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Exponential basis and exponential expanding grids third (fourth)-order compact schemes for nonlinear three-dimensional convection-diffusion-reaction equation

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Abstract

This paper addresses exponential basis and compact formulation for solving three-dimensional convection-diffusion-reaction equations that exhibit an accuracy of order three or four depending on exponential expanding or uniformly spaced grid network. The compact formulation is derived with three grid points in each spatial direction and results in a block-block tri-diagonal Jacobian matrix, which makes it more suitable for efficient computing. In each direction, there are two tuning parameters; one associated with exponential basis, known as the frequency parameter, and the other one is the grid ratio parameter that appears in exponential expanding grid sequences. The interplay of these parameters provides more accurate solution values in short computing time with less memory space, and their estimates are determined according to the location of layer concentration. The Jacobian iteration matrix of the proposed scheme is proved to be monotone and irreducible. Computational experiments with convection dominated diffusion equation, Schrödinger equation, Helmholtz equation, nonlinear elliptic Allen–Cahn equation, and sine-Gordon equation support the theoretical convergence analysis.

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Keywords: Exponential expanding grid network; Compact scheme; Exponential basis; Convection-diffusion equation; Schrödinger equation; Elliptic Allen–Cahn equation; Sine-Gordon equation; Convergence order

1 Introduction

We shall describe a numerical method to solve the general form of three-space dimensions mildly nonlinear elliptic partial differential equations

$$\epsilon\left(\frac{\partial^2 U}{\partial x^2}+\frac{\partial^2 U}{\partial y^2}+\frac{\partial^2 U}{\partial z^2}\right)=\psi\left(x,y,z,U,\frac{\partial U}{\partial x},\frac{\partial U}{\partial y},\frac{\partial U}{\partial z}\right),\quad 0<\epsilon\ll 1,(x,y,z)\in\Omega. \tag{1.1}$$

We aim to determine the solution $U=U(x,y,z)$, at the finite number of discrete grid points of the solution domain $\Omega=(0,1)^3$, with Dirichlet's boundary data

$$U(0,y,z)=f_1(y,z),\qquad U(1,y,z)=f_2(y,z),\quad 0\le y,z\le 1, \tag{1.2a}$$

$$U(x,0,z) = f_3(x,z), \qquad U(x,1,z) = f_4(x,z), \quad 0 \le x,z \le 1, \tag{1.2b}$$

$$U(x,y,0) = f_5(x,y), \qquad U(x,y,1) = f_6(x,y), \quad 0 \le x,y \le 1. \tag{1.2c}$$

We shall assume that the function $\psi(x,y,z,U,P,Q,R)$ appearing in (1.1) is continuous. Moreover, the continuity of $\partial\psi/\partial U, \partial\psi/\partial P, \partial\psi/\partial Q, \partial\psi/\partial R$ on the closed domain $\overline{\Omega}$, along with $\partial\psi/\partial U \ge 0$, ensures the unique existence of the analytic solution to (1.1)–(1.2a)–(1.2c) [18]. Elliptic partial differential equations (PDEs) appear at wide application area in natural sciences and engineering such as acoustic, chaos, boundary layer, decalescence, electricity, energy, power, force, hysteresis, resonance, opacity, refraction, conduction, propagation, and turbulence. Laplace equation, Poisson's equation, and Helmholtz equation are some of well-known second-order elliptic PDEs of linear type, and their exact solution helps in realizing the qualitative character of scientific processes. Many complex processes in which input variation is not proportional to changes in output yield a nonlinear system of elliptic PDEs, for example, spatial localization of heat and mass transfer process, crystal dislocation (sine-Gordon equation), and phase transition (elliptic Allen–Cahn equation) [39]. The treatment of such PDEs models appearing in physical phenomenon needs special attention either due to multiple character or non-existence of classical solution values. Although the theory of existence and uniqueness ensures the presence of solution, the exact solution of nonlinear elliptic PDEs, in general, is not possible alike linear PDEs. In addition to it, the exact solution cannot deal with discrete data such as the dynamic *response of the structure* in earthquake modeling. In some cases, an exact solution can serve the basis for testing computer algorithms for solving partial differential equations. Thus, to deal with nonlinear elliptic PDEs, we need to apply numerical techniques for computing approximate solution values that can optimize basic parameters depending on the requirements.

In the recent past, efficient algorithms based on high-order approximations have yielded optimal accuracies in the solution of elliptic PDEs. The forward and second central-differencing operators are commonly applied to replace first- and second-order partial derivatives. Such a discrete relation often leads to oscillatory or unbounded solution values in the case of convection dominant or low diffusion coefficient [47]. In other words, the large value of Reynolds number results in unsatisfactory solution behavior despite the well-behaved nature of the analytic solution and guaranteed existence of a unique solution. There are two ways to treat them: either employing a reasonably ample number of spatial grids or scaling down the order of local truncation error of equivalent finite-difference replacement. The utilization of a large number of spatial grid points leads to a dense sparse matrix, and handling such a matrix consumes an ample amount of memory space; moreover, computation of dense sparse matrix needs massive computing time. Therefore, enhancing accuracy to a finite-difference approximation of governing PDEs is more emphasized. The discretization processes come along with round-off and truncation errors. In the modern fast computing scenario, loss of precision in view of decimal rounding is insignificant. Therefore, we are left with the problem of minimizing discretization or truncation errors: the deviation between the analytic solution of original PDEs and numerical solution of discrete equations obtained via finite-difference replacement. A fourth-order compact finite-difference approximation, multi-grid mechanism, and non-uniform grid transformation are considered for solving boundary layer convection-diffusion equation by [9]. A detailed Maple procedure to derive nineteen-point high-order compact formulation for three space dimensional linear elliptic PDEs with variable coefficients is described in [10]. A fourth-order compact formulation on variable grid step sizes in all coordinate directions is utilized for solving a three-dimensional Poisson's equation on the domain Ω [44]. A high-order compact formulation by using exponential approximation and off-step discretization is developed for quasi-linear elliptic partial differential equations [29, 30]. Boundary value method and finite-difference discretization of spatial derivatives for solving three-dimensional elliptic PDEs are considered by [3]. A variational method for elliptic PDEs with sign-changing nonlinearity is described by [1]. *Trigonometric Fourier collocation methods, energy preserving scheme, and nonlinear stability analysis related to Klein–Gordon equations are discussed in* [41–43]. A second-order accuracy scheme with non-graded Cartesian grids is described for variable coefficient Poisson's equation by [27]. A temporary introduction of auxiliary function and converting a discretized form of 3D linear elliptic PDEs into ordinary differential equations are considered in [32]. Similar to the finite volume method, a family of the fourth-order compact differencing scheme for discretizing a semi-linear convection-diffusion equation was described by [46]. *Preconditioners based on windowed Fourier frames and multigrid method for solving elliptic PDEs are discussed in* [2, 38]. A closed-form for the eigenvalues emanating from nineteen-point compact formulation to the three-dimensional convection-diffusion equation was presented by [12]. A detailed discussion of fourth-order accurate finite-difference approximation for the 3D elliptic PDEs of mildly nonlinear type is described in [5, 11]. Recently, third-order compact formulation on variable grid spacing and fourth-order approximation on uniform grid spacing for three space elliptic boundary value problems of mildly nonlinear type have been developed by [20, 21].

On uniformly spaced grid points, the composite of averaging and central-difference operator yields second-order accuracy to the first-order partial derivatives, while the second central-difference operator results in second-order accuracy to the second-order partial derivative. Therefore, the application of second central-difference operator and composite of averaging and first central-difference operator results in a scheme having second-order truncation errors, and it is compact too since it uses minimum grid points required to discretize the presence of maximum order partial differentials in the given mathematical model. In view of the earlier observations, our aim is to improve the order of truncation errors so as to gain better accuracies in solution values in a minimal computing time as well as with less memory storage. In the next section, we shall describe a non-uniformly spaced grid network and derivations of compact operators on an exponential basis. An improved accuracy compact scheme exhibiting the third- and fourth-order of convergence is obtained in Sect. 3. In Sect. 4, irreducibility and monotonic property to the Jacobian matrix analyzes the bounds of solution error and convergence. *Experimental results about linear and nonlinear convection-diffusion* models are presented in Sect. 5. In the end, the paper is accomplished with remarks and extension of the new scheme.

2 Grid topology and compact difference operators

The non-uniform grid spacing in the discretization of PDEs influences the magnitude of truncation error that depends upon the length of adjacent grid points and derivative of absolute functional value. Thus, it is least possible to attain consistent distribution of truncation errors on an evenly spaced grid network, especially with the model that possesses boundary layer behavior or has multiple natures of solution values. The sub-domain that adds maximum derivative value will be kept with low grid spacing, while the sub-domain that has smooth functional derivative values may be arranged with comparatively large grid spacing. By this technique, one can disperse truncation errors uniformly inside the domain of integration. It is therefore advantageous to keep non-uniformity in grid spacing for discretization procedure, which results in more precise solution values of PDEs [7]. Among various variable grid spacing, an exponential expanding grid network demonstrated decent results, if the governing PDEs exhibit layer behavior of solution or singularity. This is possible because exponential grid parameters can be adjusted according to the location of the layer or singular points. The approximate solution of elliptic PDEs (1.1) using finite-difference discretizations replaces the partial derivatives by estimated difference operators, and solution values are computed at a finite number of discrete grid points. Such type of three-dimensional grid points on a unit cuboid $\Omega = \{(x, y, z) : 0 \le x, y, z \le 1\}$ may be determined by the discrete set $\{(x_i, y_j, z_k) : i = 0(1)I + 1, j = 0(1)J + 1, k = 0(1)K + 1\}$, where $(x_0, y_0, z_0) = (0, 0, 0)$, $(x_{I+1}, y_{J+1}, z_{K+1}) = (1, 1, 1)$, and interior grid points at $i = 1(1)I, j = 1(1)J, k = 1(1)K$, are obtained by the stretching relation

$$(x_i, y_j, z_k) = (x_{i-1} + \Delta x_i, y_{j-1} + \Delta y_j, z_{k-1} + \Delta z_k), \tag{2.1}$$

where the grid step sizes are given by $(\Delta x_{i+1}, \Delta y_{j+1}, \Delta z_{k+1}) = (p\Delta x_i, q\Delta y_j, r\Delta z_k)$. Here, $p, q,$ and r are the grid expansion factor (stretching parameter) in x-, y-, and z-spatial directions respectively, and its selection depends on the thickness of boundary layer in a turbulent fluid flow [4, 6]. As we knew the length of diffusion space in each spatial direction, therefore, the first grid step size can be easily determined in the following manner:

$$\begin{aligned} &\Delta x_1 = \begin{cases} \frac{p-1}{p^{I+1}-1}, & p \ne 1, \\ \frac{1}{I+1}, & p = 1, \end{cases} \qquad \Delta y_1 = \begin{cases} \frac{q-1}{q^{J+1}-1}, & q \ne 1, \\ \frac{1}{J+1}, & q = 1, \end{cases} \\ &\Delta z_1 = \begin{cases} \frac{r-1}{r^{K+1}-1}, & r \ne 1, \\ \frac{1}{K+1}, & r = 1. \end{cases} \end{aligned} \tag{2.2}$$

Such a set-up of grids is known as exponential expanding grid network, and it has been applied to the digital simulation of electrochemical phenomena by [4, 8]. Based on the exponential expanding grid, the optimal order discretization of elliptic PDEs in one and two dimensions has been described in the past by [19, 22, 23, 28].

Next, we shall define differencing operators that approximate the explicit diffusion terms and nonlinear appearance of convection term in the mathematical models (1.1). We shall denote by $U_{i,j,k}$ the exact value of $U(x, y, z)$ at grid-point (x_i, y_j, z_k), and $u_{i,j,k}$ is the approximate value obtained from the discrete relation of the proposed high accuracy compact scheme. The notations $U^x_{i,j,k} = (\partial U/\partial x)_{(x_i,y_j,z_k)}$, $U^{xx}_{i,j,k} = (\partial^2 U/\partial x^2)_{(x_i,y_j,z_k)}$, etc. will be used for derivation purpose. The x-direction difference operators are obtained on the basis $\{1, e^{\alpha x}, e^{-\alpha x}\}, \alpha \ne 0$, using three grid points set $\{x_{i-1}, x_i, x_{i+1}\}$. The exponential function spaces with basis $\mathcal{B}_x = \{1, e^{\alpha x}, e^{-\alpha x}\}$ are more flexible than polynomials basis $\mathcal{B}^*_x = \{1, x, x^2\}$. The basis $\mathcal{B}_x$ is consistent with $\mathcal{B}^*_x$ in the limiting case $\alpha \to 0$. This is investigated in the following manner:

$$\operatorname{Span}\{1, e^{\alpha x}, e^{-\alpha x}\} = \operatorname{Span}\left\{1, \frac{1}{2\alpha}\left(e^{\alpha x} - e^{-\alpha x}\right), \frac{1}{\alpha^2}\left(e^{\alpha x} + e^{-\alpha x} - 2\right)\right\} \quad \text{and}$$
$$\lim_{\alpha \to 0} \frac{1}{2\alpha}\left(e^{\alpha x} - e^{-\alpha x}\right) = x, \qquad \lim_{\alpha \to 0} \frac{1}{\alpha^2}\left(e^{\alpha x} + e^{-\alpha x} - 2\right) = x^2.$$

The frequency parameter of the exponential part in the basis optimizes the solution accuracies. This is because the C^∞-differentiability of the exponential functions compensates the loss of smoothness inherited by the polynomial functions.

Let us consider the linear combination

$$\chi \equiv a_{200}^{000} U_{i-1,j,k} + a_{000}^{000} U_{i,j,k} + a_{100}^{000} U_{i+1,j,k} - \delta x_i U_{i,j,k}^x. \tag{2.3}$$

The evaluation of χ for $U(x,y,z) = 1, e^{\alpha x}$, and $e^{-\alpha x}$ at the central grid-point location (x_i, y_j, z_k) yields three linear equations and may be solved for the three unknowns $a_{000}^{000}, a_{100}^{000}$, and a_{200}^{000} uniquely [17]. The superscript triplets in the unknowns signify the location at which derivative is calculated, while the subscript defines the central and neighboring grid locations. In this way, we can compute the approximations of $U_{i,j,k}^x$. Using the same mechanism, it is easy to obtain three-point relations of a first-order partial derivative in the x-direction at the neighboring grid locations x_{i-1} and x_{i+1}. In a similar way, for $\beta \neq 0, \gamma \neq 0$, the bases $\{1, e^{\beta y}, e^{-\beta y}\}$ and $\{1, e^{\gamma z}, e^{-\gamma z}\}$ *on the grid point* set $\{y_{j-1}, y_j, y_{j+1}\}$ and $\{z_{k-1}, z_k, z_{k+1}\}$ determine the approximations of first-order partial derivatives in y- and z-directions *respectively*. Approximations of second-order partial derivatives at the grid-point location x_i can be estimated on the same line by replacing $\delta x_i U_{i,j,k}^x$ to $\delta x_i^2 U_{i,j,k}^{xx}$ in the linear combination (2.3) and giving different names to the unknown coefficients. In this way, we can get an approximation of diffusion terms. Now, let us define

$$\begin{aligned}
\phi_1(\mu, \delta s) &= \mu\delta s\left[\cosh(\mu\delta s) - 1\right],\\
\phi_2(\mu, \sigma, \delta s) &= \mu\delta s\left[\cosh(\sigma\mu\delta s) - 1\right],\\
\phi_3(\mu, \sigma, \delta s) &= \mu\delta s\left[\cosh\left((\sigma + 1)\mu\delta s\right) - 1\right],\\
\phi_4(\mu, \sigma, \delta s) &= \phi_3(\mu, \sigma, \delta s) - \phi_2(\mu, \sigma, \delta s),\\
\phi_5(\mu, \sigma, \delta s) &= \phi_2(\mu, \sigma, \delta s) - \phi_1(\mu, \delta s),\\
\phi_6(\mu, \sigma, \delta s) &= \phi_1(\mu, \delta s) - \phi_3(\mu, \sigma, \delta s),\\
\phi_7(\mu, \delta s) &= \mu^2\delta s^2 \sinh(\mu\delta s),\\
\phi_8(\mu, \sigma, \delta s) &= \mu^2\delta s^2 \sinh(\sigma\mu\delta s),\\
\phi_9(\mu, \sigma, \delta s) &= \phi_7(\mu, \delta s) + \phi_8(\mu, \sigma, \delta s),\\
\varphi(\mu, \sigma, \delta s) &= \sinh\left((\sigma + 1)\mu\delta s\right) - \sinh(\sigma\mu\delta s) - \sinh(\mu\delta s),
\end{aligned}$$

where $\mu \in \{\alpha, \beta, \gamma\}, \sigma \in \{p, q, r\}$ and $\delta s \in \{\delta x_i, \delta y_j, \delta z_k\}$.

Next, we shall define the following three-point compact discretizations to first- and second-order partial derivatives in each coordinate direction:

$$\begin{bmatrix} \tilde{U}^x_{i+1,j+b,k+c} \\ \tilde{U}^x_{i,j+b,k+c} \\ \tilde{U}^x_{i-1,j+b,k+c} \end{bmatrix} = \frac{1}{\delta x_i \varphi(p,\alpha,\delta x_i)} \mathcal{M}(p,\alpha,\delta x_i) \begin{bmatrix} U_{i+1,j+b,k+c} \\ U_{i,j+b,k+c} \\ U_{i-1,j+b,k+c} \end{bmatrix}, \quad b,c \in \{0,\pm 1\}, \tag{2.4}$$

$$\begin{bmatrix} \tilde{U}^y_{i+a,j+1,k+c} \\ \tilde{U}^y_{i+a,j,k+c} \\ \tilde{U}^y_{i+a,j-1,k+c} \end{bmatrix} = \frac{1}{\delta y_j \varphi(q,\beta,\delta y_j)} \mathcal{M}(q,\beta,\delta y_j) \begin{bmatrix} U_{i+a,j+1,k+c} \\ U_{i+a,j,k+c} \\ U_{i+a,j-1,k+c} \end{bmatrix}, \quad a,c \in \{0,\pm 1\}, \tag{2.5}$$

$$\begin{bmatrix} \tilde{U}^z_{i+a,j+b,k+1} \\ \tilde{U}^z_{i+a,j+b,k} \\ \tilde{U}^z_{i+a,j+b,k-1} \end{bmatrix} = \frac{1}{\delta z_k \varphi(r,\gamma,\delta z_k)} \mathcal{M}(r,\gamma,\delta z_k) \begin{bmatrix} U_{i+a,j+b,k+1} \\ U_{i+a,j+b,k} \\ U_{i+a,j+b,k-1} \end{bmatrix}, \quad a,b \in \{0,\pm 1\}, \tag{2.6}$$

$$\tilde{U}^{xx}_{i,j+b,k+c} = \frac{1}{\delta x_i^2 \varphi(p,\alpha,\delta x_i)} \begin{bmatrix} \phi_7(\alpha,\delta x_i) U_{i+1,j+b,k+c} - \phi_9(p,\alpha,\delta x_i) U_{i,j+b,k+c} \\ + \phi_8(p,\alpha,\delta x_i) U_{i-1,j+b,k+c} \end{bmatrix},$$
$$(b,c) \in \{(0,0),(\pm 1,0),(0,\pm 1)\}, \tag{2.7}$$

$$\tilde{U}^{yy}_{i+a,j,k+c} = \frac{1}{\delta y_j^2 \varphi(q,\beta,\delta y_j)} \begin{bmatrix} \phi_7(\beta,\delta y_j) U_{i+a,j+1,k+c} - \phi_9(q,\beta,\delta y_j) U_{i+a,j,k+c} \\ + \phi_8(q,\beta,\delta y_j) U_{i+a,j-1,k+c} \end{bmatrix},$$
$$(a,c) \in \{(0,0),(\pm 1,0),(0,\pm 1)\}, \tag{2.8}$$

$$\tilde{U}^{zz}_{i+a,j+b,k} = \frac{1}{\delta z_k^2 \varphi(r,\gamma,\delta z_k)} \begin{bmatrix} \phi_7(\gamma,\delta z_k) U_{i+a,j+b,k+1} - \phi_9(r,\gamma,\delta z_k) U_{i+a,j+b,k} \\ + \phi_8(r,\gamma,\delta z_k) U_{i+a,j+b,k-1} \end{bmatrix},$$
$$(a,b) \in \{(0,0),(\pm 1,0),(0,\pm 1)\}, \tag{2.9}$$

where

$$\mathcal{M}(\mu,\sigma,\delta s) = \begin{bmatrix} \phi_4(\mu,\sigma,\delta s) & -\phi_3(\mu,\sigma,\delta s) & \phi_2(\mu,\sigma,\delta s) \\ \phi_1(\mu,\delta s) & \phi_5(\mu,\sigma,\delta s) & -\phi_2(\mu,\sigma,\delta s) \\ -\phi_1(\mu,\delta s) & \phi_3(\mu,\sigma,\delta s) & \phi_6(\mu,\sigma,\delta s) \end{bmatrix}.$$

Now, define the following three-point compact operators in each coordinate direction:

$$\mathcal{A}_x U_{i,j,k} = \delta x_i \tilde{U}^x_{i,j,k}, \qquad \mathcal{A}_y U_{i,j,k} = \delta y_j \tilde{U}^y_{i,j,k}, \qquad \mathcal{A}_z U_{i,j,k} = \delta z_k \tilde{U}^z_{i,j,k}, \tag{2.10}$$

$$\mathcal{B}_x U_{i,j,k} = \delta x_i^2 \tilde{U}^{xx}_{i,j,k}, \qquad \mathcal{B}_y U_{i,j,k} = \delta y_j^2 \tilde{U}^{yy}_{i,j,k}, \qquad \mathcal{B}_z U_{i,j,k} = \delta z_k^2 \tilde{U}^{zz}_{i,j,k}. \tag{2.11}$$

For $p = 1$, the grid step sizes turn out constant and grids are uniformly spaced. Moreover, in the limiting case of frequency parameters $\alpha,\beta,\gamma \to 0$, the exponential basis may be treated as a polynomial basis. Thus, in the limiting case, difference operators $\mathcal{A}_x$ and $\mathcal{B}_x$ become $\mathcal{A}_x U_{i,j,k} = 2\mu_x \delta_x = U_{i+1,j,k} - U_{i-1,j,k}$, and $\mathcal{B}_x U_{i,j,k} = \delta_x^2 = U_{i+1,j,k} - 2U_{i,j,k} + U_{i-1,j,k}$. Similarly, when $q = r = 1$ and $\beta,\gamma \to 0$, we obtain $\mathcal{A}_y = 2\mu_y\delta_y$, $\mathcal{A}_z = 2\mu_z\delta_z$ and $\mathcal{B}_y = \delta_y^2$, $\mathcal{B}_z = \delta_z^2$, where μ_x, μ_y, μ_z and δ_x, δ_y, δ_z are averaging and central difference operators respectively in x-, y-, and z-directions. With the help of Taylor's expansion, one can observe that

$$\mathcal{A}_x U_{i,j,k} = \delta x_i U^x_{i,j,k} + \frac{p}{6} \delta x_i^3 \left(U^{xxx}_{i,j,k} - \alpha^2 U^x_{i,j,k}\right) + O\left(\delta x_i^4\right) \tag{2.12}$$

and

$$\mathcal{B}_x U_{i,j,k} = \delta x_i^2 U_{i,j,k}^{xx} + \frac{1}{3}(p-1)\delta x_i^3\big(U_{i,j,k}^{xxx} - \alpha^2 U_{i,j,k}^{x}\big) + O\big(\delta x_i^4\big). \tag{2.13}$$

As a result,

$$\frac{1}{\delta x_i}\mathcal{A}_x U_{i,j,k} = U_{i,j,k}^{x} + O\big(\delta x_i^2\big), \quad \forall p, \tag{2.14}$$

$$\frac{1}{\delta x_i^2}\mathcal{B}_x U_{i,j,k} = U_{i,j,k}^{xx} + \begin{cases} O(\delta x_i), & p \neq 1, \\ O(\delta x_i^2), & p = 1. \end{cases} \tag{2.15}$$

Therefore, the operators $\mathcal{A}_x$ and $\mathcal{B}_x$ result in a first-, and second-order accuracy to first- and second-order partial derivatives on exponential expanding grid points. Similar observations for the operators $\mathcal{A}_y$, $\mathcal{B}_y$ and $\mathcal{A}_z$, $\mathcal{B}_z$ in y- and z-directions follow by applying finite series expansions. The applications of operators (2.10)–(2.11) to the mildly nonlinear elliptic PDEs (1.1) yield the system of algebraic equations

$$\begin{aligned} &\epsilon\left(\frac{\mathcal{B}_x}{\delta x_i^2} + \frac{\mathcal{B}_y}{\delta y_j^2} + \frac{\mathcal{B}_z}{\delta z_k^2}\right)U_{i,j,k} \\ &\quad = \psi\left(x_i, y_j, z_k, U_{i,j,k}, \frac{1}{\delta x_i}\mathcal{A}_x U_{i,j,k}, \frac{1}{\delta y_j}\mathcal{A}_y U_{i,j,k}, \frac{1}{\delta z_k}\mathcal{A}_z U_{i,j,k}\right). \end{aligned} \tag{2.16}$$

The truncation error associated with the difference scheme (2.16) is $O(\delta x_i + \delta y_j + \delta z_k)$, and the use of such a low order accurate finite-difference formula may not result in best possible accuracy, even if the unknown function is smooth [26]. The use of a high-order, finite-difference scheme along with suitably chosen grid step size posterior can surmount this. In the next section, we shall extend the order of truncation error that preserves the compact character of the scheme.

3 Third (fourth)-order compact scheme

We intend to formulate a third-order accurate compact difference scheme on an exponential expanding grid network for the mildly nonlinear elliptic PDEs (1.1), and for the same, we begin with Poisson's equation

$$\epsilon\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2}\right) = \psi(x,y,z), \quad (x,y,z) \in \Omega. \tag{3.1}$$

Consider the linear combination

$$\begin{aligned} \mathcal{L}\{U_{i,j,k}\} = \delta x_i^2 \delta y_j^2 \delta z_k^2\big[&\psi_{i,j,k} + \rho_x \delta x_i \psi_{i,j,k}^{x} + \rho_y \delta y_j \psi_{i,j,k}^{y} + \rho_z \delta z_k \psi_{i,j,k}^{z} \\ &+ \rho_x\rho_y \delta x_i \delta y_j \psi_{i,j,k}^{xy} + \rho_y\rho_z \delta y_j \delta z_k \psi_{i,j,k}^{yz} + \rho_x\rho_z \delta x_i \delta z_k \psi_{i,j,k}^{xz} \\ &+ \rho_{xx}\delta x_i^2 \psi_{i,j,k}^{xx} + \rho_{yy}\delta y_j^2 \psi_{i,j,k}^{yy} + \rho_{zz}\delta z_k^2 \psi_{i,j,k}^{zz}\big], \end{aligned} \tag{3.2}$$

where $\rho_x, \rho_y, \rho_z, \rho_{xx}, \rho_{yy}, \rho_{zz}$ are non-zero finite real constants, whose values are computed in such a way that the resulting difference scheme yields high order of local truncation error. The notations $\psi_{i,j,k} \equiv \psi(x_i, y_j, z_k) = U^{xx}_{i,j,k} + U^{yy}_{i,j,k} + U^{zz}_{i,j,k}$, $\psi^{x}_{i,j,k} = (\partial\psi/\partial x)_{(x_i,y_j,z_k)}$, $\psi^{xx}_{i,j,k} = (\partial^2\psi/\partial x^2)_{(x_i,y_j,z_k)}$, etc. are adopted for simplicity in presentation.

The application of difference operator formulas (2.10)–(2.11) and their composites on $\psi_{i,j,k}$ in equation (3.1) and linear combination (3.2) results in the following value of constants:

$$\begin{aligned}
&\rho_x = (p-1)/3, \qquad \rho_y = (q-1)/3, \qquad \rho_z = (r-1)/3, \\
&\rho_{xx} = \bigl(p^2 - p + 1\bigr)/3, \qquad \rho_{yy} = \bigl(q^2 - q + 1\bigr)/3, \qquad \rho_{zz} = \bigl(r^2 - r + 1\bigr)/3.
\end{aligned}$$

Now, replacing the partial derivatives by the compact difference operators

$$\begin{bmatrix} \psi^{x}_{i,j,k} \\ \psi^{y}_{i,j,k} \\ \psi^{z}_{i,j,k} \end{bmatrix} = \begin{bmatrix} \delta x_i^{-1}\mathcal{A}_x \\ \delta y_j^{-1}\mathcal{A}_y \\ \delta z_k^{-1}\mathcal{A}_z \end{bmatrix} \psi_{i,j,k}, \qquad \begin{bmatrix} \psi^{xx}_{i,j,k} \\ \psi^{yy}_{i,j,k} \\ \psi^{zz}_{i,j,k} \end{bmatrix} = \begin{bmatrix} \delta x_i^{-2}\mathcal{B}_x \\ \delta y_j^{-2}\mathcal{B}_x \\ \delta z_k^{-2}\mathcal{B}_x \end{bmatrix} \psi_{i,j,k} \tag{3.3}$$

and

$$\begin{bmatrix} \psi^{xy}_{i,j,k} \\ \psi^{yz}_{i,j,k} \\ \psi^{xz}_{i,j,k} \end{bmatrix} = \begin{bmatrix} \delta x_i^{-1}\delta y_j^{-1}\mathcal{A}_x\mathcal{A}_y \\ \delta y_j^{-1}\delta z_k^{-1}\mathcal{A}_y\mathcal{A}_z \\ \delta x_i^{-1}\delta z_k^{-1}\mathcal{A}_x\mathcal{A}_z \end{bmatrix} \psi_{i,j,k}, \tag{3.4}$$

in the linear combination (3.2), the exponential expanding grids finite-difference substitute for Poisson's equation (3.1) in three dimensions is obtained by the discrete relation

$$\epsilon\mathcal{L}\{U_{i,j,k}\} = \delta x_i^2\delta y_j^2\delta z_k^2\Biggl[\sum_{(l,m,n)\in\mathcal{M}} \mathcal{S}_{l,m,n}\psi_{l,m,n} + T_{i,j,k}\Biggr], \tag{3.5}$$

where summation runs over the set $\mathcal{M} = \{i, i+1, i-1\} \times \{j, j+1, j-1\} \times \{k, k+1, k-1\} \sim \{(i\pm 1, j\pm 1, k\pm 1)\}$. The discrete Laplacian as a sum of nearest neighbors of the central grid point is given by

$$\begin{aligned}
\mathcal{L} \equiv{}& \frac{\epsilon}{12}\delta y_j^2\delta z_k^2\bigl[\bigl\{\delta x_i^2\alpha^2\bigl(p^2-p+1\bigr)+12\bigr\}\mathcal{B}_x + 4(q-1)\mathcal{B}_x\mathcal{A}_y\bigr] \\
&+ \frac{\epsilon}{12}\delta x_i^2\delta z_k^2\bigl[\bigl\{\delta y_j^2\beta^2\bigl(q^2-q+1\bigr)+12\bigr\}\mathcal{B}_y + 4(r-1)\mathcal{B}_y\mathcal{A}_z\bigr] \\
&+ \frac{\epsilon}{12}\delta x_i^2\delta y_j^2\bigl[\bigl\{\delta z_k^2\gamma^2\bigl(r^2-r+1\bigr)+12\bigr\}\mathcal{B}_z + 4(p-1)\mathcal{B}_z\mathcal{A}_x\bigr] \\
&+ \frac{\epsilon}{9}\delta x_i^2\delta y_j^2\delta z_k^2\bigl[3\alpha^2(p-1)\mathcal{A}_x + \bigl(\alpha^2+\beta^2\bigr)(p-1)(q-1)\mathcal{A}_x\mathcal{A}_y\bigr] \\
&+ \frac{\epsilon}{9}\delta x_i^2\delta y_j^2\delta z_k^2\bigl[3\beta^2(q-1)\mathcal{A}_y + \bigl(\alpha^2+\gamma^2\bigr)(p-1)(r-1)\mathcal{A}_x\mathcal{A}_z\bigr] \\
&+ \frac{\epsilon}{9}\delta x_i^2\delta y_j^2\delta z_k^2\bigl[3\gamma^2(r-1)\mathcal{A}_z + \bigl(\beta^2+\gamma^2\bigr)(q-1)(r-1)\mathcal{A}_y\mathcal{A}_z\bigr] \\
&+ \frac{\epsilon}{12}\delta z_k^2\bigl[\bigl(1-p+p^2\bigr)\delta x_i^2 + \bigl(1-q+q^2\bigr)\delta y_j^2\bigr]\mathcal{B}_x\mathcal{B}_y \\
&+ \frac{\epsilon}{12}\delta y_j^2\bigl[\bigl(1-p+p^2\bigr)\delta x_i^2 + \bigl(1-r+r^2\bigr)\delta z_k^2\bigr]\mathcal{B}_x\mathcal{B}_z \\
&+ \frac{\epsilon}{12}\delta x_i^2\bigl[\bigl(1-r+r^2\bigr)\delta z_k^2 + \bigl(1-q+q^2\bigr)\delta y_j^2\bigr]\mathcal{B}_y\mathcal{B}_z
\end{aligned}$$

$$
\begin{aligned}
&+ \frac{\epsilon}{9}(r-1)\delta y_j^2 \delta z_k^2\big[(q-1)\mathcal{B}_x\mathcal{A}_y\mathcal{A}_z + 3\mathcal{B}_x\mathcal{A}_z\big] \\
&+ \frac{\epsilon}{9}(p-1)\delta x_i^2 \delta z_k^2\big[(r-1)\mathcal{B}_y\mathcal{A}_x\mathcal{A}_z + 3\mathcal{B}_y\mathcal{A}_x\big] \\
&+ \frac{\epsilon}{9}(q-1)\delta y_j^2 \delta x_i^2\big[(p-1)\mathcal{B}_z\mathcal{A}_y\mathcal{A}_x + 3\mathcal{B}_z\mathcal{A}_y\big]
\end{aligned}
\tag{3.6}
$$

and

$$
\begin{aligned}
\mathcal{S}_{i+1,j,k} &= \rho_x a_{100}^{000}\big(1+\rho_y b_{000}^{000}+\rho_z c_{000}^{000}\big)+\rho_{xx} d_{100}^{000}, \\
\mathcal{S}_{i-1,j,k} &= \rho_x a_{200}^{000}\big(1+\rho_y b_{000}^{000}+\rho_z c_{000}^{000}\big)+\rho_{xx} d_{200}^{000}, \\
\mathcal{S}_{i,j+1,k} &= \rho_y b_{010}^{000}\big(1+\rho_x a_{000}^{000}+\rho_z c_{000}^{000}\big)+\rho_{yy} e_{010}^{000}, \\
\mathcal{S}_{i,j-1,k} &= \rho_y b_{020}^{000}\big(1+\rho_x a_{000}^{000}+\rho_z c_{000}^{000}\big)+\rho_{yy} e_{020}^{000}, \\
\mathcal{S}_{i,j,k+1} &= \rho_z c_{001}^{000}\big(1+\rho_x a_{000}^{000}+\rho_y b_{000}^{000}\big)+\rho_{zz} f_{001}^{000}, \\
\mathcal{S}_{i,j,k-1} &= \rho_z c_{002}^{000}\big(1+\rho_x a_{000}^{000}+\rho_y b_{000}^{000}\big)+\rho_{zz} f_{002}^{000}, \\
\mathcal{S}_{i+1,j+1,k} &= \rho_x\rho_y a_{100}^{000}b_{010}^{000}, \mathcal{S}_{i+1,j,k+1} = \rho_x\rho_z a_{100}^{000}c_{001}^{000}, \mathcal{S}_{i,j+1,k+1} = \rho_y\rho_z b_{010}^{000}c_{001}^{000}, \\
\mathcal{S}_{i-1,j+1,k} &= \rho_x\rho_y a_{200}^{000}b_{010}^{000}, \mathcal{S}_{i+1,j,k-1} = \rho_x\rho_z a_{100}^{000}c_{002}^{000}, \mathcal{S}_{i,j+1,k-1} = \rho_y\rho_z b_{010}^{000}c_{002}^{000}, \\
\mathcal{S}_{i-1,j-1,k} &= \rho_x\rho_y a_{200}^{000}b_{020}^{000}, \mathcal{S}_{i,j-1,k+1} = \rho_y\rho_z b_{020}^{000}c_{001}^{000}, \mathcal{S}_{i+1,j-1,k} = \rho_x\rho_y a_{100}^{000}b_{020}^{000}, \\
\mathcal{S}_{i-1,j,k+1} &= \rho_x\rho_z a_{200}^{000}c_{001}^{000}, \mathcal{S}_{i,j-1,k-1} = \rho_y\rho_z b_{020}^{000}c_{002}^{000}, \mathcal{S}_{i-1,j,k-1} = \rho_x\rho_z a_{200}^{000}c_{002}^{000}, \\
\mathcal{S}_{i,j,k} &= 1+\rho_x a_{000}^{000}\big(1+\rho_y b_{000}^{000}\big)+\rho_y b_{000}^{000}\big(1+\rho_z c_{000}^{000}\big)+\rho_z c_{000}^{000}\big(1+\rho_x a_{000}^{000}\big) \\
&\quad + \rho_{xx} d_{000}^{000}+\rho_{yy} e_{000}^{000}+\rho_{zz} f_{000}^{000}.
\end{aligned}
$$

The values of coefficients are given by

$$
\begin{aligned}
& a_{100}^{000} = \phi_1(\alpha,\delta x_i)/\varphi(p,\alpha,\delta x_i), \qquad a_{200}^{000} = \phi_2(p,\alpha,\delta x_i)/\varphi(p,\alpha,\delta x_i), \\
& b_{010}^{000} = \phi_1(\beta,\delta y_j)/\varphi(q,\beta,\delta y_j), \qquad b_{020}^{000} = \phi_2(q,\beta,\delta y_j)/\varphi(q,\beta,\delta y_j), \\
& c_{001}^{000} = \phi_1(\gamma,\delta z_k)/\varphi(r,\gamma,\delta z_k), \qquad c_{002}^{000} = \phi_2(r,\gamma,\delta z_k)/\varphi(r,\gamma,\delta z_k), \\
& d_{100}^{000} = \phi_3(\alpha,\delta x_i)/\varphi(p,\alpha,\delta x_i), \qquad d_{200}^{000} = \phi_4(p,\alpha,\delta x_i)/\varphi(p,\alpha,\delta x_i), \\
& e_{010}^{000} = \phi_3(\beta,\delta y_j)/\varphi(q,\beta,\delta y_j), \qquad e_{020}^{000} = \phi_4(q,\beta,\delta y_j)/\varphi(q,\beta,\delta y_j), \\
& f_{001}^{000} = \phi_3(\gamma,\delta z_k)/\varphi(r,\gamma,\delta z_k), \qquad f_{002}^{000} = \phi_4(r,\gamma,\delta z_k)/\varphi(r,\gamma,\delta z_k), \\
& a_{000}^{000} = -\big(a_{100}^{000}+a_{200}^{000}\big), \qquad b_{000}^{000} = -\big(b_{010}^{000}+b_{020}^{000}\big), \qquad c_{000}^{000} = -\big(c_{001}^{000}+c_{002}^{000}\big), \\
& d_{000}^{000} = -\big(d_{100}^{000}+d_{200}^{000}\big), \qquad e_{000}^{000} = -\big(e_{010}^{000}+e_{020}^{000}\big), \qquad f_{000}^{000} = -\big(f_{001}^{000}+f_{002}^{000}\big),
\end{aligned}
$$

and truncation error is obtained as

$$
T_{i,j,k} = \begin{cases} O(\delta x_i+\delta y_j+\delta z_k)^3, & p\neq 1 \vee q\neq 1 \vee r\neq 1, \\ O(\delta x_i+\delta y_j+\delta z_k)^4, & p=q=r=1. \end{cases}
\tag{3.7}
$$

The truncation error of the nineteen-point scheme (3.5) confers third-order and fourth-order accuracy on exponential expanding and uniformly distributed grids respectively in a single formulation. Since the grid step sizes $\delta x_i, \delta y_j, \delta z_k$ are positive real values, the linear dependence of two real numbers yields $\delta y_j = \zeta_{i,j}\delta x_i$ and $\delta z_k = \eta_{i,k}\delta x_i$ for some finite constants $\zeta_{i,j}$, $\eta_{i,k}$, known as grid-ratio parameters. As a result, the truncation error $T_{i,j,k} \approx O(\delta x_i^3)$ resembles third-order accuracy on exponential expanding grids and $T_{i,j,k} \approx O(\delta x_i^4)$ presents fourth-order accuracy on uniformly distributed grids. Moreover, the new scheme is developed on a minimum number of stencils in each coordinate direction to discretize the maximum order differentials present in elliptic PDEs (1.1); thus it is compact and can be easily computed.

Next, we shall extend our scheme (3.5) to the mildly nonlinear elliptic PDEs (1.1) that involve first-order partial derivatives implicitly as a nonlinear term. For this purpose, we require some functional approximations on the set $\overline{\mathcal{M}} = \mathcal{M} \sim \{(i,j,k)\}$ defined by

$$\tilde{\psi}_{l,m,n} = \psi\left(x_l, y_m, z_n, U_{l,m,n}, \tilde{U}^x_{l,m,n}, \tilde{U}^y_{l,m,n}, \tilde{U}^z_{l,m,n}\right), \quad (l,m,n) \in \overline{\mathcal{M}}. \tag{3.8}$$

New estimates of the first-order partial derivative at a central grid point are constructed as follows:

$$\begin{aligned} \hat{U}^x_{i,j,k} &= \tilde{U}^x_{i,j,k} + \vartheta_x \delta x_i \left[\tilde{\psi}_{i+1,j,k} - \tilde{\psi}_{i-1,j,k} - \epsilon\alpha^2 (U_{i+1,j,k} - U_{i-1,j,k}) \right. \\ &\quad \left. - \epsilon\left(\tilde{U}^{yy}_{i+1,j,k} - \tilde{U}^{yy}_{i-1,j,k}\right) - \epsilon\left(\tilde{U}^{zz}_{i+1,j,k} - \tilde{U}^{zz}_{i-1,j,k}\right)\right], \end{aligned} \tag{3.9}$$

$$\begin{aligned} \hat{U}^y_{i,j,k} &= \tilde{U}^y_{i,j,k} + \vartheta_y \delta y_j \left[\tilde{\psi}_{i,j+1,k} - \tilde{\psi}_{i,j-1,k} - \epsilon\beta^2 (U_{i,j+1,k} - U_{i,j-1,k}) \right. \\ &\quad \left. - \epsilon\left(\tilde{U}^{zz}_{i,j+1,k} - \tilde{U}^{zz}_{i,j-1,k}\right) - \epsilon\left(\tilde{U}^{xx}_{i,j+1,k} - \tilde{U}^{xx}_{i,j-1,k}\right)\right], \end{aligned} \tag{3.10}$$

$$\begin{aligned} \hat{U}^z_{i,j,k} &= \tilde{U}^z_{i,j,k} + \vartheta_z \delta z_k \left[\tilde{\psi}_{i,j,k+1} - \tilde{\psi}_{i,j,k-1} - \epsilon\gamma^2 (U_{i,j,k+1} - U_{i,j,k-1}) \right. \\ &\quad \left. - \epsilon\left(\tilde{U}^{xx}_{i,j,k+1} - \tilde{U}^{xx}_{i,j,k-1}\right) - \epsilon\left(\tilde{U}^{yy}_{i,j,k+1} - \tilde{U}^{yy}_{i,j,k-1}\right)\right], \end{aligned} \tag{3.11}$$

and the updated functional at a central grid point is given by

$$\hat{\psi}_{i,j,k} = \psi\left(x_i, y_j, z_k, U_{i,j,k}, \hat{U}^x_{i,j,k}, \hat{U}^y_{i,j,k}, \hat{U}^z_{i,j,k}\right). \tag{3.12}$$

Here, ϑ_x, ϑ_y, and ϑ_z are free parameters, and their value will be determined in such a manner that the resulting difference formula yields an order of optimal accuracy. With the help of (3.5), (3.8), and (3.12), it is possible to obtain

$$\mathcal{S}_{i,j,k}\hat{\psi}_{i,j,k} + \sum_{(l,m,n)\in\overline{\mathcal{M}}} \mathcal{S}_{l,m,n}\tilde{\psi}_{l,m,n} - \sum_{(l,m,n)\in\mathcal{M}} \mathcal{S}_{l,m,n}\psi_{l,m,n} = T_{i,j,k}, \tag{3.13}$$

provided

$$\begin{aligned} \vartheta_x &= pqr\left(p^2 + p + 1\right)/\left[2\epsilon\tau(p+1)\right], \\ \vartheta_y &= pqr\left(q^2 + q + 1\right)/\left[2\epsilon\tau(q+1)\right], \\ \vartheta_z &= pqr\left(r^2 + r + 1\right)/\left[2\epsilon\tau(r+1)\right], \end{aligned}$$

where

$$\tau = 2(q+r)p^2 + 2(r+p)q^2 + 2(q+p)r^2 - (5r-2)p - (5p-2)q$$

$$- (5q - 2)r + pqr\big[2(pq + rq + pr) - 5(p + q + r) + 15\big].$$

This gives the new difference scheme

$$\epsilon\mathcal{L}\{U_{i,j,k}\} = \delta x_i^2 \delta y_j^2 \delta z_k^2 \Bigg[\mathcal{S}_{i,j,k}\hat{\psi}_{i,j,k} + \sum_{(l,m,n)\in\overline{\mathcal{M}}} \mathcal{S}_{l,m,n}\tilde{\psi}_{l,m,n} + T_{i,j,k}\Bigg]. \tag{3.14}$$

The nineteen-point extended compact finite-difference replacement (3.14) for approximating elliptic PDEs (1.1) exhibits truncation error of order three on the exponential expanding grid network, and it is fourth-order accurate on uniformly distributed grid points. The compact character of the updated scheme remains intact on either grid spacing, may be evenly spaced or unequally spaced, and can be implemented through single high accuracy formulation. The computer implementation of scheme (3.14) may be obtained after omitting the truncation error term $T_{i,j,k}$ and making use of the following boundary data:

$$U_{0,j,k} = f_1(y_j, z_k), \qquad U_{I+1,j,k} = f_2(y_j, z_k), \quad 0 \le j \le J + 1, 0 \le k \le K + 1, \tag{3.15a}$$

$$U_{i,0,k} = f_3(x_i, z_k), \qquad U_{i,J+1,k} = f_4(x_i, z_k), \quad 0 \le i \le I + 1, 0 \le j \le J + 1, \tag{3.15b}$$

$$U_{i,j,0} = f_5(x_i, y_j), \qquad U_{i,j,K+1} = f_6(x_i, y_j), \quad 0 \le i \le I + 1, 0 \le j \le J + 1. \tag{3.15c}$$

By incorporating the boundary data in the system of nonlinear difference equations (3.14), the Jacobian matrix yields block-block- tri-diagonal matrix, and it can be computed by Newton's iterative method. In case the function ψ is linear, the application of the Gauss–Seidel iterative algorithm is a suitable choice. The compact difference equation (3.14) represents four types of high-order replacement to the mildly nonlinear elliptic PDEs (1.1). When exponential fitting parameters $\alpha, \beta, \gamma \to 0$, it yields a uniform mesh fourth-order compact scheme (UM-FOCS) for the mesh parameters $p = q = r = 1$, and an exponential expanding grid third-order compact scheme (EEG-TOCS) for the mesh parameters $p \neq 1 \vee q \neq 1 \vee r \neq 1$. If the exponential fitting parameters α, β, γ are not sufficiently small, it is an exponential fitted fourth-order compact scheme (EF-FOCS) on uniformly spaced grid points and an exponential fitted third-order compact scheme (EF-EEG-TOCS) on the exponential expanding grid network.

4 Convergence analysis and bounds of discretization errors

We shall investigate the monotone and irreducible property of the Jacobian iteration matrix derived from the compact scheme (3.14) and obtain bounds of discretization error. The convergence of the scheme will follow from the fact that point-wise errors in exact and approximate solution approach to zero for sufficiently small grid step sizes. *To reduce the algebraic complexity,* we shall assume that $r \neq 1$ for maintaining exponential expanding nature of grids in z-direction and $p = q = 1$, making equally spaced grids in x- and y-direction. Therefore, we can assume $\delta x_i = \delta y_j \approx \mu_k \delta z_k$ in the following analysis. The nonlinear elliptic PDEs (1.1) at each grid point (x_i, y_j, z_k) are represented by

$$\epsilon\left(U^{xx}_{i,j,k} + U^{yy}_{i,j,k} + U^{zz}_{i,j,k}\right) = \psi\left(x_i, y_j, z_k, U_{i,j,k}, U^{x}_{i,j,k}, U^{y}_{i,j,k}, U^{z}_{i,j,k}\right). \tag{4.1}$$

The third-order accurate compact discretization (3.14) is the system of nonlinear difference equations

$$\mathcal{F}_{i,j,k} + O\big(\delta z_k^5\big) = 0, \quad 1 \le i \le I, 1 \le j \le J, 1 \le k \le K, \tag{4.2}$$

where

$$\mathcal{F}_{i,j,k} = -\epsilon \delta y_j^{-2} \delta z_k^{-2} \mathcal{L}\{U_{i,j,k}\} + \delta x_i^2 \Bigg[\mathcal{S}_{i,j,k} \hat{\psi}_{i,j,k} + \sum_{(l,m,n)\in\overline{\mathcal{M}}} \mathcal{S}_{l,m,n} \tilde{\psi}_{l,m,n} \Bigg].$$

The discrete equations (4.2) equate the mildly nonlinear equation (4.1) with local truncation accuracy of order three, since $r \neq 1$. If we denote approximate solution value of the differential equation (4.1) by $u_{i,j,k}$, then $\mathcal{E}_{i,j,k} = U_{i,j,k} - u_{i,j,k}$ is referred to as point-wise solution error at the grid point (x_i, y_j, z_k). As a notational ease, the vector $\boldsymbol{\mathcal{G}} = \boldsymbol{\mathcal{E}}, \boldsymbol{T}, \boldsymbol{U}, \boldsymbol{u}, \boldsymbol{\mathcal{F}}$ in lexical order is defined as

$$\begin{aligned}
\boldsymbol{\mathcal{G}} = {} & [\mathcal{G}_{111}, \mathcal{G}_{121}, \dots, \mathcal{G}_{1J1}, \mathcal{G}_{211}, \mathcal{G}_{221}, \dots, \mathcal{G}_{2J1}, \dots, \mathcal{G}_{I11}, \mathcal{G}_{I21}, \dots, \mathcal{G}_{IJ1}, \\
& \mathcal{G}_{112}, \mathcal{G}_{122}, \dots, \mathcal{G}_{1J2}, \mathcal{G}_{212}, \mathcal{G}_{222}, \dots, \mathcal{G}_{2J2}, \dots, \mathcal{G}_{I12}, \mathcal{G}_{I22}, \dots, \mathcal{G}_{IJ2}, \\
& \vdots \\
& \mathcal{G}_{11K}, \mathcal{G}_{12K}, \dots, \mathcal{G}_{1JK}, \mathcal{G}_{21K}, \mathcal{G}_{22K}, \dots, \mathcal{G}_{2JK}, \dots, \mathcal{G}_{I1K}, \mathcal{G}_{I2K}, \dots, \mathcal{G}_{IJK}]^{\mathrm{T}}.
\end{aligned}$$

The matrix representation of the difference equation (4.2) is given by

$$\boldsymbol{\mathcal{F}}(\boldsymbol{U}) + \boldsymbol{T} = \mathbf{0}_{IJK\times IJK}, \tag{4.3}$$

where $\boldsymbol{T}$ is a vector of fifth-order truncation error in the approximate scheme (4.2). For the numerical solution, we drop the truncation error $\boldsymbol{T}$ and receive approximate solution vector $\boldsymbol{u}$ that satisfies

$$\boldsymbol{\mathcal{F}}(\boldsymbol{u}) = \mathbf{0}_{IJK\times IJK}. \tag{4.4}$$

Like approximations (3.8) and (3.12) defined for the exact solution, we can measure the function ψ with approximate solution values by defining

$$\tilde{\psi}_{l,m,n} = \psi\left(x_l, y_m, z_n, u_{l,m,n}, \tilde{u}^x_{l,m,n}, \tilde{u}^y_{l,m,n}, \tilde{u}^z_{l,m,n}\right) \approx \Psi_{l,m,n}, \quad (l,m,n) \in \overline{\mathcal{M}}, \tag{4.5}$$

and

$$\hat{\psi}_{i,j,k} = \psi\left(x_i, y_j, z_k, u_{i,j,k}, \hat{u}^x_{i,j,k}, \hat{u}^y_{i,j,k}, \hat{u}^z_{i,j,k}\right) \approx \Psi_{i,j,k}. \tag{4.6}$$

In this way, we can compute the difference of exact and estimated functional values as

$$\tilde{\Gamma}_{l,m,n} = \tilde{\psi}_{l,m,n} - \Psi_{l,m,n}, \quad (l,m,n) \in \overline{\mathcal{M}}, \qquad \hat{\mathcal{E}}_{i,j,k} = \hat{\psi}_{i,j,k} - \Psi_{i,j,k}. \tag{4.7}$$

This implies

$$\begin{aligned}\tilde{\Gamma}_{l,m,n} &= \psi\big(x_l, y_m, z_n, u_{l,m,n}, \tilde{u}^x_{l,m,n}, \tilde{u}^y_{l,m,n}, \tilde{u}^z_{l,m,n}\big) \\ &\quad - \psi\big(x_i, y_j, z_k, U_{l,m,n}, \tilde{U}^x_{l,m,n}, \tilde{U}^y_{l,m,n}, \tilde{U}^z_{l,m,n}\big) \\ &= \psi\big(x_l, y_m, z_n, u_{l,m,n}, \tilde{u}^x_{l,m,n}, \tilde{u}^y_{l,m,n}, \tilde{u}^z_{l,m,n}\big) \\ &\quad - \psi\big(x_l, y_m, z_n, u_{l,m,n} + \mathcal{E}_{l,m,n}, \tilde{u}^x_{l,m,n} + \tilde{\mathcal{E}}^x_{l,m,n}, \tilde{u}^y_{l,m,n} + \tilde{\mathcal{E}}^y_{l,m,n}, \tilde{u}^z_{l,m,n} + \tilde{\mathcal{E}}^z_{l,m,n}\big).\end{aligned} \tag{4.8}$$

Expanding the function ψ containing point-wise error $\mathcal{E}_{l,m,n}$ and its derivatives, we obtain

$$\tilde{\Gamma}_{l,m,n} = A_{l,m,n}\mathcal{E}_{l,m,n} + B_{l,m,n}\tilde{\mathcal{E}}^x_{l,m,n} + C_{l,m,n}\tilde{\mathcal{E}}^y_{l,m,n} + D_{l,m,n}\tilde{\mathcal{E}}^z_{l,m,n} + O\big(\mathcal{E}^2_{l,m,n}\big), \tag{4.9}$$

where $A_{l,m,n} = -(\partial\psi/\partial u_{l,m,n})$, $B_{l,m,n} = -(\partial\psi/\partial\tilde{u}^x_{l,m,n})$, $C_{l,m,n} = -(\partial\psi/\partial\tilde{u}^y_{l,m,n})$, and $D_{l,m,n} = -(\partial\psi/\partial\tilde{u}^z_{l,m,n})$ are finite real constants. Dropping the $O(\mathcal{E}^2_{l,m,n})$ terms from equation (4.9) does not affect the error analysis, because we will take $\mathcal{E}_{l,m,n} \to 0$ later, and in that case $O(\mathcal{E}^2_{l,m,n})$ automatically vanishes. Hence, it is enough to write (4.9) as

$$\tilde{\Gamma}_{l,m,n} = A_{l,m,n}\mathcal{E}_{l,m,n} + B_{l,m,n}\tilde{\mathcal{E}}^x_{l,m,n} + C_{l,m,n}\tilde{\mathcal{E}}^y_{l,m,n} + D_{l,m,n}\tilde{\mathcal{E}}^z_{l,m,n}. \tag{4.10}$$

Similarly, the error equation at the central grid point is given by

$$\hat{\Gamma}_{i,j,k} = A_{i,j,k}\mathcal{E}_{i,j,k} + B_{i,j,k}\hat{\mathcal{E}}^x_{i,j,k} + C_{i,j,k}\hat{\mathcal{E}}^y_{i,j,k} + D_{i,j,k}\hat{\mathcal{E}}^z_{i,j,k}. \tag{4.11}$$

Explicit expressions for $\tilde{\mathcal{E}}^x_{l,m,n}, \tilde{\mathcal{E}}^y_{l,m,n}, \tilde{\mathcal{E}}^z_{l,m,n}$ and $\hat{\mathcal{E}}^x_{i,j,k}, \hat{\mathcal{E}}^y_{i,j,k}, \hat{\mathcal{E}}^z_{i,j,k}$ are determined from approximations (2.4)–(2.6) and (3.9)–(3.11) respectively upon replacing U by $\mathcal{E}$. In this way, we obtain a system of discrete equations for discretization errors as follows:

$$\begin{aligned}&\boldsymbol{\mathcal{F}}(\boldsymbol{u}) - \boldsymbol{\mathcal{F}}(\boldsymbol{U}) \\ &\quad = \Bigg[-\epsilon\,\delta y_j^{-2}\delta z_k^{-2}\mathcal{L}\{\mathcal{E}_{i,j,k}\} \\ &\qquad + \delta x_i^2\Bigg[\mathcal{S}_{i,j,k}\hat{\Gamma}_{i,j,k} + \sum_{(l,m,n)\in\overline{\mathcal{M}}}\mathcal{S}_{l,m,n}\tilde{\Gamma}_{l,m,n}\Bigg]\Bigg]_{i=1(1)I,j=1(1)J,k=1(1)K};\end{aligned} \tag{4.12}$$

that is,

$$\boldsymbol{\mathcal{F}}(\boldsymbol{u}) - \boldsymbol{\mathcal{F}}(\boldsymbol{U}) = \boldsymbol{\mathcal{H}}\boldsymbol{\mathcal{E}}. \tag{4.13}$$

Now, combining equations (4.3), (4.4), and (4.13), one obtains

$$\boldsymbol{\mathcal{H}}\boldsymbol{\mathcal{E}} = \boldsymbol{T}, \tag{4.14}$$

where $\boldsymbol{\mathcal{H}} = [\mathcal{H}_{l,m}], l,m = 1(1)IJK$ is a block-block tri-diagonal matrix. Since the convergence is analyzed in the limiting case, when $\max_k \delta z_k \to 0$, the block-block tri-diagonal coefficient matrix is estimated to be $\boldsymbol{\mathcal{H}} = [\boldsymbol{\mathcal{H}_l}\ \boldsymbol{\mathcal{H}_m}\ \boldsymbol{\mathcal{H}_u}]$, where $\boldsymbol{\mathcal{H}_l} = [\boldsymbol{\mathcal{H}^l_l}\ \boldsymbol{\mathcal{H}^l_m}\ \boldsymbol{\mathcal{H}^l_u}]$, $\boldsymbol{\mathcal{H}_m} =$

$[\boldsymbol{\mathcal{H}_l^m}\ \boldsymbol{\mathcal{H}_m^m}\ \boldsymbol{\mathcal{H}_u^m}]$, and $\boldsymbol{\mathcal{H}_u} = [\boldsymbol{\mathcal{H}_l^u}\ \boldsymbol{\mathcal{H}_m^u}\ \boldsymbol{\mathcal{H}_u^u}]$. Here, the bold subscript and superscript $(\boldsymbol{l}, \boldsymbol{m}, \boldsymbol{u})$ represent the lower, main, and upper tri-diagonal or block-tri-diagonal matrices. The finite-order Taylor series expansion to the elements of each tri-diagonal matrices results in the following form:

$$\begin{aligned}
\boldsymbol{\mathcal{H}_l^l} &= \boldsymbol{\mathcal{H}_u^l} = \left[0, -\frac{\mu_k^2 - r^2 + r + 1}{r+1} + O(\delta z_k), 0\right], \\
\boldsymbol{\mathcal{H}_m^l} &= \left[-\frac{\mu_k^2 - r^2 + r + 1}{r+1} + O(\delta z_k), -\frac{4(2\mu_k^2 + r^2 - r - 1)}{r+1} + O(\delta z_k), \right. \\
&\quad \left. -\frac{\mu_k^2 - r^2 + r + 1}{r+1} + O(\delta z_k)\right], \\
\boldsymbol{\mathcal{H}_l^m} &= \boldsymbol{\mathcal{H}_u^m} = \left[-1 + O(\delta z_k), -\frac{-\mu_k^2 + r^2 + r + 1}{r} + O(\delta z_k), -1 + O(\delta z_k)\right], \\
\boldsymbol{\mathcal{H}_m^m} &= \left[-\frac{-\mu_k^2 + r^2 + r + 1}{r} + O(\delta z_k), \frac{4\{2\mu_k^2 + (r+1)^2\}}{r} + O(\delta z_k), \right. \\
&\quad \left. -\frac{-\mu_k^2 + r^2 + r + 1}{r} + O(\delta z_k)\right], \\
\boldsymbol{\mathcal{H}_l^u} &= \boldsymbol{\mathcal{H}_u^u} = \left[0, -\frac{\mu_k^2 + r^2 + r - 1}{r(r+1)} + O(\delta z_k), 0\right], \\
\boldsymbol{\mathcal{H}_m^u} &= \left[-\frac{\mu_k^2 + r^2 + r - 1}{r(r+1)} + O(\delta z_k), -\frac{4\{2\mu_k^2 - r^2 - r + 1\}}{r(r+1)} + O(\delta z_k), \right. \\
&\quad \left. -\frac{\mu_k^2 + r^2 + r - 1}{r(r+1)} + O(\delta z_k)\right].
\end{aligned}$$

The main diagonal elements $4\{2\mu_k^2 + (r+1)^2\}/r + O(\delta z_k)$ of the matrix $\boldsymbol{\mathcal{H}}$ are positive in the limiting value of $\delta z_k \to 0$ for all k, since the grid expansion parameter r and the grid-ratio parameter μ_k are positive real numbers. Also, all of non-diagonal entries are either zero or negative provided $|r - \sqrt{5}/2| < 1/2$ and $\max_r\{(1 + r - r^2)/2, (-1 + r + r^2)/2\} \leq \mu_k^2 \leq 1 + r + r^2$. The positive diagonal entries and non-positive off-diagonal entries of the matrix $\boldsymbol{\mathcal{H}}$ make it irreducible, and it can be visualized via the connected graph associated with the matrix $\boldsymbol{\mathcal{H}}$. With a prescribed set of IJK distinct points in a plane, draw a directed line segment from point l to m for each non-zero entry $\mathcal{H}_{l,m}$ in the matrix $\boldsymbol{\mathcal{H}}$. In this way, we observe that the two distinct locations represented by the points l and m are either directly connected or there is a finite number of directed line segments that join them. This proves the strongly connected property of the graph of matrix $\boldsymbol{\mathcal{H}}$. As a consequence, the matrix $\boldsymbol{\mathcal{H}}$ is irreducible [14, 40, 45].

Next, we will prove that the real square matrix $\boldsymbol{\mathcal{H}}$ is monotone. Given that the matrix $\boldsymbol{\mathcal{H}}$ contains either zero or negative real values at non-diagonal and positive main diagonal elements, it suffices to establish the weak row elements sum criterion. For this purpose, we suppose $A = \min A_{i,j,k}, B = \min B_{i,j,k}, C = \min C_{i,j,k}, D = \min D_{i,j,k}, i = 1(1)I, j = 1(1)J, k = 1(1)K$. Let ϑ_l $(l = 1(1)IJK)$ be the sum of elements from each lth row in the irreducible matrix $\boldsymbol{\mathcal{H}}$. For sufficiently small grid step size (assuming $\delta z = \max_k \delta z_k$) and $|r - \sqrt{5}/2| < 1/2$, one finds

$$\vartheta_1 \geq \lambda_1 > 0, \qquad \vartheta_l \geq \lambda_2 > 0, \quad l = 2(1)I - 1, \qquad \vartheta_I \geq \lambda_3 > 0,$$

$m = 2(1)J-1$:

$$\vartheta_{I(m-1)+1} \geq \lambda_4 > 0, \qquad \vartheta_{I(m-1)+l} \geq \lambda_5 > 0, \quad l = 2(1)I-1, \qquad \vartheta_{I(m-1)+I} \geq \lambda_6 > 0,$$

$$\vartheta_{I(J-1)+1} \geq \lambda_7 > 0, \qquad \vartheta_{I(J-1)+l} \geq \lambda_8 > 0, \quad l = 2(1)I-1, \qquad \vartheta_{I(J-1)+I} \geq \lambda_9 > 0,$$

$n = 2(1)K-1$:

$$\vartheta_{(n-1)JI+1} \geq \lambda_{10} > 0, \qquad \vartheta_{(n-1)JI+l} \geq \lambda_{11} > 0, \quad l = 2(1)I-1,$$

$$\vartheta_{(n-1)JI+I} \geq \lambda_{12} > 0,$$

$m = 2(1)J-1$:

$$\vartheta_{(n-1)JI+(m-1)I+1} \geq \lambda_{13} > 0,$$

$$\vartheta_{(n-1)JI+(m-1)I+l} \geq \lambda_{14} \geq 0, \quad l = 2(1)I-1, \qquad \vartheta_{(n-1)JI+(m-1)I+I} \geq \lambda_{15} > 0,$$

$$\vartheta_{(n-1)JI+I(J-1)+1} \geq \lambda_{16} > 0,$$

$$\vartheta_{(n-1)JI+I(J-1)+l} \geq \lambda_{17} > 0, \quad l = 2(1)I-1, \qquad \vartheta_{(n-1)JI+I(J-1)+I} \geq \lambda_{18} > 0,$$

$$\vartheta_{JI(K-1)+1} \geq \lambda_{19} > 0, \qquad \vartheta_{JI(K-1)+l} \geq \lambda_{20} > 0, \quad l = 2(1)I-1,$$

$$\vartheta_{JI(K-1)+I} \geq \lambda_{21} > 0,$$

$m = 2(1)J-1$:

$$\vartheta_{JI(K-1)+I(m-1)+1} \geq \lambda_{22} > 0,$$

$$\vartheta_{JI(K-1)+I(m-1)+l} \geq \lambda_{23} > 0, \quad l = 2(1)I-1, \qquad \vartheta_{JI(K-1)+I(m-1)+I} \geq \lambda_{24} > 0,$$

$$\vartheta_{JI(K-1)+I(J-1)+1} \geq \lambda_{25} > 0,$$

$$\vartheta_{JI(K-1)+I(J-1)+l} \geq \lambda_{26} > 0, \quad l = 2(1)I-1, \qquad \vartheta_{JI(K-1)+I(J-1)+I} \geq \lambda_{27} > 0,$$

where the expressions of λ_ζ for $\zeta = 1(1)27$ are given in the Appendix.

Therefore, except leaving the principal diagonal of irreducible matrix $\boldsymbol{\mathcal{H}}$, the sum of entries from each row in $\boldsymbol{\mathcal{H}}$ is positive real values for an adequately small value of δz. Also, the sum of row elements corresponding to the main diagonal is zero or positive depending on the value of constant A. Hence, the condition $A \geq 0$ makes all of the row sums strictly positive and that associated with the principal diagonal becomes non-negative. This proves that the irreducible matrix $\boldsymbol{\mathcal{H}}$ is monotone [14]. As a result, the square matrix $\boldsymbol{\mathcal{H}}$ is invertible and each entry of $\boldsymbol{\mathcal{H}}^{-1}$ is either a negative real number or zero.

Let us denote $\boldsymbol{\mathcal{H}}^{-1} = [\mathcal{H}^{-1}_{l,m}]_{l,m=1(1)IJK}$. Applying the matrix identity $\boldsymbol{\mathcal{H}}^{-1}(\boldsymbol{\mathcal{H}}\boldsymbol{\mathcal{I}}) = \boldsymbol{\mathcal{I}}$, where $\boldsymbol{\mathcal{I}}$ is column vector of order $IJK \times 1$ having each value as one, we get

$$\sum_{m=1(1)IJK} \mathcal{H}^{-1}_{l,m}\vartheta_m = 1, \quad l = 1(1)IJK. \tag{4.15}$$

Therefore, by the use of Taylor's expansions, one can compute the upper bounds on the non-positive elements of matrix $\boldsymbol{\mathcal{H}}^{-1}$ in the following manner:

For $l = 1(1)IJK$:

$$
\begin{aligned}
&\mathcal{H}_{l,1}^{-1} \le 1/\vartheta_1 \le \lambda_1^{-1} + O(\delta z),\\
&\sum_{b=2}^{I-1} \mathcal{H}_{l,b}^{-1} \le 1/\operatorname*{Min}_{b=2(1)I-1} \vartheta_b \le \lambda_2^{-1} + O(\delta z),\\
&\mathcal{H}_{l,I}^{-1} \le 1/\vartheta_I \le \lambda_3^{-1} + O(\delta z),\\
&\sum_{b=2}^{J-1} \mathcal{H}_{l,I(b-1)+1}^{-1} \le 1/\operatorname*{Min}_{b=2(1)J-1} \vartheta_{I(b-1)+1} \le \lambda_4^{-1} + O(\delta z),\\
&\sum_{b=2}^{J-1}\sum_{a=2}^{I-1} \mathcal{H}_{l,I(b-1)+a}^{-1} \le 1/\operatorname*{Min}_{b=2(1)J-1,a=2(1)I-1} \vartheta_{I(b-1)+a} \le \lambda_5^{-1} + O(\delta z),\\
&\sum_{b=2}^{J-1} \mathcal{H}_{l,I(b-1)+I}^{-1} \le 1/\operatorname*{Min}_{b=2(1)J-1} \vartheta_{I(b-1)+I} \le \lambda_6^{-1} + O(\delta z),\\
&\mathcal{H}_{l,I(J-1)+1}^{-1} \le 1/\vartheta_{I(J-1)+1} \le \lambda_7^{-1} + O(\delta z),\\
&\sum_{a=2}^{I-1} \mathcal{H}_{l,I(J-1)+a}^{-1} \le 1/\operatorname*{Min}_{a=2(1)I-1} \vartheta_{I(J-1)+a} \le \lambda_8^{-1} + O(\delta z),\\
&\mathcal{H}_{l,I(J-1)+I}^{-1} \le 1/\vartheta_{I(J-1)+I} \le \lambda_9^{-1} + O(\delta z),\\
&\sum_{c=2}^{K-1} \mathcal{H}_{l,(c-1)JI+1}^{-1} \le 1/\operatorname*{Min}_{c=2(1)K-1} \vartheta_{(c-1)JI+1} \le \lambda_{10}^{-1} + O(\delta z),\\
&\sum_{c=2}^{K-1}\sum_{a=2}^{I-1} \mathcal{H}_{l,IJ(c-1)+a}^{-1} \le 1/\operatorname*{Min}_{a=2(1)I-1,c=2(1)K-1} \vartheta_{IJ(c-1)+a} \le \lambda_{11}^{-1} + O(\delta z),\\
&\sum_{c=2}^{K-1} \mathcal{H}_{l,IJ(c-1)+I}^{-1} \le 1/\operatorname*{Min}_{c=2(1)K-1} \vartheta_{IJ(c-1)+I} \le \lambda_{12}^{-1} + O(\delta z),\\
&\sum_{c=2}^{K-1}\sum_{b=2}^{J-1} \mathcal{H}_{l,IJ(c-1)+I(b-1)+1}^{-1}\\
&\quad \le 1/\operatorname*{Min}_{b=2(1)J-1,c=2(1)K-1} \vartheta_{IJ(c-1)+I(b-1)+1} \le \lambda_{13}^{-1} + O(\delta z),\\
&\sum_{c=2}^{K-1}\sum_{b=2}^{J-1}\sum_{a=2}^{I-1} \mathcal{H}_{l,IJ(c-1)+I(b-1)+a}^{-1}\\
&\quad \le 1/\operatorname*{Min}_{a=2(1)I-1,b=2(1)J-1,c=2(1)K-1} \vartheta_{(c-1)JI+(b-1)I+a} \le \lambda_{14}^{-1} + O(\delta z),\\
&\sum_{c=2}^{K-1}\sum_{b=2}^{J-1} \mathcal{H}_{l,IJ(c-1)+I(b-1)+I}^{-1}\\
&\quad \le 1/\operatorname*{Min}_{b=2(1)J-1,c=2(1)K-1} \vartheta_{IJ(c-1)+I(b-1)+I} \le \lambda_{15}^{-1} + O(\delta z),\\
&\sum_{c=2}^{K-1} \mathcal{H}_{l,(c-1)JI+I(J-1)+1}^{-1} \le 1/\operatorname*{Min}_{c=2(1)K-1} \vartheta_{(c-1)JI+I(J-1)+1} \le \lambda_{16}^{-1} + O(\delta z),
\end{aligned}
$$

$$
\begin{aligned}
&\sum_{c=2}^{K-1}\sum_{a=2}^{L-1}\mathcal{H}^{-1}_{l,IJ(c-1)+I(J-1)+a} \\
&\quad\le 1/\underset{a=2(1)I-1,c=2(1)K-1}{\mathrm{Min}}\vartheta_{IJ(c-1)+I(J-1)+a} \le \lambda_{17}^{-1} + O(\delta z), \\
&\sum_{c=2}^{K-1}\mathcal{H}^{-1}_{l,IJ(c-1)+I(J-1)+I} \le 1/\underset{c=2(1)K-1}{\mathrm{Min}}\vartheta_{IJ(c-1)+I(J-1)+I} \le \lambda_{18}^{-1} + O(\delta z), \\
&\mathcal{H}^{-1}_{l,JI(K-1)+1} \le 1/\vartheta_{JI(K-1)+1} \le \lambda_{19}^{-1} + O(\delta z), \\
&\sum_{a=2}^{I-1}\mathcal{H}^{-1}_{l,JI(K-1)+a} \le 1/\underset{a=2(1)I-1}{\mathrm{Min}}\vartheta_{JI(K-1)+a} \le \lambda_{20}^{-1} + O(\delta z), \\
&\mathcal{H}^{-1}_{l,IJ(K-1)+I} \le 1/\vartheta_{IJ(K-1)+I} \le \lambda_{21}^{-1} + O(\delta z), \\
&\sum_{b=2}^{J-1}\mathcal{H}^{-1}_{l,JI(K-1)+I(b-1)+1} \le 1/\underset{b=2(1)J-1}{\mathrm{Min}}\vartheta_{JI(K-1)+(b-1)I+1} \le \lambda_{22}^{-1} + O(\delta z), \\
&\sum_{b=2}^{K-1}\sum_{a=2}^{I-1}\mathcal{H}^{-1}_{l,JI(K-1)+(b-1)I+a} \\
&\quad\le 1/\underset{a=2(1)I-1,b=2(1)J-1}{\mathrm{Min}}\vartheta_{JI(K-1)+(b-1)I+a} \le \lambda_{23}^{-1} + O(\delta z), \\
&\sum_{b=2}^{J-1}\mathcal{H}^{-1}_{l,(K-1)IJ+I(b-1)+I} \le 1/\underset{b=2(1)J-1}{\mathrm{Min}}\vartheta_{JI(K-1)+I(b-1)+I} \le \lambda_{24}^{-1} + O(\delta z), \\
&\mathcal{H}^{-1}_{l,JI(K-1)+I(J-1)+1} \le 1/\vartheta_{JI(K-1)+I(J-1)+1} \le \lambda_{25}^{-1} + O(\delta z), \\
&\sum_{a=2}^{I-1}\mathcal{H}^{-1}_{l,(K-1)IJ+(J-1)I+a} \le 1/\underset{a=2(1)I-1}{\mathrm{Min}}\vartheta_{(K-1)IJ+(J-1)I+a} \le \lambda_{26}^{-1} + O(\delta z), \\
&\mathcal{H}^{-1}_{l,JI(K-1)+I(J-1)+I} \le 1/\vartheta_{JI(K-1)+I(J-1)+I} \le \lambda_{27}^{-1} + O(\delta z).
\end{aligned}
$$

Incorporating the above inequalities in the error equation (4.14), we get

$$
\begin{aligned}
\|\boldsymbol{\mathcal{E}}\|_\infty &\le \left\|\boldsymbol{\mathcal{H}}^{-1}\right\|_\infty \cdot \|\boldsymbol{T}\|_\infty \le \left(\lambda_{14}^{-1} + \sum_{\substack{t=1\\ t\ne 14}}^{27}\lambda_t^{-1}\right) O\left(\delta z^5\right) \\
&\le \begin{cases} \delta z^3\epsilon/(6A\mu^2) + O(\delta z^5), & A > 0, \\ O(\delta z^5), & A = 0. \end{cases}
\end{aligned}
\tag{4.16}
$$

That is to say,

$$
\|\boldsymbol{\mathcal{E}}\|_\infty \le \mathrm{Min}\left\{\delta z^3\epsilon/\left(6A\mu^2\right) + O\left(\delta z^5\right), O\left(\delta z^5\right)\right\} = O\left(\delta z^3\right), \quad A \ge 0. \tag{4.17}
$$

This proves that the discretization errors $\|\boldsymbol{\mathcal{E}}\| \to 0$, as $\delta z \to 0^+$.

Inequality (4.17) establishes the maximum truncation error appearing in the high-order discretization formula (3.14). An accuracy of third order can be achieved by choosing the value of one or all of the grid expansion parameters as not equal to one. In the above proof, we have assumed that $A \ge 0$, which suggests that $\partial\psi/\partial U \ge 0$, as an essential criterion for the convergence. By the same arguments, one can establish that the compact scheme (3.14) achieves accuracy of order four if grid points are chosen equally spaced. We summarize the above result in the following manner:

Theorem 4.1 *The exponential basis compact scheme* (3.14) *on the exponential expanding grid network has third order of convergence, provided* $\partial\psi/\partial U \geq 0$, $p, q, r \in (\frac{\sqrt{5}-1}{2}, \frac{\sqrt{5}+1}{2})$, *and* $p \neq 1, q \neq 1$, *or* $r \neq 1$.

5 Numerical simulations

We briefly test the empirical execution of the third-order scheme and affirm that the character of approximate solution values corresponds to the theoretical analysis. In each experiment, the domain of integration is a unit cube, and known analytic solution regulates Dirichlet's boundary data as well as right-hand side function, if any. The maximum absolute error $\mathfrak{l}_{\infty}^{(I,J,K)}$ and root-mean-square error $\mathfrak{l}_{2}^{(I,J,K)}$, with I, J, and K number of grid points in x-, y-, and z-direction and corresponding computational order of convergence (Θ_{∞}) and (Θ_2), are examined for two types of fourth-order schemes: UM-FOCS and EF-FOCS on uniformly spaced grid points with standard basis and exponential basis respectively. The experiments with exponential basis third-order compact scheme on exponential expanding grid points (EF-EEG-TOCS) and third-order scheme on exponential expanding grid points (EEG-TOCS) with standard basis will provide superior accuracies compared with UM-FOCS and EF-FOCS.

$$\mathfrak{l}_{\infty}^{(I,J,K)} = \max_{i,j,k}\left|U(x_i, y_j, z_k) - u_{i,j,k}\right|, \tag{5.1}$$

$$\mathfrak{l}_{2}^{(I,J,K)} = \sqrt{\sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K}\frac{1}{IJK}\left|U(x_i, y_j, z_k) - u_{i,j,k}\right|^2}, \tag{5.2}$$

$$\Theta_{\infty} = \log_2\left[\frac{\mathfrak{l}_{\infty}^{(I,J,K)}}{\mathfrak{l}_{\infty}^{(2I+1,2J+1,2K+1)}}\right], \qquad \Theta_2 = \log_2\left[\frac{\mathfrak{l}_{2}^{(I,J,K)}}{\mathfrak{l}_{2}^{(2I+1,2J+1,2K+1)}}\right]. \tag{5.3}$$

For solving a linear system of difference equations, the Gauss–Seidel iterative algorithm is applied, while solutions to the nonlinear difference equations are obtained by employing the Newton–Raphson method [13, 24, 37]. The error tolerance as a stopping criterion is taken to be $\leq 10^{-10}$ along with zero vector as an initial solution guess. The optimum values of frequency parameters α, β, γ, and grid expansion factors p, q, r are acquired from the simulations with $I = J = K$. The computational convergence order for the uniformly spaced grid points is four and the same reverberates in the tabulated results. But that convergence order of truncation error does not reflect when the grids are dispersed unevenly [16]. Maple programs are implemented for deriving nonlinear algebraic equations, optimized code generation, and symbolic computations. The C programs demonstrate the numerical calculations. All the computing is performed on 2.6 GHz Intel Core i7 processor on the Mac operating system.

Example 5.1 The study of steady-state convection, diffusion, and reactive phenomena is significant in heat and mass transfer. The behavior of physical quantities in fluid flow follows the convection-diffusion model, for example, heat and momentum; diffusion process in an environment such as pollutant transport in groundwater and atmosphere are some

Table 1a Errors and order for UM-FOCS in Example 5.1

	$\tau = 1.0$		$\tau = 0.1$		$\tau = 0.01$	
$L+1$	$l_2^{(I,J,K)}$	Θ_2	$l_2^{(I,J,K)}$	Θ_2	$l_2^{(I,J,K)}$	Θ_2
4	5.67e–04	–	4.36e–02	–	1.02e+01	–
8	2.86e–05	4.3	2.82e–03	4.0	2.32e+00	2.1
16	6.55e–07	5.4	1.70e–04	4.0	4.65e–01	2.3

Table 1b Errors and order for UM-FOCS in Example 5.1

	$\tau = 1.0$		$\tau = 0.1$		$\tau = 0.01$	
$L+1$	$l_2^{(I,J,K)}$	Θ_2	$l_2^{(I,J,K)}$	Θ_2	$l_2^{(I,J,K)}$	Θ_2
4	4.83e–04	–	4.13e–02	–	1.02e+01	–
8	2.38e–05	4.30	2.61e–03	4.0	2.31e–00	2.2
16	1.34e–06	4.10	1.55e–04	4.1	4.61e–01	2.3

Table 1c Errors for the EF-EEG-TOCS in Example 5.1

$L+1$	p	q	r	α	β	γ	$l_2^{(I,J,K)}$	Θ_∞
$\tau = 0.1$								
4	1.50	1.10	0.80	11	1	2	8.19e–04	–
8	1.20	1.10	0.90	9	1	2	8.45e–05	3.3
16	1.09	1.06	0.98	82	1	2	5.87e–06	3.8
$\tau = 0.01$								
4	1.60	1.40	0.90	1	1	1	2.80e–01	–
8	1.40	1.30	0.70	1	1	1	3.30e–02	3.1
16	1.20	1.30	0.80	1	1	1	1.84e–03	4.2

Table 1d Errors for the EF-EEG-TOCS in Example 5.1 at $\tau = 0.01$

$L+1$	p	q	r	α	β	γ	$l_2^{(I,J,K)}$	Θ_∞
4	1.50	1.50	0.90	1	1	1	9.13e–01	–
8	1.50	1.50	0.70	1	1	1	4.81e–02	4.2
16	1.20	1.20	0.80	1	1	1	1.99e–03	4.6

of the important application areas. The mathematical model derived from such models is given by

$$\epsilon\left(\frac{\partial^2 U}{\partial x^2}+\frac{\partial^2 U}{\partial y^2}+\frac{\partial^2 U}{\partial z^2}\right)=aU+b\frac{\partial U}{\partial x}+c\frac{\partial U}{\partial y}+d\frac{\partial U}{\partial z}+g(x,y,z), \tag{5.4}$$

where $U(x,y,z)=[1-(1-x)e^{-x/\tau}]\cos(\pi\{y+z\})$ denotes the theoretical steady-state temperature distribution on a unit cube in analytic form. We shall determine $U(x,y,z)$ numerically when the temperature of each lateral surface is known. The source function $g(x,y,z)$ will be obtained for given $U(x,y,z)$, known values of a, $b=\rho uc_p$, $c=\rho vc_p$, $d=\rho wc_p$, and they are functions of $(x,y,z)\in\Omega\subseteq\mathbb{R}^3$. The physical quantities ϵ, c_p, and ρ denote thermal conductivity, specific heat, and specific mass respectively for the conducting material. The velocity component in x-, y-, and z-directions is u, v, and w respectively [35, 36]. Since the solution changes sharply with a change in the value of parameter τ, we analyze them for $\epsilon = 1$ and different values of τ in the following cases.

Case-1: When $a = 0$, it represents a convection-diffusion phenomenon, and errors in Table 1a with $b = c = d = 1$ and Table 1b with $b = x + y, c = y + z, d = x + z$, at $\tau = 1, 0.1$ and 0.01, show degenerate solution in particular at small value $\tau = 0.01$ by using UM-

Table 1e Errors and order for UM-FOCS in Example 5.1

	$\tau = 1.0$		$\tau = 0.1$		$\tau = 0.01$	
$L+1$	$\mathrm{I}_2^{(I,J,K)}$	Θ_2	$\mathrm{I}_2^{(I,J,K)}$	Θ_2	$\mathrm{I}_2^{(I,J,K)}$	Θ_2
4	5.51e–04	–	4.26e–02	–	9.99-00	–
8	2.78e–05	4.3	2.76e–03	3.9	2.28-00	2.1
16	6.45e–07	5.4	1.67e–04	4.0	4.58e–01	2.3

Table 1f Errors and order for UM-FOCS in Example 5.1

	$\tau = 1.0$		$\tau = 0.1$		$\tau = 0.01$	
$L+1$	$\mathrm{I}_2^{(I,J,K)}$	Θ_2	$\mathrm{I}_2^{(I,J,K)}$	Θ_2	$\mathrm{I}_2^{(I,J,K)}$	Θ_2
4	4.69e–04	–	4.02e–02	–	9.99e–00	–
8	2.31e–05	4.30	2.55e–03	4.0	2.26e–00	2.1
16	1.30e–06	4.10	1.51e–04	4.1	4.54e–01	2.3

Table 1g Errors and order for EEG-TOCS in Example 5.1 at $\tau = 0.01$

$L+1$	p	q	r	$\mathrm{I}_\infty^{(I,J,K)}$	Θ_∞	$\mathrm{I}_2^{(I,J,K)}$	Θ_2
4	1.59	0.82	1.02	7.41e–01	–	2.88e–01	–
8	1.35	0.74	1.13	9.09e–02	3.0	1.70e–02	4.1
16	1.17	0.82	1.07	8.07e–03	3.5	1.28e–03	3.7

Table 1h Errors for the EF-EEG-TOCS in Example 5.1 at $\tau = 0.01$

$L+1$	p	q	r	α	β	γ	$\mathrm{I}_2^{(I,J,K)}$	Θ_∞
4	1.50	1.50	0.90	1	1	1	8.99e–01	–
8	1.50	0.90	0.70	1	1	1	5.62e–02	4.0
16	1.30	0.90	0.80	1	1	1	2.45e–03	4.5

FOCS. Significant improvement in the solution values at $\tau = 0.01$ by using EF-EEG-TOCS is presented in Table 1c and Table 1d for $b = c = d = 1$ and $b = x + y, c = y + z, d = x + z$, respectively.

Case-2: When $a = 1$, it is convection-diffusion-reaction equation, and errors in Table 1e with $b = c = d = 1$ and Table 1f with $b = x + y, c = y + z, d = x + z$, at $\tau = 1, 0.1$ and 0.01, show degenerate solution for significantly small value $\tau = 0.01$ by using UM-FOCS. An intense improvement in the solution values at $\tau = 0.01$ by using EF-EEG-TOCS is observed in Table 1g and Table 1h for $b = c = d = 1$ and $b = x + y, c = y + z, d = x + z$, respectively.

Example 5.2 Consider the linear convection-diffusion equation

$$\epsilon\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2}\right) + \frac{\partial U}{\partial x} + \frac{\partial U}{\partial y} + \frac{\partial U}{\partial z} = 0, \quad (x, y, z) \in \Omega. \tag{5.5}$$

We will determine boundary values from the analytic solution $U(x, y, z) = e^{-x/\epsilon} + e^{-y/\epsilon} + e^{-z/\epsilon}$. A solution of (5.5) independent of small parameter ϵ was discussed by [15, 21]. Experiments with $\epsilon = 1, 2^{-2}, 2^{-4}$ exhibit uniform solution behavior with UM-FOCS, and implementing a variable structure of grids or exponential fitting results in almost the same solution behavior. Further diminishing values of $\epsilon = 2^{-5}$ and 2^{-6} require exponential expanding grid spacing and exponential fitted method due to deteriorating errors and numerical order. In Table 2a, we have presented root-mean-square errors and order at $\epsilon = 2^{-5}$

Table 2a Errors and order for UM-FOCS and EEG-TOCS in Example 5.2

$L+1$	p	q	r	$\mathrm{L}_2^{(I,J,K)}$	Θ_∞	p	q	r	$\mathrm{L}_2^{(I,J,K)}$	Θ_∞
4	1.0	1.0	1.0	1.81e–01	–	1.40	1.40	1.30	1.89e–01	–
8	1.0	1.0	1.0	3.65e–02	2.3	1.30	1.20	1.20	1.21e–02	4.0
16	1.0	1.0	1.0	3.40e–03	3.4	1.10	1.10	1.40	8.39e–04	3.8
32	1.0	1.0	1.0	2.15e–04	4.0	1.10	1.10	1.03	3.90e–05	4.4

Table 2b Errors and computational rate for the EF-EEG-TOCS in Example 5.2

$L+1$	p	q	r	α	β	γ	$\mathrm{L}_2^{(I,J,K)}$	Θ_∞
4	1.40	1.40	1.30	20	33	34	2.98e–02	–
8	1.30	1.20	1.20	32	32	31	1.67e–03	4.2
16	1.10	1.10	1.40	32	32	33	1.34e–04	3.6
32	1.09	1.09	1.10	32	32	33	9.15e–06	3.9

Table 2c Errors and order for UM-FOCS and EEG-TOCS in Example 5.2

$L+1$	p	q	r	$\mathrm{L}_2^{(I,J,K)}$	Θ_∞	p	q	r	$\mathrm{L}_2^{(I,J,K)}$	Θ_∞
4	1.0	1.0	1.0	3.37e–01	–	1.59	1.60	1.60	3.61e–01	–
8	1.0	1.0	1.0	1.37e–01	1.3	1.40	1.40	1.40	2.82e–02	3.7
16	1.0	1.0	1.0	2.57e–02	2.4	1.12	1.21	1.21	1.84e–03	3.9
32	1.0	1.0	1.0	2.40e–03	3.4	1.05	1.06	1.05	2.44e–04	3.1

Table 2d Errors and computational rate for the EF-EEG-TOCS in Example 5.2

$L+1$	p	q	r	α	β	γ	$\mathrm{L}_2^{(I,J,K)}$	Θ_∞
4	1.40	1.40	1.40	65	64	63.9	1.95e–03	–
8	1.30	1.20	1.30	64	64	63.9	1.29e–04	3.9
16	1.10	1.10	1.20	64	64	63.9	1.64e–05	3.0
32	1.01	1.01	1.09	64	64	63.9	1.98e–06	3.0

for both uniform grids fourth-order and exponential expanding grid third-order compact schemes without an exponential fitting operator, that is, by taking $\alpha, \beta, \gamma \to 0$ in scheme (3.14). Considering the exponential expanding grid network, a slight improvement reflects in the root-mean-squared errors. Additionally, the exponential fitted operator method EF-EEG-TOCS reflects almost true behavior of exact solution values in Table 2b at $\epsilon = 2^{-5}$. A similar observation can be drawn by using uniform and exponential expanding grid network high-order compact schemes from Table 2c and EF-EEG-TOCS from Table 2d at $\epsilon = 2^{-6}$.

Example 5.3 Consider the singular Schrödinger equation describing the quantum effect in a physical system and motion of an electron in the Coulomb field of a nucleus:

$$\epsilon\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2}\right) + \left(1 + \frac{\xi}{x^2 + y^2 + z^2}\right)U = g(x, y, z), \quad (x, y, z) \in \Omega. \tag{5.6}$$

The application of exponential basis quasi-variable meshes high-order compact scheme (3.14) to the Schrödinger equation (5.6) with $\xi > 0$ and $\epsilon = 1$, involving singular coefficient $a(x, y, z) = 1 + \xi/[x^2 + y^2 + z^2]$, needs special attention [20]. This is because the application of scheme (3.14) to the singular equation (5.6) yields $a(x_{i-1}, y_{j-1}, z_{k-1}) = 1 + \xi/[x_{i-1}^2 + y_{j-1}^2 + z_{k-1}^2]$, and at $i = j = k = 1$, we come across $a(x_0, y_0, z_0) = 1 + \xi/[x_0^2 + y_0^2 + z_0^2]$, which leads to

Table 3a Errors and order for UM-FOCS and EEG-TOCS in Example 5.3

$L+1$	p	q	r	$\mathfrak{l}_2^{(I,J,K)}$	Θ_∞	p	q	r	$\mathfrak{l}_2^{(I,J,K)}$	Θ_∞
4	1.0	1.0	1.0	9.06e–04	–	1.20	1.30	1.30	8.75e–05	–
8	1.0	1.0	1.0	5.96e–05	3.9	1.20	1.10	1.10	5.86e–06	3.9
16	1.0	1.0	1.0	3.69e–06	4.0	1.10	1.10	1.00	7.34e–07	3.0

Table 3b Errors and computational rate for the EF-EEG-TOCS in Example 5.3

$L+1$	p	q	r	α	β	γ	$\mathfrak{l}_2^{(I,J,K)}$	Θ_∞
4	1.20	1.30	1.30	0.9	0.6	0.8	6.10e–05	–
8	1.20	1.10	1.10	0.1	0.2	0.1	5.92e–06	3.4
16	1.09	1.09	1.02	0.1	0.1	0.1	4.91e–07	3.6

Table 3c Errors and computational rate for the EF-EEG-TOCS in Example 5.3

$L+1$	p	q	r	α	β	γ	$\mathfrak{l}_2^{(I,J,K)}$	Θ_∞
4	0.62	0.62	0.62	0.10	0.10	0.10	9.17e–03	–
8	0.62	0.62	0.62	0.10	0.10	0.10	2.14e–03	2.1
16	0.62	0.62	0.62	0.10	0.10	0.10	6.74e–04	1.7

zero divisors. In such situations, we substitute $x_{i-1}^{-1} = x_i^{-1} + x_i^{-2}\delta x_i + x_i^{-3}\delta x_i^2 + x_i^{-4}\delta x_i^3 + O(\delta x_i^4)$, (similarly for y_{j-1}^{-1} and z_{k-1}^{-1}) in the scheme and drop the higher-order terms for computing purpose, as it forms a part of truncation error. More precisely, we can express $U_{l,m,n}$, $(l,m,n) \in \overline{\mathcal{M}}$ in terms of compact operators defined by (2.10)–(2.11) and their composites. Such a replacement of $U_{l,m,n}$, $(l,m,n) \in \overline{\mathcal{M}}$ in terms of compact operators in the numerical scheme may consist of the terms like $\delta x_i^3 \mathcal{S}_x \mathcal{S}_y \mathcal{S}_z U_{i,j,k} = O(\delta x_i^3 \delta x_i^2 \delta y_j^2 \delta z_k^2) \approx O(\delta x_i^9)$ and must be omitted, as it again forms a part of truncation error. To test the accuracies, analytical solution $U(x,y,z) = (\frac{2}{\pi})^{3/4} e^{-x^2-y^2-z^2}$ is taken so as to satisfy the normalizing condition $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |U(x,y,z)|^2\,dx\,dy\,dz = 1$ [33]. Numerical simulations are performed in Table 3a with UM-FOCS and EEG-TOCS for $\xi = 10$ in the limiting case $\alpha, \beta, \gamma \to 0$. Results in Table 3b that exhibit better accuracies compared with Table 3a are obtained by EF-EEG-TOCS. At $\xi = 20$, both UM-FOCS and EEG-TOCS fail, while EF-EEG-TOCS computes the solution with reasonably good accuracies, see Table 3c.

Example 5.4 The nonlinear three-dimensional elliptic Allen–Cahn equation describes the reaction-diffusion process of phase separation in a multi-component alloy system, including order-disorder transitions [33, 39]. The equations take the form

$$\epsilon\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2}\right) = U - U^3 + g(x,y,z), \quad (x,y,z) \in \Omega. \tag{5.7}$$

To test the new high-order compact difference scheme, we have chosen theoretical solution as $U(x,y,z) = e^3(e^{1-2z} - ze^{-z})\sin(x)\sin(y)$ and $\epsilon = 1$. Root-mean-square errors, computational order, and the number of iterations to achieve the error tolerance of 10^{-10} are presented in Tables 4a–4c for UM-FOCS, EEG-TOCS, and EF-EEG-TOCS to illustrate the efficiency in a comparative manner.

Table 4a Errors and computational rate for the UM-FOCS in Example 5.4

$L+1$	p	q	r	α	β	γ	Itr	$l_2^{(I,J,K)}$	Θ_∞
4	1.00	1.00	1.00	0.01	0.01	0.01	20	3.78e–04	–
8	1.00	1.00	1.00	0.01	0.01	0.01	58	2.00e–05	3.9
16	1.00	1.00	1.00	0.01	0.01	0.01	145	1.14e–06	4.0

Table 4b Errors and computational rate for the EEG-TOCS in Example 5.4

$L+1$	p	q	r	α	β	γ	Itr	$l_2^{(I,J,K)}$	Θ_∞
4	1.10	1.00	1.03	0.01	0.01	0.01	14	4.97e–05	–
8	1.10	1.00	1.00	0.01	0.01	0.01	39	4.79e–06	3.3
16	1.05	1.00	1.00	0.01	0.01	0.01	88	2.80e–07	3.9

Table 4c Errors and computational rate for the EF-EEG-TOCS in Example 5.4

$L+1$	p	q	r	α	β	γ	Itr	$l_2^{(I,J,K)}$	Θ_∞
4	1.10	1.00	1.03	1.00	2.00	2.00	15	1.46e–05	–
8	1.10	1.00	1.00	2.00	1.00	1.00	36	1.57e–06	3.3
16	1.05	1.00	1.00	2.00	1.00	1.00	55	9.23e–08	3.9

Example 5.5 We consider the celebrated elliptic sine-Gordon elliptic PDEs with a small parameter, appearing in condensed matter physics, plane rotator spin model, Josephson effect, statistical mechanics, and spin waves in ferromagnetisms [12, 39]. The dimensionless form of the equation is

$$\epsilon\left(\frac{\partial^2 U}{\partial x^2}+\frac{\partial^2 U}{\partial y^2}+\frac{\partial^2 U}{\partial z^2}\right)=\sin(U)+g(x,y,z), \quad (x,y,z)\in\Omega. \tag{5.8}$$

To analyze the solution accuracies, forcing function g and boundary data are obtained using the theoretic solution

$$U(x,y,z)=\frac{1}{\sinh(\frac{\sqrt{1+4\epsilon}}{2\epsilon})}\sinh\left(\frac{\sqrt{1+4\epsilon}}{2\epsilon}x\right)\sin\left(\frac{\sqrt{1+4\epsilon}}{2\epsilon}y\right)\sin\left(\frac{\sqrt{1+4\epsilon}}{2\epsilon}z\right).$$

Computed root-mean-squared errors and convergence order are presented in Tables 5a–5e for the various arrangement of grid spacing. The tabulated results are in agreement with theoretical estimates exhibiting the importance of exponential basis and exponential expanding grids. It is noted that for $\epsilon = 1$ and 0.1, the fourth-order compact scheme with $p = q = r = 1$ yields accurate solution values with the small value of fitted parameters $\alpha = \beta = \gamma = 0.01$. A further small value of $\epsilon = 0.01$ results in drops in computational order with the fourth-order compact scheme and non-zero exponential fitted parameters. Combination of exponential fitted parameters and grid expansion factors generates accurate solution values along with expected computational order. In Table 5a, when $\epsilon = 1$, the UM-FOCS can be easily considered due to smoothness in the solution. However, as the value of ϵ decreases to 0.1, a small improvement in solution is observed by EF-EEG-TOCS (Table 5c) over UM-FOCS (Table 5b). A further diminishing value of $\epsilon = 0.01$, the errors, and computational order observed by UM-FOCS (Table 5d) are unsatisfactory. Significant improvement by EF-EEG-TOCS is observed in Table 5e since it reduces errors and iteration number significantly.

Table 5a Errors and order for UM-FOCS in Example 5.5 at $\epsilon = 1$

$L+1$	p	q	r	α	β	γ	Itr	$l_2^{(I,J,K)}$	Θ_∞
4	1.00	1.00	1.00	0.01	0.01	0.01	10	3.45e–07	–
8	1.00	1.00	1.00	0.01	0.01	0.01	21	1.75e–08	4.0
16	1.00	1.00	1.00	0.01	0.01	0.01	31	5.41e–10	4.6

Table 5b Errors and order for UM-FOCS in Example 5.5 at $\epsilon = 0.1$

$L+1$	p	q	r	α	β	γ	Itr	$l_2^{(I,J,K)}$	Θ_∞
4	1.00	1.00	1.00	0.01	0.01	0.01	10	1.04e–03	–
8	1.00	1.00	1.00	0.01	0.01	0.01	21	9.07e–05	3.5
16	1.00	1.00	1.00	0.01	0.01	0.01	31	5.60e–06	4.0

Table 5c Errors and order for EF-EEG-TOCS in Example 5.5 at $\epsilon = 0.1$

$L+1$	p	q	r	α	β	γ	Itr	$l_2^{(I,J,K)}$	Θ_∞
4	0.90	0.90	1.00	1.00	1.00	1.00	9	5.04e–04	–
8	0.88	0.92	1.00	1.00	1.00	1.00	18	3.34e–05	3.9
16	0.90	1.00	1.00	1.00	1.00	1.00	26	2.15e–06	4.0

Table 5d Errors and order for UM-FOCS in Example 5.5 at $\epsilon = 0.01$

$L+1$	p	q	r	α	β	γ	Itr	$l_2^{(I,J,K)}$	Θ_∞
4	1.00	1.00	1.00	0.01	0.01	0.01	10	1.65e–01	–
8	1.00	1.00	1.00	0.01	0.01	0.01	21	7.49e–02	1.1
16	1.00	1.00	1.00	0.01	0.01	0.01	31	3.29e–03	4.5

Table 5e Errors and order for EF-EEG-TOCS in Example 5.5 at $\epsilon = 0.01$

$L+1$	p	q	r	α	β	γ	Itr	$l_2^{(I,J,K)}$	Θ_∞
4	0.90	0.70	1.00	023	1.00	1.00	5	5.59e–02	–
8	0.89	0.64	1.01	200	1.00	1.00	8	3.66e–03	2.5
16	1.20	1.00	1.00	042	1.00	1.00	9	1.88e–04	4.2

Example 5.6 Consider the nonlinear elliptic PDEs appearing in the steady-state combustion process and mass transfer in inhomogeneous anisotropic media

$$\epsilon\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2}\right) = \left(U^x + U^y + U^z\right)U + g(x,y,z), \quad (x,y,z) \in \Omega. \tag{5.9}$$

The source function $g(x,y,z)$ and boundary values are determined from the analytic solution $U(x,y,z) = e^x \sinh(\frac{\pi y}{2})\sin(\frac{\pi z}{2})$ [21, 30, 31, 34]. By using the uniformly spaced grids fourth-order scheme, the accuracies and computational order remain intact for $\epsilon = 1$ and 0.1. However, as the ϵ becomes smaller, say $\epsilon = 0.01$ and 0.001, the accuracy measures, namely numerical order and root-mean-square error, grow; as a result, it is necessary to implement quasi-variables meshes and exponential fitted third-order scheme, and the improved results are tabulated in Table 6 at $\alpha = \beta = \gamma = 0.1$.

6 Conclusion and remarks

The proposed high-order compact schemes numerically solve the three-space dimensional elliptic partial differential equations with small parameters. With necessary mod-

Table 6 Errors and order for UM-FOCS and EEG-TOCS in Example 5.6

$L+1$	p	q	r	$l_2^{(I,J,K)}$	Θ_∞	p	q	r	$l_2^{(I,J,K)}$	Θ_∞
4	1.6	1.00	1.00	4.22e–03	–	1.5	1.00	1.30	7.54e–03	–
8	1.3	1.20	1.30	3.64e–04	3.5	1.1	1.20	1.10	7.58e–04	3.3
16	1.0	1.07	1.14	2.68e–05	3.8	1.0	1.11	1.18	6.57e–05	3.5

ifications and with the help of compact operators, it is possible to solve singular elliptic equations without loss of order and accuracies. The third-order compact formulation with an exponential basis and exponential expanding grids generate improved solution accuracies in comparison with fourth-order uniformly spaced grid network. In the limiting case $\alpha, \beta, \gamma \to 0$ and $p = q = r = 1$, the proposed third-order exponential basis scheme on the exponential expanding grid network returns a fourth-order accurate scheme on uniformly spaced grid points, and therefore, the new scheme may be regarded as a generalization to the existing high-order compact formulation. *The proposed nineteen-point high-order compact discretization produces a stable scheme which is efficient in terms of operation count and does not experience difficulties near boundaries* [25]. To the great extent, a general non-uniform distribution of grid points can be received by exchanging grid expansion factors p, q, r to p_i, q_j, r_k respectively in the suggested third-order compact scheme. It is feasible to extend such high-order compact discretization for hyperbolic and parabolic PDEs.

Appendix: Values of $\lambda_t, t = 1(1)26$ appearing in Section 4

$$\lambda_1 = \lambda_3 = \lambda_7 = \lambda_9 = \bigl(10\mu^2 + 2r^2 + 9r + 9\bigr)/(r+1) + O(\delta z),$$
$$\lambda_2 = \lambda_4 = \lambda_6 = \lambda_8 = \bigl(11\mu^2 + r^2 + 5r + 5\bigr)/(r+1) + O(\delta z),$$
$$\lambda_5 = 12\mu^2/(r+1) + O(\delta z), \qquad \lambda_{10} = \lambda_{12} = \lambda_{16} = \lambda_{18} = 11 + O(\delta z),$$
$$\lambda_{11} = \lambda_{13} = \lambda_{15} = \lambda_{17} = 6 + O(\delta z),$$
$$\lambda_{14} = \begin{cases} 6A\mu^2\delta z^2/\epsilon + O(\delta z^3), & A \neq 0, \\ 0, & A = 0, \end{cases}$$
$$\lambda_{19} = \lambda_{21} = \lambda_{25} = \lambda_{27} = \bigl(10\mu^2 + 9r^2 + 9r + 2\bigr)/\bigl[r(r+1)\bigr] + O(\delta z),$$
$$\lambda_{20} = \lambda_{22} = \lambda_{24} = \lambda_{26} = \bigl(11\mu^2 + 5r^2 + 5r + 1\bigr)/\bigl[r(r+1)\bigr] + O(\delta z).$$

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