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A modified cubic B-spline differential quadrature method for three-dimensional non-linear diffusion equations

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Abstract: This paper employs a differential quadrature scheme for solving non-linear partial differential equations. Differential quadrature method (DQM), along with modified cubic B-spline basis, has been adopted to deal with three-dimensional non-linear Brusselator system, enzyme kinetics of Michaelis-Menten type problem and Burgers' equation. The method has been tested efficiently to three-dimensional equations. Simple algorithm and minimal computational efforts are two of the major achievements of the scheme. Moreover, this methodology produces numerical solutions not only at the knot points but also at every point in the domain under consideration. Stability analysis has been done. The scheme provides convergent approximate solutions and handles different cases and is particularly beneficial to higher dimensional non-linear PDEs with irregularities in initial data or initial-boundary conditions that are discontinuous in nature, because of its capability of damping specious oscillations induced by high frequency components of solutions.

Keywords: Brusselator system, Michales-Menten system, Burgers' Equation, Modified cubic B-spline DQM, SSP-RK43 method

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1 Introduction

In this work, we have extended an earlier approach [1] to obtain the numerical solutions of three-dimensional non-linear reaction-diffusion equations and three-dimensional Burgers' equation. Reaction-diffusion models appear very frequently while investigating biological and chemical phenomena and time-dependent PDEs are adopted to model them naturally i.e. reaction-diffusion equations. The non-linear reaction-diffusion system is made up of two different terms: (a) diffusion term, involving the random motion of every particular component because of turbulent nature of the governing field flow and (b) reaction term, which describes the interactions between biological and physical species that are involved [2]. Over the past decades, reaction-diffusion systems have attained enormous interest from researchers because of their complexity and behavioral dynamics such as periodicity in solution, formation of patterns, and chaos [3–5]. We have discussed some well known and reaction-diffusion models appearing very frequently: the Brusselator model [4] and the Michaelis-Menten model [6]. A number of authors have emphasized the significance of oscillations in biochemical systems, e.g. Turing [7] observed that a stable spatial arrangement can possibly be obtained by coupling the diffusion process with certain reactions leading to the idea of morphogenesis.

The development and analysis of the behavior of a non-linear oscillator related to chemical system

$$\begin{aligned} B_{in} &\Longrightarrow X_1, \\ A_{in} + X_1 &\Longrightarrow X_2 + D_1, \\ 2X_1 + X_2 &\Longrightarrow 3X_1, \\ X_1 &\Longrightarrow D_2, \end{aligned} \tag{1}$$

was developed and analysed by the Brussels schools [8]. Here A_{in}, B_{in}, D_1 and D_2 denote the input and output chemicals, respectively. X_1 and X_2 are intermediates. The system (1) consists of only two dependent variables and admits limit cycle oscillations. The trimolecular reaction step in (1) appears in manifold coupling between modes in laser and plasma physics [9, 10], during enzymatic reactions, ozone formation by atomic oxygen by triple collision. The three-dimensional Brusselator system is written as

$$\frac{\partial \mathbf{u}}{\partial t} = A + \mathbf{u}^2\mathbf{v} - (B+1)\mathbf{u} + \alpha\nabla^2\mathbf{u}, \tag{2a}$$

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$$\frac{\partial \mathbf{v}}{\partial t} = B\mathbf{u} - \mathbf{u}^2\mathbf{v} + \alpha\nabla^2\mathbf{u}, \quad (\mathbf{x}, \mathbf{t}) \in \Omega \times (\mathbf{0}, \mathbf{T}] \tag{2b}$$

together with initial conditions

$$(\mathbf{u}(\mathbf{x}, \mathbf{0}), \mathbf{v}(\mathbf{x}, \mathbf{0})) = (\mathbf{g_1}(\mathbf{x}), \mathbf{g_2}(\mathbf{x})), \quad \mathbf{x} \in \Omega \tag{3}$$

and no flux conditions on boundary.

Here, $\mathbf{u}(\mathbf{x}, t) = u(x, y, z, t)$ and $\mathbf{v}(\mathbf{x}, t) = v(x, y, z, t)$ represents the concentrations of two reactants in the dimensionless form. A and B are constant concentrations of the two reactants, α is coefficient of diffusivity. For Brusselator system (2), if $1 - A + B^2 > 0$, then solution reaches the point of equilibria $(B, A/B)$ in steady state, given the values of coefficient of diffusivity α are kept very small.

Michaelis-Menten model is one of the best models known for enzyme kinetics. It involves an enzyme binding to a substrate S that results in the formation of an enzyme-substrate complex that is reduced in a product P and enzyme. The model transforms into an equation that describes the rate of enzymatic reactions by setting a relationship between reaction rate v to the concentration of substrate S. The formula is given by

$$v = \frac{d[P]}{dt} = \frac{V_{max}S}{K_M + S}.$$

Here, V_{max} represents the highest rate of the system at the highest substrate concentrations. K_M, known as the Michaelis constant, gives the substrate concentration at which rate of reaction is half of V_{max} [12]. Biochemical reactions that involve only one substrate are usually taken to follow kinetics of Michaelis-Menten, with no consideration to underlying assumptions of the model. The three-dimensional counterpart of Michaelis-Menten type one-dimensional problem discussed in [11] is given and reads as:

$$\frac{\partial u}{\partial t} = d\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) - \frac{u}{1-u}, 0 < x, y, z < 1, t > 0, \tag{4}$$

together with initial condition

$$u(x, y, z, 0) = f_1(x, y, z), 0 \le x, y, z \le 1. \tag{5}$$

and homogeneous boundary conditions.

In the present scenario, reaction-diffusion systems have gained significant concern as a model for formation of patterns. The stripes, hexagons, targets, spirals, fronts and dissipative soliton patterns are seen in many types of reaction-diffusion systems despite huge differences e.g. in the local reaction term. The reaction-diffusion processes are found to be significant bases for processes correlated to morphogenesis in biology [13]. Wound healing [14], tumor growth [15], spread of epidemics [16], ecological invasions [17] etc. are some of fields in which reaction-diffusion systems are applicable.

Burgers' equation has been extensively studied to portray many types of phenomena like mathematical model of turbulence [18], traveling of shock waves in viscous fluid [19], etc. One can take it as Navier-Stokes equation [20, 21] in a simplified version, because of the form of non-linear convective term and the appearance of the viscosity term.

Therefore, study of Burgers' equation is useful in understanding the convection-diffusion phenomena. Moreover, the study relates to many problems in physics such as acoustic transmission [22], traffic and aerofoil flow theory [23], gravity effect on sedimentation of two types of particles in fluid suspensions [24] as well as a prerequisite to the Navier-Stokes equations [25].

The Burgers' equation in one dimension is likewise to the Navier-Stokes equations in one dimension barring the stress term. A significant amount of research has been done in the recent years to numerically solve the Burgers' equation efficiently for varying kinematic viscosity values. Many numerical approaches to solve Burgers' equation such as Galerkin finite element method [26], finite volume method [27], iterative methods [28], automatic differentiation method [29] have been introduced in literature.

The three-dimensional Burgers' equation is

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - u\frac{\partial u}{\partial y} - u\frac{\partial u}{\partial z} + \frac{1}{R}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 z}{\partial t^2}\right), \tag{6}$$

with prescribed initial and boundary conditions.

2 Differential quadrature method

Differential quadrature method [30] is a numerical approach to approximate numerically the solutions of ODEs and PDEs. The derivatives of the unknown functions are approximated numerically using DQM at some predefined discrete points as a weighted sum of functional values in the complete domain. Computational inexpensiveness, accuracy and ease of application makes the technique more preferable. By employing differential quadrature method, we are capable of approximating the derivatives of functions in space at any of the given knots with the weighted linear sum of function values at all knots in the domain under consideration. To apply DQM in three dimensions, firstly we discretize the domain $\Omega = \{(x, y, z) : 0 \le x, y, z \le 1\}$ as $D^1 = \{(x_i, y_j, z_k), i = 1, 2, ...N; j = 1, 2, ..., M; k = 1, 2, ...L\}$ by taking step length $\Delta x = x_i - x_{i-1}$ in x-axis direction, $\Delta y = y_j - y_{j-1}$ in y-axis direction and $\Delta z = z_k - z_{k-1}$ in z-axis direction. Approximation of the partial derivative of order one of functional $u(x, y, z, t)$ along $x - axis$, at point x_i, keeping y_j and z_k fixed, is given

as follows

$$u_x(x_i, y_j, z_k, t) = \sum_{r=1}^{N} a_{ir}^{(1)} u(x_r, y_j, z_k, t), \quad i = 1, 2, \ldots, N \tag{7}$$

where $a_{ir}^{(1)}$ represent the the weighting coefficients to be determined to approximate the partial derivatives of order one in the direction of x. Various approaches are available in literature that can compute these weighting coefficients, e.g. Shu's approach [31], Quan and Chang's approach [32, 33], etc. Korkmaz and Daĝ [34, 35] used DQM based on cosine expansion and sinc DQM for many non-linear PDEs. Lagrange interpolation and sine-cosine expansion based quadrature methods has been very frequently used in literature. A differential quadrature method based on polynomials have been suggested by Mittal *et al.* [36] for numerical approximation of the the solutions of PDEs both linear and non-linear in nature. The idea of iterative DQM has been introduced by Tomasiello [37–40]. In her work, iterative DQM and the stability of DQ solutions have been discussed. Korkmaz [41] in his work employed DQM for solution of KdV equation. Arora and Singh [42] worked on one-dimensional Burgers' equation, whereas Jiwari and Yuan [43] worked on two-dimensional Brusselator model employing DQM. Bashan *et al.* [44] used Quintic B-splines DQM to approximate KdVB equation, whereas Korkmaz and Daĝ [45] employed both quartic and quintic B-splines for solving advection-diffusion equations. DQM based on Hermite radial basis function has been used by Krowick [46] to deal with higher order equations and DQM based on quasi-interpolation has been employed by Barrera *et al.* [47]. Shukla *et al.* [48–50] worked extensively on DQM to solve two and three-dimensional PDEs. In the present work, weighting coefficients of DQM are determined using a methodology that employs modified cubic B-spline functions. In this work, we have used cubic B-splines as basis functions and weighting coefficients are computed accordingly.

2.1 Modified cubic B-spline functions

Computation of weighting coefficients is a key procedure which is of paramount importance. In this work, the authors have computed the weighting coefficients $a_{ir}^{(1)}$, $a_{jr}^{(1)}$ and $a_{kr}^{(1)}$ by adopting modified cubic B-spline functions. These functions can be written as:

$$\varphi_m(x) = \frac{1}{h^3} \begin{cases} (x - x_{m-2})^3 & x \in [x_{m-2}, x_{m-1}) \\ (x - x_{m-2})^3 - 4(x - x_{m-1})^3 & x \in [x_{m-1}, x_m) \\ (x_{m+2} - x)^3 - 4(x_{m+1} - x)^3 & x \in [x_m, x_{m+1}) \\ (x_{m+2} - x)^3 & x \in [x_{m+1}, x_{m+2}) \\ 0 & \text{elsewhere} \end{cases} \tag{8}$$

Here, $\{\varphi_0(x), \varphi_1(x), \ldots, \varphi_{N+1}(x)\}$ defines a basis over the computational domain [a, b]. Table 1 comprises the values of original cubic B-splines and their derivatives at the knots. The B-spline functions are modified in a particular manner in which the diagonal dominance of the resultant matrix can be preserved. Jain [51] defines the modified cubic B-spline basis functions at the knot points as:

$$\begin{aligned} \phi_1(x) &= \varphi_1(x) + 2\varphi_0(x), \\ \phi_2(x) &= \varphi_2(x) - \varphi_0(x), \\ \phi_l(x) &= \varphi_l(x), l = 3, 4, \ldots., N-2, \\ \phi_{N-1} &= \varphi_{N-1}(x) - \varphi_{N+1}(x) \\ \phi_N(x) &= \varphi_N(x) + 2\varphi_{N+1}(x) \end{aligned} \tag{9}$$

The function $\phi_l(x)$, $l = 1, 2, \ldots., N$ again forms a basis over the interval [a, b].

Table 1: Values of $\varphi_m(x)$ and its derivatives at the nodal points

	x_{m-2}	x_{m-1}	x_m	x_{m+1}	x_{m+2}
$\varphi_m(x)$	0	1	4	1	0
$\varphi_m'(x)$	0	$3/h$	0	$3/h$	0
$\varphi_m''(x)$	0	$6/h^2$	$-12/h^2$	$6/h^2$	0

2.2 Determination of weighting coefficients

Korkmaz and Daĝ [52] used classic cubic B-spline functions and Korkmaz and Akmaz [53] used exponential cubic B-spline functions to compute the weighting coefficients. In their work, the resultant algebraic equation systems has $(N + 2)$ equations in $(N + 4)$ unknowns. Therefore, two more equations has to be added in the system. But, in the present study this is not the case. Determining the weighting coefficients $a_{ir}^{(1)}$ and using modified B-spline functions $\phi_m(x_i)$, $m = 1, 2, \ldots, N$ in Eq. (7), gives

$$\phi_m'(x_i) = \sum_{k=1}^{N} a_{ik} \phi_m(x_k), i = 1, 2, \ldots., N$$

To compute the weighting coefficients $a_{ir}^{(1)}$, we fix $y - axis$ and $z - axis$ in Eq. (7) as done in [1]. "Thomas algo-

rithm" is adopted to solve the resultant tri-diagonal system and the weighting coefficients $a_{11}^{(1)}, a_{12}^{(1)}, \ldots, a_{1N}^{(1)}$ are computed. Similarly, the weighting coefficients for each knot $i = 2, 3, \ldots, N$ can be computed. With these coefficients, we can approximate partial derivatives of order one in the direction of $x - axis$. The following recurrence relation is used to compute derivatives of higher order [31].

$$a_{ir}^{(p)} = r\left[a_{ir}^{(1)} a_{ii}^{(p-1)} - \frac{a_{ir}^{(p-1)}}{x_i - x_r}\right], \text{ for } i \neq r \tag{10}$$
$$i, r = 1, 2, \ldots, N; \quad p = 2, 3, \ldots, N-1$$

$$a_{ii}^{(p)} = -\sum_{r=1, r\neq i}^{N} a_{ir}^{(p)}, \qquad \text{for } i = r \tag{11}$$

Here $a_{ir}^{(p-1)}$ represents the weighting coefficients of partial derivatives of order $(p-1)$ w.r.t. x and $a_{ir}^{(p)}$ represents the weighting coefficients of derivatives of order (p) w.r.t. x. Following the same methodology, we can determine the weighting coefficients $a_{jr}^{(1)}$ and $a_{kr}^{(1)}$ of partial derivatives of order one in the direction of $y - axis$ and $z - axis$ using cubic B-spline functions in modified form. Recurrence formula can be successfully applied to calculate the derivatives of order two and higher.

2.3 Partition and denotations

For time-step discretization, τ is time increment and $\exists$ two positive integers N_1 and n such that $\tau = T/N_1$, $t_n = nt$, $0 \leq n \leq N_1$. For spatial approximations, let h_x, h_y and h_z be $x-$, $y-$ and $z-$ dimensional spatial increments, such that $h_x = (b_1 - a_1)/N$, $h_y = (b_2 - a_2)/M$, $h_z = (b_3 - a_3)/L$ for positive integers N, M, and L. In this way the set $\Omega_h = \{(x_i, y_j, z_k) | 1 \leq i \leq N-1, 1 \leq j \leq M-1, 1 \leq k \leq L-1\}$ is composed of the spatial nodes $(x_i, y_j, z_k) = (a_1 + ih_x, a_2 + jh_y, a_3 + kh_z)$, which are denoted by x_{ijk}.

3 Three-dimensional reaction-diffusion systems

3.1 Brusselator system

For numerical treatment of Brusselator system rewriting Eq. (2) in the first order system, discretizing the derivatives in space using MCB-DQM, we achieve the following system of non-linear ODEs

$$\frac{du_{ijk}}{dt} = A + u_{ijk}^2 v_{ijk} - (B+1)u_{ijk} \tag{12a}$$
$$+ \mu\left(\sum_{r=1}^{N} a_{ir}^{(2)} u(x_r, y_j, z_k, t) + \sum_{r=1}^{M} a_{jr}^{(2)} u(x_i, y_r, z_k, t) + \sum_{r=1}^{L} a_{kr}^{(2)} u(x_i, y_j, z_r, t)\right)$$

$$\frac{dv_{ijk}}{dt} = Bu_{ijk} - u_{ijk}^2 v_{ijk} + \alpha\left(\sum_{k=1}^{N} a_{ir}^{(2)} v(x_r, y_j, z_k, t) + \sum_{r=1}^{M} a_{jr}^{(2)} v(x_i, y_r, z_k, t) + \sum_{r=1}^{L} a_{kr}^{(2)} v(x_i, y_j, z_r, t)\right), \tag{12b}$$

$$\omega \in (x_i, y_j, z_k) / \quad 0 < x_i, y_j, z_k < 1, t > 0 \tag{12c}$$

subject to initial conditions

$$u(x_i, y_j, z_k, 0) = u_0(x_i, y_j, z_k) \tag{13}$$
$$v(x_i, y_j, z_k, 0) = v_0(x_i, y_j, z_k)$$

and no flux boundary conditions.

3.2 Michaelis-Menten type reaction-diffusion equation

For numerical treatment of Michaelis-Menten system rewriting Eq. (4) in the first order system, discretizing the spatial derivatives by using MCB-DQM, we obtain the following system of non-linear ODEs

$$\frac{du_{ijk}}{dt} = d\left(\sum_{r=1}^{N} a_{ir}^{(2)} u(x_r, y_j, z_k, t) + \sum_{r=1}^{M} a_{jr}^{(2)} u(x_i, y_r, z_k, t) \sum_{r=1}^{L} a_{kr}^{(2)} u(x_i, y_j, z_r, t)\right) - \frac{u_{ijk}}{1 - u_{ijk}}, \quad 0 < x, y, z < 1, \quad t > 0, \tag{14}$$

together with homogeneous Dirichlet's boundary conditions and suitable initial conditions.

4 Discretization of three-dimensional non-linear Burgers' equation and stability analysis

For numerical treatment of Burgers' equation rewriting Eq. (6) in the first order system, discreting the spatial derivatives using MCB-DQM, we obtain the following system of non-linear ODEs

$$\frac{du_{ijk}}{dt} = -u_{ijk}\left(\sum_{r=1}^{N} a_{ir}^{(1)} u(x_r, y_j, z_k, t)\right) \tag{15}$$

$$+\sum_{r=1}^{M} a_{jr}^{(1)} u(x_i, y_r, z_k, t) + \sum_{r=1}^{L} a_{kr}^{(1)} u(x_i, y_j, z_r, t)\Big)$$
$$+\frac{1}{R}\Big(\sum_{r=1}^{N} a_{ir}^{(2)} u(x_r, y_j, z_k, t) + \sum_{r=1}^{M} a_{jr}^{(2)} u(x_i, y_r, z_k, t)$$
$$+\sum_{r=1}^{L} a_{kr}^{(2)} u(x_i, y_j, z_r, t)\Big)$$

with given initial and boundary conditions. Von Neumann stability analysis can be easily done when one is working with the classical finite difference. As with the case here, Von Neumann stability criterion can not be used with differential quadrature method discretized systems. For this purpose, matrix stability or energy stability methods have been extensively discussed in literature [38–40].

Let us consider a problem that is time-dependent along with a set of suitable initial and boundary conditions, given as

$$\frac{\partial V}{\partial t} = l(V) \tag{16}$$

Here, l is the operator in space. Discretizing Eq. (16), we attain a system of ODEs:

$$\frac{dv}{dt} = [D_c]v + \bar{b} \tag{17}$$

where v represents unknown functional at knots except at boundaries, D_c denotes the coefficient matrix and $\bar{b}$ is the non-homogeneous part. Stability conditions of the computational method for solving the Eq. (16) are dependent on the stability of ODEs in Eq. (17). The matrix D_c plays an inevitable part as its eigenvalues directly determine the exact solutions. Therefore, the whole scenario can be well described using the eigenvalues of the coefficient matrix. When the real part of all the eigenvalues of D_c, $R(\lambda_i) \le 0$, it shows the stable exact solutions as $t \to \infty$. The matrix D_c can be determined as $[D_{ij}] = -\alpha(a_{ir}^{(1)} + a_{jr}^{(1)} + a_{kr}^{(1)}) + \frac{1}{R}(a_{ir}^{(2)} + a_{jr}^{(2)} + a_{kr}^{(2)})$, where $\alpha = u_{ijk}$.

The stable solution for t tending to infinity requires

1. for real eigenvalues $-2.78 < \Delta t.\lambda_i < 0$,
2. for eigenvalues having complex part only, $-2\sqrt{2} < \Delta t.\lambda_i < 2\sqrt{2}$,
3. For complex eigenvalues, $\Delta t.\lambda_i$ should lie in the sector shown in Figure 1.

For complex eigenvalues, real parts can be small enough positive numbers that lie within a prescribed tolerance limit. [54]. For linearization, we have assumed $\alpha = u_{ijk}$, α constant therefore, the eigenvalues need to be calculated for every problems. As it will induce changes in the entries of the coefficient matrix D. Eigenvalues have been calculated for different grid sizes and have been found in region of stability.

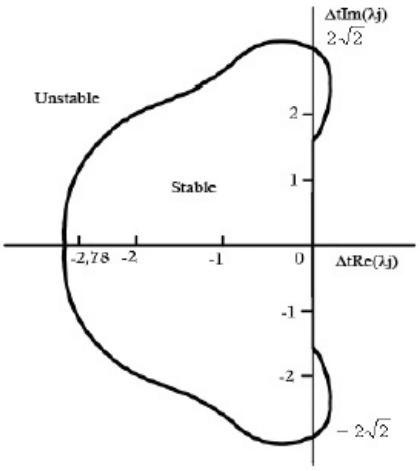

Figure 1: Stability region

5 Boundary conditions with MCB-DQM

Whenever Dirichlet's boundary conditions are given, they can be used directly at the boundary without any manipulation. In the case of Neumann or mixed type boundary conditions, they can be discretized adopting MCB-DQM. They are simplified into solutions at boundary points. Dirichlet's boundary conditions for Michaelis-Menten and Burgers' equation are given as:

$$u(a_1, j, k) = f_1(y_j, z_k, t), \quad u(b_1, j, k) = f_2(y_j, z_k, t) \tag{18}$$
$$u(i, a_2, k) = g_1(x_i, z_k, t), \quad u(i, b_2, k) = g_2(x_i, z_k, t)$$
$$u(i, j, a_3) = s_1(x_i, y_j, t), \quad u(i, j, b_3) = s_1(x_i, y_j, t),$$
$$(x_i, y_j, z_k) \in \Omega$$

Neumann boundary conditions at $x = a_1$ and $x = b_1$ can be approximated as

$$\sum_{r=1}^{N} a_{1r}^{(1)} u(x_r, y_j, z_k, t) = f_1(y_j, z_k, t), \tag{19}$$
$$\sum_{r=1}^{N} a_{Nr}^{(1)} u(x_r, y_j, z_k, t) = f_2(y_j, z_k, t),$$
$$j = 1, 2, \ldots, M, \quad k = 1, 2, \ldots, L \tag{20}$$

Rewritting the above system as:

$$a_{11}^{(1)} u_{(1jk)} + a_{N1}^{(1)} u_{(Njk)} = f_1 - \sum_{r=2}^{N-1} a_{1r}^{(1)} u(x_r, y_j, z_k, t),$$
$$a_{N1}^{(1)} u_{(1jk)} + a_{NN}^{(1)} u_{(Njk)} = f_2 - \sum_{r=2}^{N-1} a_{Nr}^{(1)} u(x_r, y_j, z_k, t),$$
$$j = 1, 2, \ldots, M, \quad k = 1, 2, \ldots, L$$

Solving for u_{1jk} and u_{Njk} we get approximate values at the boundary points $x = a_1$ and $x = b_1$. Similarly, boundary conditions at other boundary points can be calculated. The system of non-linear ODEs can not be solved directly by SSP-RK43 method.

The systems of ordinary differential equations given in system (12), (14) and (15) can be solved using various methods. Using the optimal stability preserving Runge-Kutta method of order three and stage four [SSP-RK43] [55], we solve the system of ODEs. It is not possible to solve this non-linear system of initial-boundary ODEs directly by SSP-RK43 scheme. So, it is dealt by first applying boundary conditions on the system, then a system of non-linear ODEs is obtained. Here, the system in Eqs. (12), (14) and (15) integrated from time t_0 to $t_0 + \Delta t$ through the following operations.

$$\begin{aligned} v^{(1)} &= v^m + \frac{\Delta t}{2} L(v^m) \\ v^{(2)} &= v^{(1)} + \frac{\Delta t}{2} L(v^{(1)}) \\ v^{(3)} &= \frac{2}{3} v^m + \frac{u(2)}{3} + \frac{\Delta t}{6} L(v^{(2)}) \\ v^{(m+1)} &= v^{(3)} + \frac{\Delta t}{2} L(v^{(3)}) \end{aligned} \tag{21}$$

Hence, giving solution v at any specified time level. Here $L(v^m)$ is the right hand side of resultant equation after space discretization at the initial time.

6 Why SSP-RK method

SSP methods [55, 56] also sometimes termed as TVD (total variation diminishing) time discretization sometimes are used for solving a system of ODEs. In [57], a general Runge-Kutta method of order m is formulated as:

$$\begin{aligned} v^{(0)} &= v^n, \\ v^{(i)} &= \sum_{k=1}^{i-1} \left(\alpha_{i,k} v^{(k)} + \Delta t \beta_{i,k} L(v^{(k)}) \right), \alpha_{i,k} \geq 0, \\ i &= 1, \ldots, m \\ v^{(n+1)} &= v^{(m)}. \end{aligned} \tag{22}$$

For the sake of consistent system $\sum_{k=0}^{i-1} \alpha_{i,k} = 1$. The hyperbolic conservation law,

$$\frac{\partial u}{\partial t} = -f(u)_x,$$

where the spatial derivative, $f(u)_x$ is discretized using TVD finite difference with method of lines approximation results into a system of ODEs

$$\frac{d}{dt} u = L(u),$$

We invariably assume that the discretization in space $-L(u)$ posses the attribute that when it combines with forward first-order Euler time discretization,

$$u^{n+1} = u^n + \Delta t L(u^n),$$

then, for a small enough time step governed by the CFL (Courant-Friedrichs-Lewy) condition,

$$\Delta t \leq c \Delta t_{FE},$$

the total variation in discrete solution does not increase in time, where $c = \min_{i,k} \frac{\alpha i,k}{\beta i,k}$, provided $\beta_{i,k} L$ is replaced by $\beta_{i,k} \bar{L}$ whenever $\beta_{i,k}$ is negative. The prime objective of multistep time discretization or high-order SSP Runge-Kutta is to achieve temporal accuracy of higher order and to maintain strong stability property. In short, idea behind SSP methods is to start with a method-of-lines semi-discretization, which is strongly stable in a certain norm, semi-norm, or convex functional under forward Euler time stepping, with suitably restricted time step Δt, and then go for a higher order time discretization maintaining strong stability for the given norm, perhaps under a different time step restriction.

7 Test cases

In this section, the numerical approximations are obtained by implementing MCB-DQM for some examples of both reaction-diffusion system and Burgers' equation. The illustration of the solutions have been done especially for the same parametric values as taken by researchers in their studies for the sake of valid comparison. The computations are carried out with programming in DEV C++. Availability of analytical solutions aids in analyzing the accuracy and reliability of the proposed scheme.

Error analysis is done by using L_∞ and L_2 errors for the computed solutions defined below:

$$L_\infty(u) \cong \max_{1 \leq i \leq M, 1 \leq j \leq M, 1 \leq k \leq L} |u_{ijk} - U_{ijk}|$$

and

$$L_2(u) \cong \sqrt{\sum_{i=1,j=1,k=1}^{i=N,j=M,k=L} |u_{ijk} - U_{ijk}|^2}$$

where u_{ijk} is the approximate solution computed by the proposed scheme and U_{ijk} is the exact solution at the corresponding mesh points (x_i, y_j, z_k) at time t.

7.1 Reaction-diffusion systems

The following section presents some numerical experiments for three-dimensional problems. The calculated results are compared with exact solutions available in literature or compared our result with the work done by researchers in the same field.

Problem 1. Brusselator model The three-dimensional analogue of present one-dimensional Brusselator system [59]:

$$\frac{\partial u}{\partial t} = A + u^2 v - (B+1)u + \alpha \nabla^2 u, \tag{23a}$$

$$\frac{\partial v}{\partial t} = Bu - u^2 v + \alpha \nabla^2 u, \quad \mathbf{x} \in \Omega \times (\mathbf{0}, \mathbf{T}] \tag{23b}$$

with no flux boundary conditions and following initial conditions

$$u(x, y, z, 0) = 1 + sin(2\pi x) sin(2\pi y) sin(2\pi z),$$

$$v(x, y, z, 0) = 3,$$

To compare our results with those given in [59], the parameters are set accordingly. We have taken $A = 2.0$, $B = 1.0$, $h = 0.01$, $k = 0.001$, and $\mu = 0.02$. Here $\Delta x = \Delta y = \Delta z = h$ and k is the time step. Table 2 shows that at every grid point, the value of u and v approach 2 and 0.5, respectively as t increases. The plots of approximate values of u and v at the grid point (0.5, 0.5) along z-direction vs. time t are shown in Figure 2. It can be seen from Figure 2 that $(u, v) \in$ (2.0, 0.5) along z-direction as time t increases. These observations comply with the theoretical results of [30], which claims that whenever the parameters A and B are chosen such that $1-A+B^2 \geq 0$, then the values of u and v approach B and A/B, respectively.

Table 2: Approximated solution for Problem 1 with $A = 1.$, $B = 2.$, $\mu = 0.02$ at different mesh points and different values of t

t	(0.2, 0.2, 0.2)		(0.8, 0.9, 0.8)	
	u	v	u	v
1.0	2.951770	0.326131	3.006090	0.329108
2.0	2.292070	0.422134	2.303350	0.419887
3.0	2.077210	0.473946	2.078890	0.473407
4.0	2.017370	0.493274	2.017580	0.493198
5.0	2.003430	0.498565	2.003450	0.498556
6.0	2.000620	0.499953	2.000100	0.499729
7.0	2.000100	0.422134	2.303350	0.499953
8.0	2.00002	0.499992	2.00002	0.499992
9.0	2.000000	0.499999	2.000000	0.499999
10.0	2.000000	0.500000	2.000000	0.500000
↓	↓	↓	↓	↓
∞	2.000000	0.500000	2.000000	0.500000

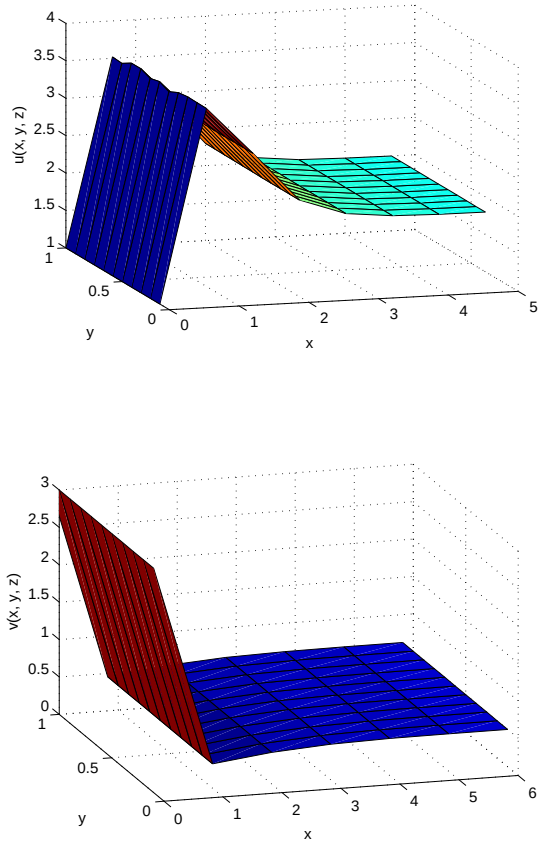

Figure 2: Plot of $u(0.3, 0.3, :)$ and $v(0.3, 0.3, :)$ vs. time with parameters $A = 1.0$, $B = 2.0$, $h = 0.1$, time step $k = 0.001$ and α

Figure 3 represents the values of u and v for the same step-length, time-step and μ, but for different values of A and B. Here we have taken $A = 3.$ and $B = 1.$ The values of u and v are approximated until time $t = 60$. The solutions are found to be oscillatory and not convergent to any fixed concentration. The outcome shows compliance with the observation in [59], that the solution does not converge to any fixed concentration, whenever the parameters A and B are chosen such that $1 - A + B^2 \leq 0$

Problem 2. [59] In this problem, the three-dimensional Brusselator system is studied. The exact solution is:

$$\begin{cases} u(x, y, z, t) = exp(-x - y - z - 0.5t) \\ v(x, y, z, t) = exp(x + y + z + 0.5t) \end{cases} \tag{24}$$

Table 3 gives the L_2 and L_∞ errors for the concentrations u and v, taking the parametric values as $B = 1.0$, $A = 0$, $\alpha = 1.0/6.0$ at different t values. The errors have been calculated with $N = M = L = 21$.

Table 3: Errors of Problem 2 with $A = 0.$, $B = 1.$, $\mu = 1/6$ at for varying time

t	L_2 Error		L_∞ Error	
	u	v	u	v
0.1	1.90385E-005	4.00995E-005	2.19122E-005	4.723245E-005
1.0	2.08566E-005	9.03154E-005	1.47474E-005	7.70677E-005
2.0	1.27933E-005	1.49674E-004	8.94614E-006	1.12714E-004
3.0	7.76417E-006	2.47037E-004	5.42659E-006	2.09640E-004
4.0	4.71003E-006	4.07456E-004	3.29150E-006	3.45643E-004
5.0	2.85838E-006	6.71543E-004	1.99741E-006	5.69587E-004
10.0	2.34522E-007	8.18585E-004	1.62877E-007	6.94249E-004

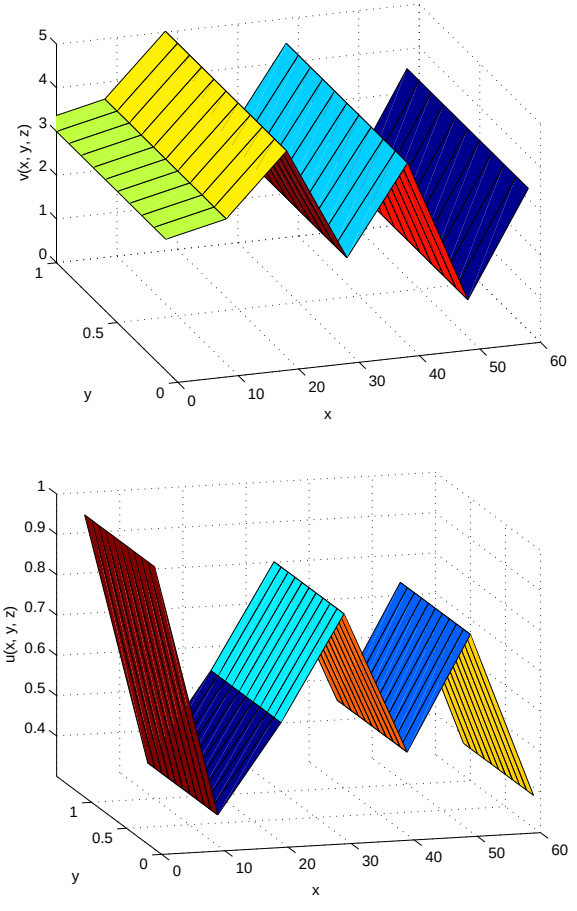

Figure 3: Plot of $u(0.3, 0.3, :)$ and $v(0.3, 0.3, :)$ vs. time with parameters $A = 3.0$, $B = 1.0$, $h = 0.1$, time step $k = 0.001$ and α

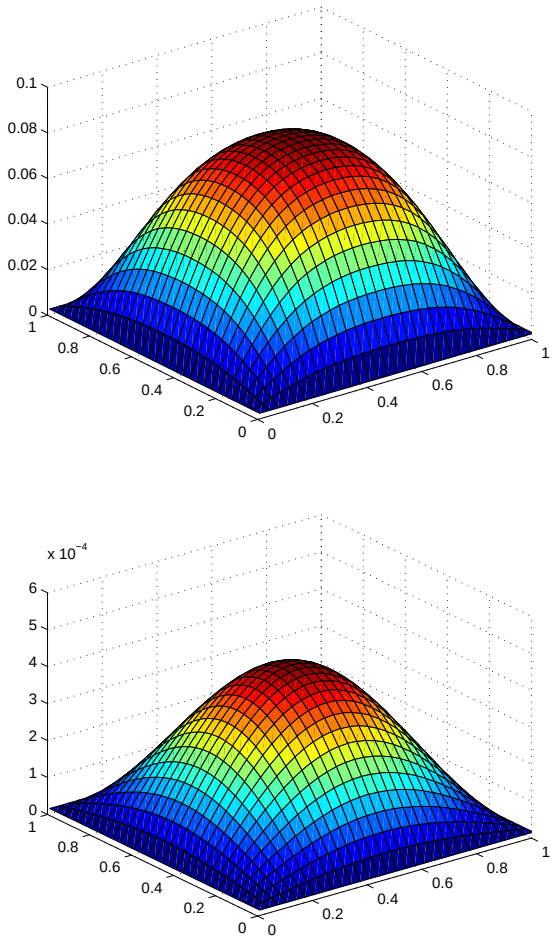

Figure 4: Numerical solution of Problem 3 with $N = 30$ and time step 0.001 for final time $t = 0.1$ and 1

Problem 3. In this example, the three-dimensional Michaelis-Menten system is considered with homogeneous Dirichlet's boundary and initial condition [59]:

$$u(x, y, z, 0) = 1, 0 \le x, y, z \le 1.$$

In the problem, there exists a discontinuity between given initial and boundary conditions, that causes solutions to show spurious oscillations. This problem solved with MCB-DQM shows that this scheme has a capability of damping specious oscillations caused by high frequency components in the solution. The computations are carried out for $t = 1$, 2 and $t = 3$. Figure 4 and 5 depicts the results

Table 4: Error estimation for problem 4 for different times and different values of R

R	$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 10$
R = 1, h = 1/10, $\Delta t = 0.001$	2.38653E-006	1.00550E-006	2.29000E-006	1.74900E-007	2.23800E-010
R = 10, h = 1/10, $\Delta t = 0.001$	3.54000E-004	3.29200E-005	4.46100E-014	4.48000E-014	4.48400E-014
R = 50, h = 1/20, $\Delta t = 0.010$	2.30000E-003	5.15700E-006	9.03100E-015	9.03900E-015	8.97000E-015
R = 100, h = 1/20, $\Delta t = 0.010$	2.41000E-002	1.32000E-006	7.79900E-015	8.11500E-015	8.08900E-015
R = 500, h = 1/20, $\Delta t = 0.010$	2.24615E-001	4.21000E-003	4.13300E-008	5.53000E-014	8.27170E-015

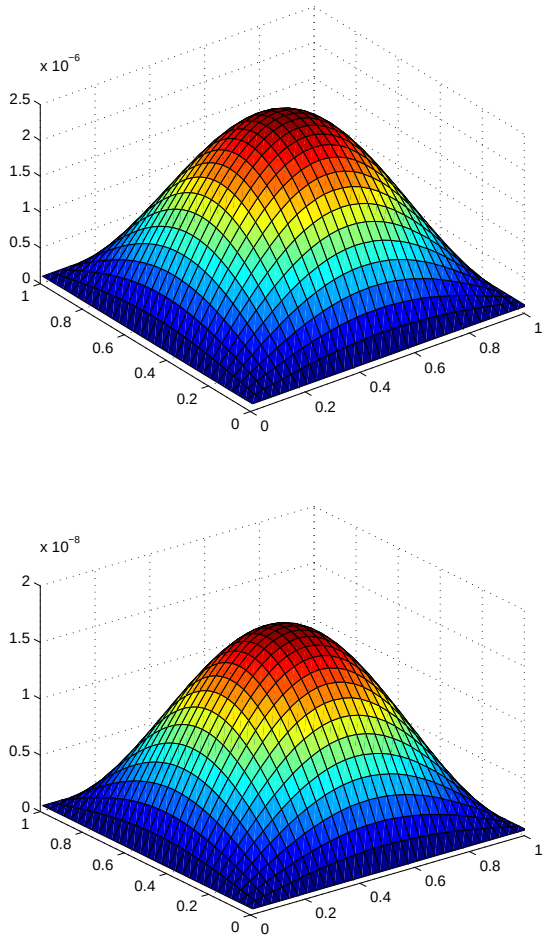

Figure 5: Numerical solution of Problem 3 with $N = 30$ and time step 0.001 for final time $t = 2$ and 3

with time-step 0.001 and mesh-size $N = M = L = 31$. The value of d is taken as 0.2.

Problem 4. Three-dimensional Burgers' equation: Here we consider the three-dimensional Burgers' equation over the domain $[-0.5, 0.5]\times[-0.5, 0.5]\times[-0.5, 0.5]$, initial and boundary conditions have been taken from the exact solution

$$u(x, y, t) = 1 - tanh\left(\frac{(x + y + z - 2t)R}{3}\right)$$

We have obtained numerical solution for $t = 0.1, 1, 3, 5$ and 10. Table 4 gives the error estimation for varying values of R.

8 Conclusion

In this work, differential quadrature method based on a modification in cubic B-spline functions have been applied for the first time to non-linear three-dimensional reaction-diffusion equations and Burgers' equation. The method employed in this work elaborates an approach to numerically approximate solutions for three-dimensional equations. The method efficiently provides accurate approximations for variable sets of parametric values. The efficiency and reliability of the approach have been evaluated for test problems under consideration. Different error norms are calculated for varying times or the results present in literature are compared with the numerical solutions achieved by the used method. The approximated solutions and the corresponding error norms are presented in tables for varying time levels and for varying sets of parametric values. We also note that for large values of R, Burgers' equation behaves merely as hyperbolic partial differential equation, and the problem becomes very difficult to solve as a steep shock-like wave front is developed. The results show that error decreases with the increase in time. We see that the solutions become better with decreasing values of time step. The method gives convergent solutions and for different cases, handles the equations efficiently even for non-linear ones. The obtained approximations are satisfactory and in compliance with the results available in the literature. The strong point of the method is its ease of implementation and less complexity and calculations. The method is economically cheap and can be relied upon. Therefore, it is suggested that the method can be used as an alternative for the class of three-dimensional reaction-diffusion equation. The possibility of extending

present approach may be useful to solve partial differential equations of higher order appearing in various applications of engineering and science.

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References

[1] Mittal R.C., Dahiya S., et al., Numerical simulation on hyperbolic diffusion equations using modified cubic B-spline differential quadrature methods, Computers and Mathematics with Applications, 2015, 70.5, 737-749.

[2] Zhao S., Ovadia J., Liu X., Zhang Y.T., Nie Q., et al., Operator splitting implicit integration factor methods for stiff reaction–diffusion–advection systems, J. Comput. Phys., 2011, 230(15), 5996-6009.

[3] Marek M., and Schreiber I., Chaotic behaviour of deterministic dissipative systems (Vol. 1). Cambridge University Press, 1995.

[4] Nicolis G., and Prigogine I., Self-organization in nonequilibrium systems (Vol. 191977). Wiley, New York, 1977.

[5] Ersoy O., Daĝ I., et al., Numerical solutions of the reaction diffusion system by using exponential cubic B-spline collocation algorithms. Open Phys., 2015, 13: 414-427.

[6] Cherruault Y., Choubane M., Valleton J.M., Vincent J.C., et al., Stability and asymptotic behavior of a numerical solution corresponding to a diffusion-reaction equation solved by a finite difference scheme (Crank-Nicolson), Computers and Mathematics with Applications, 1990, 20(11), 37-46.

[7] Turing A.M., The chemical basis of morphogenesis, Philosophical Transactions of the Royal Society of London B: Biological Sciences, 237(641), 1952, 37-72.

[8] Lefever R., Nicolis G., et al., Chemical instabilities and sustained oscillations, Journal of theoretical Biology, 1971, 30(2), 267-284.

[9] Twizell E.H., Gumel A.B., Cao Q., et al., A second-order scheme for the Brusselator reaction–diffusion system, J. Math. Chem., 1999, 26(4), 297-316.

[10] Adomian G., The diffusion-Brusselator equation. Computers and Mathematics with Applications, 1995, 29(5), 1-3.

[11] Cherruault Y., Choubane M., Valleton J.M., Vincent J.C., et al., Stability and asymptotic behavior of a numerical solution corresponding to a diffusion–reaction equation solved by a finite difference scheme (Crank–Nicolson Scheme), Comput. Math. Appl., 1990, 20 (11), 37-46.

[12] http://www.worthington-biochem.com/introbiochem/substrateconc.html

[13] L.G. Harrison, Kinetic Theory of Living Pattern, Cambridge University Press, 1993.

[14] Sherratt J.A., Murray J.D., et al., Models of epidermal wound healing, Proc. R. Soc. Lond. B, 1990, 241, 29-36..

[15] Chaplain M.A.J., Reaction-diffusion pre-patterning and its potential role in tumour invasion, J. Bio. Systems, 1995, 3, 929-936.

[16] Murray J.D., Stanley E.A., Brown D.L., et al., On the Spatial Spread of Rabies among Foxes, Proc. R. Soc. Lond. B, 1986, 229, 111-150.

[17] Holmes E.E., Lewis M.A., Banks J.E., Veit R.R., et al., Spatial Interactions and Population Dynamics, Ecology, 1994, 75(1), 17—29.

[18] Burgers J.M., A mathematical model illustrating the theory of turbulence, Advances in applied mechanics, 1948, 1, 171-199.

[19] Khater A.H., Temsah R.S., Hassan M.M., et al., A Chebyshev spectral collocation method for solving Burgers'-type equations, J. Comput. Appl. Math., 2008, 222(2), 333-350.

[20] Ames W.F. (Ed.). Nonlinear partial differential equations in engineering (Vol. 1). Academic press, 1965.

[21] Karpman V.I. Non-Linear Waves in Dispersive Media: International Series of Monographs in Natural Philosophy (Vol. 71). Elsevier, 2016.

[22] Ali A., Haq S., et al., A computational meshfree technique for the numerical solution of the two-dimensional coupled Burgers' equations, International Journal for Computational Methods in Engineering Science and Mechanics, 2009, 10(5), 406-422.

[23] Perko J., Sarler B., et al., Weight function shape parameter optimization in meshless methods for non-uniform grids, Computer Modeling in Engineering and Sciences, 19(1), 2007, 55.

[24] Nee J., Duan J., et al., Limit set of trajectories of the coupled viscous Burgers' equations. Applied mathematics letters, 1998, 11(1), 57-61.

[25] Zhang W, Zhang C.H., Guang X., et al., An explicit Chebyshev pseudospectral multigrid method for incompressible Navier–Stokes equations. Computers and Fluids, 2010, 39, 1, 178-188.

[26] Dogan A., A Galerkin finite element approach to Burgers' equation. Appl. Math. Comput., 2004, 157(2), 331-346.

[27] Kumar Pany A., Nataraj, N., Singh, S., et al., A new mixed finite element method for Burgers' equation, Journal of Applied Mathematics and Computing, 2007, 23(1-2), 43-55.

[28] Golmankhaneh A.K., Khatuni T., Porghoveh N.A., Baleanu D., et al,. Comparison of iterative methods by solving nonlinear Sturm-Liouville, Burgers and Navier-Stokes equations, Central European Journal of Physics, 2012, 10(4), 966-976.

[29] Asaithambi A., et al., Numerical solution of the Burgers' equation by automatic differentiation, Appl. Math. Comput., 2010, 216, 2700-2708.

[30] Bellman R., Kashe B.G., Casti J., et al., Differential quadrature: a technique for the rapid solution of non-linear partial differential equations, J. Comput. Phys., 1972, 10, 40-52.

[31] Shu C., Differential Quadrature and its Application in Engineering, Athenaeum Press Ltd., Great Britain, 2000.

[32] Quan J.R., Chang C.T., et al., Newinsights in solving distributed system equations by the quadrature methods, I. Comput. Chem. Eng., 1989, 13, 779 - 788.

[33] Quan J.R., Chang C.T., et al., Newinsights in solving distributed system equations by the quadrature methods-II, Comput. Chem. Eng., 1989, 13, 1017-1024.

[34] Korkmaz A., Daĝ I., et al., Shock wave simulations using Sinc DQM, Eng. Comput., 2011, 28(6), 654 - 674.

[35] Korkmaz A., Daĝ, I., et al., A differential quadrature algorithm for nonlinear Schrödinger equation. Nonlinear Dynamics, 2009, 56(1-2), 69-83.

[36] Mittal R.C., Jiwari R., Sharma K.K., et al., A numerical scheme based on differential quadrature method to solve time depen-

dent Burgers' equation. Engineering Computations, 2012, 30(1), 117-131.
[37] Tomasiello S., Solving 2D-wave problems by the iterative differential quadrature method, Int. J. Comput. Math., 2011, 88(12), 2550-2566.
[38] Tomasiello S., Stability and accuracy of the iterative differential quadrature method. International journal for numerical methods in engineering, 2003, 58(9), 1277-1296.
[39] Tomasiello S., Numerical solutions of the Burgers-Huxley equation by the IDQ method, Int. J. Comput. Math, 2010, 87(1), 129-40.
[40] Tomasiello S., Numerical stability of DQ solutions of wave problems, Numerical Algorithms, 2011, 57(3), 289-312.
[41] Korkmaz A., Numerical algorithms for solutions of Korteweg-de Vries equation. Numer. Methods Partial Differential Equations, 2010, 26(6), 1504-1521.
[42] Arora G., Singh B.K., et al., Numerical solution of Burgers' equation with modified cubic B-spline differential quadrature method, Applied Mathematics and Computation, 2013, 224, 166-177.
[43] Jiwari R., Yuan J., et al., A computational modeling of two dimensional reaction–diffusion Brusselator system arising in chemical processes, 2014, 52(6), 1535-1551.
[44] Bashan A., Karakoc S.B.G., Geyikli T., et al., Approximation of the KdVB equation by the quintic B-spline differential quadrature method, Kuwait Journal of Science, 2015, 42(2).
[45] Korkmaz A., Daĝ I., et al., Quartic and quintic B-spline methods for advection-diffusion equation, Appl. Math. Comput., 2016, 274, 201-219.
[46] Krowick A., Hermite type radial basis finction-based differential quadrature method for higher order equations, Applied Mathematical modelling, 2016, 40(3), 2421-2430.
[47] Barrera D., Gonzàlez P., Ibàñez F., Ibàñez M.J., et al., A general soline differential quadrature method based on quasi-interpolation, J Comput. Appl. Math., 2015, 275, 465-479.
[48] Shukla H.S., Tamsir M., Srivastava V.K., Kumar J., et al., Numerical solution of two dimensional coupled viscous Burger equation using modified cubic B-spline differential quadrature method, AIP Advances, 2014, 4, 117-134.
[49] Shukla H.S., Tamsir M., Srivastava V.K., et al., Numerical simulation of two dimensional sine-Gordon solitons using modified cubic B-spline differential quadrature method, AIP Advances, 2015, 5, 017121.
[50] Shukla H.S., Tamsir M., Srivastava V.K., Rashidi M. M. et al., Modified cubic B-spline differential quadrature method for numerical solution of three-dimensional coupled viscous Burger equation, Modern Physics Letters B 30(11), Modern Physics Letters B, 2016, 30(11), 16501 10-27.
[51] Mittal R.C., Jain R.K., et al., Numerical solutions of nonlinear Burgers' equation with modified cubic B-splines collocation method, Appl. Math. Comput., 2012, 218, 7839-7855.
[52] Korkmaz A., Daĝ I., Cubic B-spline differential quadrature method for advection-diffusion equations. International Journal of Numerical Methods for Heat and Fluid flow, 2012, 22(8), 1021-1036.
[53] Korkmaz A., Akmaz H.K., et al., Numerical simulations for transport of conservative pollutants, Selcuk Journal of Applied Mathematics, 2015, 16(1).
[54] Jain M.K., Numerical Solution of Differential Equations, 2nd ed.,Wiley, New York, NY, 1983.
[55] Ruuth S.J., and Spiteri R.J., et al., A new class of optimal high-order strongstability-preserving time-stepping schemes, SIAM J. Numer. Anal., 2002, 40 (2), 469-491.
[56] Shu C., Total-variation-diminishing time discretizations, SIAM J. Sci. Statist. Comput., 1988, 9, 1073-1084.
[57] Ruuth S.J., Spiteri R.J., et al., Two barriers on strong-stability-preserving time discretization methods, J. Sci. Comp., 2002, 17, 211-220.
[58] Stenger F., Numerical methods based on Wittaker cardinal or sinc functions, SIAM Review, 1983, 23, 165-224.
[59] Bhatt H.P., Khaliq A.Q.M., et al., The locally extrapolated exponential time differencing LOD scheme for multidimensional reaction–diffusion systems, J. Comput. Appl. Math., 2015, 285, 256 - 278.