (2.1) with \( w(u) = 0 \) and the following exact solution [28] where the computational domain is 
\[
D = \{(x,y,t) \in R^2 \times R | 0 \leq x, y \leq 1 \text{ and } t \in [0, t_f]\}
\]. The initial and boundary conditions can be taken from the exact solution (4.6). We observe that all our theoretical error expectations are satisfied for all values of the direction parameter \( \theta \). Natural solution behavior (4.6) drops rapidly from one to zero when the

| \( \varepsilon \) | Method           | Step | \( \|E\|_{\infty} \) |
|----------------|-----------------|------|-----------------|
| \( \varepsilon = 1 \) | IELDTM-ChCSM \( K = 3 \) | 500  | 8.5E-09         |
|                      | IELDTM-ChCSM \( K = 4 \) | 354  | 8.5E-09         |
|                      | IELDTM-ChCSM \( K = 5 \) | 101  | 8.5E-09         |
|                      | \textit{ode45}-ChCSM | 493  | 8.0E-09         |
|                      | \textit{ode15s}-ChCSM | 243  | 8.6E-09         |
| \( \varepsilon = 0.1 \) | IELDTM-ChCSM \( K = 3 \) | 266  | 2.0E-08         |
|                      | IELDTM-ChCSM \( K = 4 \) | 189  | 2.0E-08         |
|                      | IELDTM-ChCSM \( K = 5 \) | 88   | 2.0E-08         |
|                      | \textit{ode45}-ChCSM | 596  | 2.0E-08         |
|                      | \textit{ode15s}-ChCSM | 163  | 2.0E-08         |
| \( \varepsilon = 0.01 \) | IELDTM-ChCSM \( K = 3 \) | 583  | 1.2E-05         |
|                      | IELDTM-ChCSM \( K = 4 \) | 413  | 1.2E-05         |
|                      | IELDTM-ChCSM \( K = 5 \) | 126  | 1.2E-05         |
|                      | \textit{ode45}-ChCSM | 839  | 1.2E-05         |
|                      | \textit{ode15s}-ChCSM | 253  | 1.2E-05         |

Table 2 Comparison of the numerical results produced with \( t_f = 0.1, \varepsilon = 0.1 \) and \( dt = 0.001 \)

| \( x \) | WGFEM \[37\] \( N = 40 \) | GFEM \[38\] \( N = 40 \) | ChCM-IELDTM \( (\theta = 0.5/K = 1) \) \( N = 20 \) | ChCM-IELDTM \( (\theta = 0.5/K = 3) \) \( N = 20 \) | Exact          |
|---------|-----------------|-----------------|-----------------|-----------------|-----------------|
| \( x = 0.1 \) | 0.22346         | 0.2234492260    | 0.2234492160    | 0.2234495335    | 0.2234495335    |
| \( x = 0.3 \) | 0.62514         | 0.6251179353    | 0.6251179207    | 0.6251182341    | 0.6251182333    |
| \( x = 0.5 \) | 0.87728         | 0.8772800857    | 0.8772800822    | 0.8772796533    | 0.8772796530    |
| \( x = 0.7 \) | 0.83686         | 0.8369228762    | 0.8369228771    | 0.8369225592    | 0.8369225599    |
| \( x = 0.9 \) | 0.36573         | 0.36575425470   | 0.3657542612    | 0.3657544560    | 0.3657544557    |
| \( \|E\|_{\infty} \) | 5.57E-07        | 8.97E-10        |                   |                   |                 |

\[ u(x,y,t) = \frac{1}{1 + e^{(x+y-t)/\varepsilon}} \] (4.6)

The direction parameter \( \theta \) plays a critical role in terms of both accuracy and stability. Exponential convergence of the current algorithm for both \( \varepsilon = 1 \) and \( \varepsilon = 0.1 \) is illustrated for various \( \theta \) values as seen in Fig. 4. We observe that all our theoretical error expectations are satisfied for all values of the direction parameter \( \theta \). Natural solution behavior (4.6) drops rapidly from one to zero when the
viscosity constant approaches zero. Thus, many numerical solvers fail to produce non-oscillatory results in the regions in which the rapid changes occur. In Fig. 5, it has been shown that the present ChCM-IELDTM technique has ability to accurately capture the shock behavior for both $\varepsilon = 0.01$ and $\varepsilon = 0.005$. In Table 3, our motivation is to compare the current IELDTM integration method with the MATLAB solvers, ode45 and ode15s, in terms of both accuracy and computational cost. As seen in the table, the present IELDTM-ChCM provides optimal results with less number of time steps than the rival schemes.

Fig. 4 Order refinement results of the ChCM-IELDTM at $t_f = 0.5$ for various values of the direction parameter $\theta$ with the parameter values $a$ $\varepsilon = 1, N = M = 10$ and $dt = 0.005$  $b$ $\varepsilon = 0.1, N = M = 20$ and $dt = 0.005$

Fig. 5 The ChCM-IELDTM solutions of Problem 2 at various times for the parameter values $a$ $\varepsilon = 0.01, N = M = 40, \theta = 0.5, K = 4$ and $dt = 0.01$ $b$ $\varepsilon = 0.005, N = M = 80, \theta = 0.5, K = 4$ and $dt = 0.01$
Table 3  Number of time steps and the maximum pointwise errors of the time-adaptive ChCM-IELDTM method for various values of the viscosity constant $\varepsilon$ and time approximation order $K$ with $\theta = 0.5$, $t_f = 0.5$ and $tol = E - 15$

| $\varepsilon$ | Method       | Step | $\|E\|_{\infty}$   |
|---------------|--------------|------|---------------------|
| $\varepsilon = 1$ $N = M = 10$ | IELDTM-ChCSM $K = 3$ | 222  | 1.84E-14            |
|               | IELDTM-ChCSM $K = 4$ | 178  | 1.48E-14            |
|               | IELDTM-ChCSM $K = 5$ | 149  | 2.35E-14            |
|               | ode45-ChCSM   | 7023 | 1.87E-14            |
|               | ode15s-ChCSM  | 94   | 2.25E-14            |

| $\varepsilon = 0.1$ $N = M = 20$ | IELDTM-ChCSM $K = 3$ | 274  | 8.93E-10            |
|                                | IELDTM-ChCSM $K = 4$ | 220  | 9.02E-10            |
|                                | IELDTM-ChCSM $K = 5$ | 183  | 9.02E-10            |
|                                | ode45-ChCSM     | 19,919 | 9.02E-10          |
|                                | ode15s-ChCSM    | 504   | 9.02E-10            |

| $\varepsilon = 0.01$ $N = M = 40$ | IELDTM-ChCSM $K = 3$ | 378  | 2.50E-03            |
|                                 | IELDTM-ChCSM $K = 4$ | 311  | 2.60E-03            |
|                                 | IELDTM-ChCSM $K = 5$ | 268  | 2.60E-03            |
|                                 | ode45-ChCSM     | 55,436 | 2.60E-03        |
|                                 | ode15s-ChCSM    | 4327  | 2.60E-03            |

**Problem 3** Aro [40] To test the performance of the currently proposed numerical algorithm, we consider a real-life chemistry model represented by a coupled advection–diffusion-reaction equation. Let $u(x, t)$ denote the chemical concentration of atomic oxygen ($[O]$) and let $v(x, t)$ denote the concentration of molecular ozone ($[O_3]$) in the earth’s atmosphere. Let us represent the concentration of molecular oxygen ($[O_2]$) with $r = 3.7 \times 10^{16}$ as a constant value since $[O_2] \gg [O]$ and $[O_2] \gg [O_3]$ in the earth’s atmosphere. By considering the transport of chemicals through advection and diffusion, the Chapman model of $[O] - [O_2] - [O_3]$ reaction system with transport phenomena can be described by the following ADR equations [40],

$$u_t + u_x = u_{xx} + 2k_3(t)r + k_4(t)v - k_1ru - k_2uv$$  \hspace{1cm} (4.7)

$$v_t + v_x = v_{xx} + k_1ru - k_2uv - k_4(t)v$$  \hspace{1cm} (4.8)

where $x \in [0, 1]$ and $t \in [0, 864000]$. Initial conditions are considered as $u(x, 0) = 10^5$ and $v(x, 0) = 10^{12}$. Periodic boundary conditions with $u(0, t) = u(1, t)$, $u_x(0, t) = u_x(1, t)$, $v(0, t) = v(1, t)$ and $v_x(0, t) = v_x(1, t)$ are also assumed. The constant reaction rates occurred in Eqs. (4.7), (4.8) are $k_1 = 1.63 \times 10^{-16}$ and $k_2 = 4.66 \times 10^{-16}$. The time-dependent reaction rates for chemical reactions driven by the absorption of sunlight can be expressed as follows

$$k_i(t) = \begin{cases} 
\exp\left(\frac{-a_i}{\sin(\omega t - 2\pi i)}\right), & \sin(\omega t - 2\pi i) \\
0, & \sin(\omega t - 2\pi i) \leq 0
\end{cases}$$  \hspace{1cm} (4.9)

where $i = 3, 4$, $a_3 = 22.62$, $a_4 = 7.601$, and $\omega = \frac{\pi}{31200}$. The test problem is sufficiently stiff to handle and has challenging numerical characteristics that are not easy to handle by the conventional numerical algorithms.
The numerical analysis of the Chapman chemistry problem is performed with the time-adaptive ChCM-IELDTM, and the results are illustrated in Figs. 6 and 7. As mentioned in literature [40], the dynamical responses of the concentrations of the atomic oxygen $[O]$ and molecular ozone $([O_3])$ are observed up to $t_f = 864000$ (10 days) with the currently derived IELDTM. The time adaptive procedure here needs special attention due to the relatively long time interval. For the numerical solution of the reduced

**Fig. 6** The time-adaptive ChCM-IELDTM solution profile of the Chapman chemistry problem at $x = 0.5$ up to $t_f = 864000$ with the spatial polynomials of order $N = 20$

**Fig. 7** $[O]$ and $[O_3]$ surfaces for the Chapman chemistry problem over 10 days obtained by the time-adaptive ChCM-IELDTM with the spatial polynomials of order $N = 20$
ODE system (like Eq. (2.20)) obtained by applying the ChCM to Eqs. (4.7), (4.8), we have used the following adaptive procedure

\[
\Delta t_i = \frac{\min(\|\vec{\beta}_i(0)\|) \text{tol}}{\|\vec{\beta}_i(2)\|}, \text{ if } \Delta t_i > 1 \text{ with } \theta = K = 1 \text{ (the backward IELDTM)},
\]

\[
\Delta t_i = \left( \frac{2\min(\|\vec{\beta}_i(0)\|) \text{tol}}{\|\vec{\beta}_i(3)\|} \right)^{\frac{1}{3}}, \text{ otherwise with } \theta = 0.5 \text{ and } K = 1 \text{ (the central IELDTM)},
\]

(4.10)

(4.11)

where \( \vec{\beta}_i(k) = [\vec{U}_i(k), \vec{V}_i(k)]^T \), \( \vec{U}_i(k) \) and \( \vec{V}_i(k) \) are the local differential transforms of the functions \( u(x, t) \) and \( v(x, t) \) at any local time \( t = t_i \). The terms \( \min(\|\vec{\beta}_i(0)\|) \) in the numerators of estimations (4.10), (4.11) are occurred due to the controlling of the relative errors with the \( \text{tol} \) values. Since the concentrations of both chemicals are higher than \( 10^6 \), \( \text{tol} = 10^3 \) is chosen as the local maximum relative error bound in simulations. By applying adaptivity Eqs. (4.10), (4.11), the IELDTM requires 41,137 time steps to integrate the reduced ODE system up to \( t_f = 864000 \).

The numerical behaviors of the concentrations of oxygen ([O]) and molecular ozone ([O_3]) are illustrated up to 10 days with at the middle point of the spatial interval in Fig. 5. Monotonically increasing profile of [O_3] and oscillatory profile of [O] are observed over 10 days period from the illustrations. The stiff dynamics for the [O] is accurately captured at the early times. The corresponding surface plots for the space–time numerical behaviors of both chemicals are presented in Fig. 6. The transport phenomena with advection and diffusion are seen to lead to the wave-like distribution of the solution profiles in \( x \)-direction (with highly small wave amplitude of [O_3]).

5 Conclusions and recommendation

In this study, one-step implicit-explicit local differential transform method (IELDTM) has been derived for the temporal integration of problems represented by nonlinear advection–diffusion-reaction Processes. The Chebyshev spectral collocation method (ChCM) has been considered for the spatial part of the considered PDEs due to computational efficiency of the method. The global error analysis of the IELDTM together with the stability analysis has been utilized and adaptivity equations have been proposed. The exponential convergence of the current numerical algorithm has been proven both theoretically and experimentally. The central case of the IELDTM, with the selection of \( \theta = 0.5 \), has been observed to be both more accurate and stability preserved. It has been proven that the IELDTM overcomes the shortcomings of the existing numerical techniques, such as the inaccuracy disadvantages of the \( \theta \)-method and the instability drawbacks of the DTM-based methods. It has also been presented that the current time integration scheme

\[ \Delta t_i = \frac{\min(\|\vec{\beta}_i(0)\|) \text{tol}}{\|\vec{\beta}_i(2)\|}, \text{ if } \Delta t_i > 1 \text{ with } \theta = K = 1 \text{ (the backward IELDTM)}, \]

\[ \Delta t_i = \left( \frac{2\min(\|\vec{\beta}_i(0)\|) \text{tol}}{\|\vec{\beta}_i(3)\|} \right)^{\frac{1}{3}}, \text{ otherwise with } \theta = 0.5 \text{ and } K = 1 \text{ (the central IELDTM)}, \]

(4.10)

(4.11)
achieves optimum accuracy by using fewer time steps than the commonly used time integrators of MATLAB such as ode45 and ode15s. It has also been shown here that the ChCM-IELDTM can solve advection dominated problems without producing any unwanted oscillation in both one and two dimensions. The Chapman oxygen-ozone ADR model has been numerically investigated with the present time adaptive ChCM-IELDTM hybridization. The proposed algorithm has been proven to have the ability to solve this stiff problem, which is an important chemical application, with optimum costs.

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Declarations

Conflict of interest The authors have no conflicts of interest to declare.

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