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Numerical simulation of reaction-diffusion systems by modified cubic B-spline differential quadrature method

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ABSTRACT

In this paper, we have applied modified cubic B-spline based differential quadrature method to get numerical solutions of one dimensional reaction-diffusion systems such as linear reaction-diffusion system, Brusselator system, Isothermal system and Gray-Scott system. The models represented by these systems have important applications in different areas of science and engineering. The most striking and interesting part of the work is the solution patterns obtained for Gray Scott model, reminiscent of which are often seen in nature. We have used cubic B-spline functions for space discretization to get a system of ordinary differential equations. This system of ODE's is solved by highly stable SSP-RK43 method to get solution at the knots. The computed results are very accurate and shown to be better than those available in the literature. Method is easy and simple to apply and gives solutions with less computational efforts.

1. Introduction

We consider time dependent nonlinear reaction-diffusion system

$$\begin{cases} \dfrac{\partial u}{\partial t} = a_1 \dfrac{\partial^2 u}{\partial x^2} + f_1(u, v) \\ \dfrac{\partial v}{\partial t} = a_2 \dfrac{\partial^2 v}{\partial x^2} + f_2(u, v) \end{cases} \tag{1}$$

with Dirichlet or Neumann boundary conditions in the domain [a, b]. Here u(x, t) and v(x, t) are real valued functions while a_1 and a_2 are constants, known as diffusion coefficients. Basically, reaction-diffusion systems are mathematical models which correspond to several physical phenomena. Reaction-diffusion systems have great applications in chemistry and also describe dynamical processes in non-chemical areas such as biology, geology, physics (neutron diffusion theory) and ecology. We can see that when reaction-diffusion system is represented mathematically, it takes the form of semi-linear parabolic partial differential Eq. (1) which include Brusselator [1], Isothermal [2], Gray Scott [3] and Schnakenberg [4] models and many others. Recently many researchers have been attracted to solve reaction-diffusion systems numerically. Sahin [5] applied B-spline finite element method to get numerical solutions of such systems. Numerical study of these systems can be found in [6–8] by different methods. The solutions of reaction-diffusion systems display a wide range of behaviours, including the formation of traveling waves [9] and wave-like phenomena as well as other self-organized patterns like stripes, hexagons or more intricate structures like dissipative solitons.

B-spline based differential quadrature method has never been used to solve reaction-diffusion systems. The study of literature on the numerical solutions of reaction-diffusion systems shows that such type of systems have been solved by using exponential cubic B-splines collocation algorithms [10]. Ruuth [11] studied reaction-diffusion systems by implicit-explicit methods to obtain patterns which have great applications in biology. In [12] Zegeling and Kok presented adaptive moving mesh method for solution of reaction-diffusion system. Lopez and Ramos [2] applied linearized methods to study isothermal reaction-diffusion system. Turing [13] considered some reaction-diffusion systems in case of an isolated ring of cells. He considered a reaction-diffusion system on a sphere also. It can be seen that chemical reactions and diffusion systems produce spatial patterns of chemical concentrations under specific conditions. Such type of patterns are of great importance in biology [14–17].

In seeking efficient discretization technique to obtain accurate numerical solutions using considerably small number of grid points, Bellman et al. [18] introduced the method of differential quadrature. In this method partial derivative of a function with respect to coordinate direction is expressed as a linear weighted sum of all the functional values at all the mesh points along that direction. The key to differential quadrature is to determine weighting coefficients for discretization of derivatives of any order. Bellman et al. [18] used two approaches for the calculation of weighting

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coefficients. Later Quan and Chang [19,20] and Shu and Richards [21] derived a recursive formula which does not depend on the number and sampling of grid points. The DQ method can yield highly accurate solution with relatively little computational effort because it needs to be applied at a few number of grid points. To calculate weighting coefficients, we use base functions. There are many functions which can be used as base functions such as Lagrange polynomials, splines, sinc functions, Bernstein polynomials and cosine functions. In our work, cubic B-splines have been used for space discretization to obtain a system of ordinary differential equations. The solution of system of ordinary differential equations is found by using SSP-RK43 [22] method.

Differential quadrature method has been successfully applied to solve various linear and nonlinear 1D and 2D PDE's of engineering, chemistry and physics problems. Feng and Bert [23] used differential quadrature to study flexural vibration of a geometrically nonlinear beam. Tomasiello [24] applied Lagrange polynomial based differential quadrature method. Mittal and Jiwari [25] used differential quadrature to solve two dimensional Burgers' equation. Korkmaz et al. used cosine expansion based differential quadrature method to solve RLW equation [26]. Sinc differential quadrature for the solution of Burgers' equation has been used by Kormaz and Dag [27]. A polynomial Differential quadrature method has been applied by Mittal and Jiwari [28]. Mittal and Bhatia [29] studied hyperbolic telegraph equation by modified B-spline differential quadrature method (Table 1). Bashan et al. [30] used quintic B-spline differential quadrature method to solve the Korteweg de veries Burgers' equation while Jiwari and Verma [31] applied cosine functions as base functions in differential quadrature method to solve two dimensional hyperbolic equations. Ali Bashan [32] and Korkmaz [33] used differential quadrature method for numerical study of modified Burgers' equation and transport of conservative pollutants respectively. Some more work on DQM can be seen in [34–36].

The outline of the paper is as follows. In Section 2, cubic B-spline and modified cubic B-spline functions are explained. In Section 3, procedure for implementation of the cubic B-spline differential quadrature method to Eq. (1) is explained. Implementation of boundary conditions is also discussed in the same section. We present 4 reaction-diffusion systems to check the adaptability and accuracy of the proposed method computationally in Section 4. Stability analysis for the method is done in Section 5. In Section 6, numerical results are discussed. last section contains some concluding remarks.

2. Cubic B-spline functions

A spline is a function that is piecewise defined by polynomial functions and possesses high degree of smoothness at the places where polynomial pieces connect. A B-spline is a spline function that has minimal support with respect to given degree smoothness and domain partition.We consider a uniform partition of the domain $a \le x \le b$ by the knots x_i, $i = 1, 2 \ldots N$ such that $x_i - x_{i-1} = h$ is the length of each interval. The cubic B-spline functions are defined as follows

$$B_j(x) = \frac{1}{h^3}\begin{cases} (x - x_{j-2})^3, & x \in [x_{j-2}, x_{j-1}], \\ (x - x_{j-2})^3 - 4(x - x_{j-1})^3, & x \in [x_{j-1}, x_j], \\ (x_{j+2} - x)^3 - 4(x_{j+1} - x)^3, & x \in [x_j, x_{j+1}], \\ (x_{j+2} - x)^3, & x \in [x_{j+1}, x_{j+2}], \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

where the collection $\{B_0(x), B_1(x), B_2(x), ..., B_N(x), B_{N+1}(x)\}$ forms a basis over the considered interval [37,38].

Modified cubic B-spline basis functions [39] at the knots are defined by

$$\tilde{B_1}(x) = B_1(x) + 2B_0(x), \quad j = 1 \tag{3}$$

Table 1
Cubic B-spline and its derivatives at the knots.

x	x_{j-2}	x_{j-1}	x_j	x_{j+1}	x_{j+2}
$B_i(x)$	0	1	4	1	0
$B_i^{'}(x)$	0	$\frac{3}{h}$	0	$\frac{-3}{h}$	0
$B_i^{''}(x)$	0	$\frac{6}{h^2}$	$\frac{-12}{h^2}$	$\frac{6}{h^2}$	0

$$\tilde{B_2}(x) = B_2(x) - B_0(x), \quad j = 2 \tag{4}$$

$$\tilde{B_i}(x) = B_i(x), \quad j = 3, 4, 5 \ldots ..N - 2 \tag{5}$$

$$\tilde{B}_{N-1}(x) = B_{N-1}(x) - B_{N+1}(x), \quad j = N - 1 \tag{6}$$

$$\tilde{B_N}(x) = B_N(x) + 2B_{N+1}(x), \; j = N \tag{7}$$

where $\left\{\tilde{B_1}(x), \tilde{B_2}(x), \ldots .\tilde{B_N}(x)\right\}$ forms a basis over the considered interval. The B-splines are modified to (2.2) – (2.6), so that the boundary conditions given in terms of u or $\frac{\partial u}{\partial x}$ can be put easily. Moreover, the resulting matrices for $\frac{\partial u}{\partial x}$ and $\frac{\partial^2 u}{\partial x^2}$ etc at different points are also diagonally dominant.

3. Description of the method

Differential quadrature method is a numerical technique [18] to solve ordinary and partial differential equations. In DQM, we approximate the derivatives of unknown function with respect to any coordinate direction by using linear sum of functional values along that direction in the whole domain. The main task in DQM is the calculation of weighting coefficients.

3.1. Calculation of weighting coefficients

The first order derivatives at the knots are approximated as

$$\tilde{B_l'}(x_i) = \sum_{j=1}^{N} w_{ij}^{(1)} \; \tilde{B_l}(x_j), \; i = 1, 2..N \text{ and } l = 1, 2, 3 \ldots .N$$

at the first knot

$$\tilde{B_l'}(x_1) = \sum_{j=1}^{N} w_{1j}^{(1)} \; \tilde{B_l}(x_j) \text{ , l=1,2,3....N}$$

we obtain following matrix

$$\begin{pmatrix} 6 & 1 & & & & & \\ 0 & 4 & 1 & & & & \\ & 1 & 4 & 1 & & & \\ .. & .. & .. & .. & .. & .. & .. \\ & & & 1 & 4 & 1 & \\ & & & & 1 & 4 & 0 \\ & & & & & 1 & 6 \end{pmatrix} \times \begin{pmatrix} w_{11}^{(1)} \\ w_{12}^{(1)} \\ . \\ . \\ . \\ . \\ w_{1N}^{(1)} \end{pmatrix} = \begin{pmatrix} \frac{-6}{h} \\ \frac{6}{h} \\ 0 \\ . \\ . \\ . \\ 0 \end{pmatrix}$$

This is a tridiagonal system and contains N unknowns $w_{11}^{(1)}, w_{12}^{(1)}, .., w_{1N}^{(1)}$ which can be evaluated by solving the above system by Thomas algorithm. Similarly, at the second knot we obtain

$$\tilde{B_l'}(x_2) = \sum_{j=1}^{N} w_{2j}^{(1)} \; \tilde{B_l}(x_j), \; l = 1, 2, 3 \ldots .N$$

which produces the following tridiagonal system of equations

$$\begin{pmatrix} 6 & 1 & & & & & \\ 0 & 4 & 1 & & & & \\ & 1 & 4 & 1 & & & \\ .. & .. & .. & .. & .. & .. & .. \\ & & & 1 & 4 & 1 & \\ & & & & 1 & 4 & 0 \\ & & & & & 1 & 6 \end{pmatrix} \times \begin{pmatrix} w_{21}^{(1)} \\ w_{22}^{(1)} \\ . \\ . \\ . \\ . \\ w_{2N}^{(1)} \end{pmatrix} = \begin{pmatrix} \frac{-3}{h} \\ 0 \\ \frac{3}{h} \\ . \\ . \\ . \\ 0 \end{pmatrix}$$

This system again contains N unknowns $w_{21}^{(1)}$, $w_{22}^{(1)}$,....,$w_{2N}^{(1)}$. We solve this system by Thomas algorithm. Similarly, we proceed to