Chaos, Solitons and Fractals 103 (2017) 422–439

Contents lists available at ScienceDirect

Chaos, Solitons and Fractals

Nonlinear Science, and Nonequilibrium and Complex Phenomena

journal homepage: www.elsevier.com/locate/chaos

Numerical simulation to capture the pattern formation of coupled reaction-diffusion models

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ARTICLE INFO

Article history:
Received 1 March 2017
Revised 9 June 2017
Accepted 19 June 2017

Keywords:
Coupled reaction-diffusion models
Trigonometric cubic B-spline functions
Differential quadrature method
Thomas algorithm
Travailing wave solution

ABSTRACT

This work deals to capture the different types of patterns of nonlinear time dependent coupled reaction-diffusion models. To accomplish this work, a new differential quadrature (DQ) algorithm is developed with the help of modified trigonometric cubic B-spline functions. The stability part of the developed algorithm is studied by matrix stability analysis method. In the experimental part, different types of patterns of Gray–Scott, Schnakenberg, Isothermal Chemical and Brusselator Models are captured which are similar to the existing patterns of the models.

1. Introduction

Turing patterns play very important role to study the characteristics of biological and chemical reactions. To capture Turing patterns of various phenomena become popular after the famous work by Turing [1]. Mathematical modelling of biological and chemical phenomena lies under the category of reaction-diffusion models. Reaction-diffusion models are very important for chemical species which produce a variety of patterns, represent chemical exchange reactions, pattern formation of biological phenomenon, reminiscent of those often seen in nature. Recently, numerical simulation of reaction-diffusion models has become interested area of research to capture the patterns of chemical exchange reactions, dynamical transitions of Turing patterns, interaction of pulses, Self replicating pulse patterns and dynamic pulse-splitting process.

In this work, the authors attempt to capture the patterns of nonlinear time dependent coupled reaction-diffusion of one and two dimensional models. Generally, $(n+1)$ dimensional time dependent coupled reaction-diffusion models can be defined as

$$\begin{aligned}
\frac{\partial u}{\partial t} &= a_1\Delta u + a_2 u + a_3 v + a_4 + f(u,v),\\
\frac{\partial v}{\partial t} &= b_1\Delta v + b_2 u + b_3 v + b_4 + g(u,v),\\
(X,t) &= (x_1, x_2, \ldots, x_n, t) \in \Omega\times[0,T]
\end{aligned} \tag{1.1}$$

where n is a positive integer, $u(X,t)$, $v(X,t)$ are the concentrations of two chemical species, Δ is the Laplacian operator in n spatial dimensions, $\Omega = [a_1,\ b_1]\times[a_2,\ b_2]\times\ldots\times[a_n,\ b_n]\subseteq\Re^n$, $a_i, b_i, i = 1, 2, \ldots, n$ are constant parameters The initial and boundary conditions associated with Eq. (1.1) are given by

$$\begin{cases} u(X,0) = f_1(X), \\ v(X,0) = f_2(X), \qquad X\in\Omega \end{cases} \tag{1.2a}$$

$$\begin{cases} Bu(X,t) \\ Bv(X,t), \qquad X\in\partial\Omega \end{cases} \tag{1.2b}$$

where B Dirichlet or Neumann operator.

The Eq. (1.1) is connexion of many well known reaction-diffusion mathematical models such as Gray Scott [2], Isothermal [3], Glycolysis [4], Brusselator [4,5], Schnakenberg [6] models and many others.

Analytical and numerical solutions perusal of reaction-diffusion models is an interesting and challenging area of research. The solution study of these models helps to capture their patterns and species interact with each other. Many authors [7–10,42–51] studied these type of models numerically as well as analytically. The solutions of reaction-diffusion models exhibit a wide range of behaviours of natural phenomenon in form of wave-like phenomena and traveling waves [11] as well as other self-organized patterns like stripes, hexagons, or more complex structures like dissipative solitons.

In this article, the authors used a new type of basis functions modified trigonometric cubic B-spline to find the weight coeffi-

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http://dx.doi.org/10.1016/j.chaos.2017.06.023
0960-0779/

cients of DQ method different from the traditional techniques of Lagrange interpolation and cubic B-spline functions [12–15] and developed a new DQ approach to simulate the patterns of coupled reaction-diffusion models. The approach converts the coupled system into a system of ordinary differential equations (ODEs). Finally, the obtained system is solved by four-stage RK4 scheme [16]. The stability of the new approach is discussed with the help of matrix stability analysis method. In the computational part, some well known coupled reaction-diffusion models are considered to check the accuracy and efficiency of the proposed approach.

2. Basic description of differential quadrature method

In last some decades, DQ methods become popular for solving partial differential equations. These methods approximate the spatial derivatives of unknown function over one dimensional domain $\Omega = [a, b]$ in the following way

$$u_x(x_i, t) = \sum_{j=1}^{N} \omega_{ij}^{(1)} u(x_j, t), \quad i = 1, 2, ...N \tag{2.1}$$

$$u_{xx}(x_i, t) = \sum_{j=1}^{N} \omega_{ij}^{(2)} u(x_j, t), \quad j = 1, 2, ...N \tag{2.2}$$

where $\omega_{ij}^{(1)}$ and $\omega_{ij}^{(2)}$ are unknown weighting coefficients of first and second derivatives respectively and $x_i,\ i = 1, 2, ..., N$ are uniform or non-uniform grid points lies in the domain. In these methods, the first task is to find out the weighting coefficients $\omega_{ij}^{(1)}$ and $\omega_{ij}^{(2)}$. There are various techniques based on functions such as Legendre polynomials, Lagrange interpolation polynomials, spline functions, Lagrange interpolated cosine functions, radial basis functions [17–28] etc. to calculate these coefficients. In this work, we have calculated the weighting coefficients with the help of new test functions trigonometric cubic B-spline by some modifications.

2.1. Cubic trigonometric B-spline functions

Consider a mesh which is equally divided by knots x_i into N subintervals $[x_i,\ x_{i+1}],\ i = 0, 1, ..., N-1$ such that $a = x_0 < x_1, ..., < x_N = b$ as a uniform partition of the solution domain $a \le x \le b$ with step length $h = x_{i+1} - x_i = \frac{b-a}{N},\ i = 0, 1, ..., N-1$. The piecewise cubic trigonometric B-spline basis functions $TB_j(x)$ over the uniform mesh defined as [29]:

$$TB_j(x) = \frac{1}{\omega}\begin{cases} p^3(x_i), & x \in [x_{i-2},\ x_{i-1}) \\ p(x_i)(p(x_i)q(x_{i+2}) \\ \quad +q(x_{i+3})p(x_{i+1})) \\ \quad +q(x_{i+4})p^2(x_{i+1}), & x \in [x_{i-1},\ x_i) \\ q(x_{i+4})(p(x_{i+1})q(x_{i+3}) \\ \quad +q(x_{i+4})p(x_{i+2})) \\ \quad +p(x_i)q^2(x_{i+3}), & x \in [x_i,\ x_{i+1}) \\ q^3(x_{i+4}), & x \in [x_{i+1},\ x_{i+2}) \\ 0, & otherwise \end{cases} \tag{2.3}$$

where

$$p(x_i) = \sin\left(\frac{x - x_i}{2}\right), \quad q(x_i) = \sin\left(\frac{x_i - x}{2}\right),$$
$$\omega = \sin\left(\frac{h}{2}\right)\sin(h)\sin\left(\frac{3h}{2}\right).$$

Table 2.1
Coefficient of trigonometric cubic B-splines and its derivatives at knots x_j.

x	x_{j-2}	x_{j-1}	x_j	x_{j+1}	x_{j+2}
$TB_j(x)$	0	a_1	a_2	a_1	0
$TB'_j(x)$	0	a_3	0	a_4	0
$TB''_j(x)$	0	a_5	a_6	a_5	0

The set $\{TB_{-1}(x), TB_0(x), ..., TB_N(x), TB_{N+1}(x)\}$ forms a basis over the region $a \le x \le b$. Each trigonometric cubic B-splines cover four elements.

The values of $TB_j(x)$ and its derivative are tabulated in Table 2.1.

where

$$a_1 = \frac{\sin^2\left(\frac{h}{2}\right)}{\sin(h)\sin\left(\frac{3h}{2}\right)}, \quad a_2 = \frac{2}{1 + 2\cos(h)}, \quad a_3 = \frac{-3}{4\sin\left(\frac{3h}{2}\right)},$$
$$a_4 = \frac{3}{4\sin\left(\frac{3h}{2}\right)}, a_5 = \frac{3(1 + 3\cos(h))}{16\sin^2\left(\frac{h}{2}\right)\left(2\cos\left(\frac{h}{2}\right) + \cos\left(\frac{3h}{2}\right)\right)},$$
$$a_6 = \frac{3\cos^2\left(\frac{h}{2}\right)}{2\sin^2\left(\frac{h}{2}\right)(1 + 2\cos(h))}.$$

2.2. Modified cubic trigonometric B-spline functions

In this work, we have done the following modification in cubic trigonometric B-splines basis functions defined in (2.3) to compute the weighting coefficients of DQ method. The modified basis functions are as follows:

$$\left.\begin{aligned} &T\tilde{B}_0(x) = TB_0(x) + 2TB_{-1}(x), \quad j = 0 \\ &T\tilde{B}_1(x) = TB_1(x) - TB_{-1}(x), \quad j = 1 \\ &T\tilde{B}_j(x) = TB_j(x), \ \ j = 2, 3, ..., N-2 \\ &T\tilde{B}_{N-1}(x) = TB_{N-1}(x) - TB_{N+1}(x), \quad j = N-1 \\ &T\tilde{B}_N(x) = TB_N(x) + 2TB_{N+1}(x), \quad j = N \end{aligned}\right\} \tag{2.4}$$

The modified functions $\{T\tilde{B}_j(x)\},\ j = 0, 1, ..., N$ are also linear independent and form a family of basis functions on [a, b].

2.3. Calculation of weighting coefficients for one dimensional modified cubic trigonometric B-spline DQ method

Put the modified functions $\{T\tilde{B}_j(x)\},\ j = 0, 1, ..., N$ in Eq. (2.1). The equations can be written in the matrix form as

$$\begin{cases} Aw_0^{(1)} = B_0 \\ Aw_1^{(1)} = B_1 \\ . \\ . \\ Aw_{N-1}^{(1)} = B_{N-1} \\ Aw_N^{(1)} = B_N \end{cases} \tag{2.5}$$

where A is $(N+1) \times (N+1)$ coefficient matrix

$$A = \begin{bmatrix} a_2 + 2a_1 & a_1 & & & & & \\ 0 & a_2 & a_1 & & & & \\ & a_1 & a_2 & a_1 & & & \\ & & . & . & . & & \\ & & & . & . & . & \\ & & & & . & . & . \\ & & & & a_1 & a_2 & 0 \\ & & & & & a_1 & a_2 + 2a_1 \end{bmatrix},$$