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Efficient numerical method for the Fitzhugh-Nagumo equations with Neumann boundary conditions

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Abstract

The objective of this work is to construct a new efficient numerical scheme to solve the Fitzhugh-Nagumo model. For the space discretization, Chebyshev spectral method proposed on Legendre orthogonal approximations on Gauss- Chebyshev- Lobatto points. A high-order Runge-Kutta algorithm was used in the time direction. The full-discrete scheme was expressed explicitly and was easy to be implemented with the Neumann boundary conditions. Numerical experiments are discussed to validate the accuracy and reliability of the proposed method.

Keywords: Chebyshev spectral method; FitzHugh-Nagumo equation; Neumann boundary condition

1. Introduction

The early Fitzhugh equation was a mathematical model of excitable media applied to neuronal dynamics [1]. Then, Nagumo developed the Fitzhugh equation to the Fitzhugh–Nagumo (FN) equation which simplified the Hodgkin–Huxley dynamics model [2]. Over four decades, the FN equation has been widely extended to describe various sciences phenomena such as autocatalytic chemical reaction, branching Brownian motion process, nuclear reactor theory, neurophysiology, logistic population growth and study of reentry in heart tissue [2-3].

In this work, we consider the following FN equation with diffusion

$$\begin{cases} \dfrac{\partial u}{\partial t} = K_u \Delta u + u(1-u)(u-a) - v, \\ \dfrac{\partial v}{\partial t} = \varepsilon(\beta u - \gamma v - \delta), \end{cases} \tag{1.1}$$

subject to the initial conditions

$$u(x,y,0) = u_0(x,y), \quad v(x,y,0) = v_0(x,y), \tag{1.2}$$

with Neumann boundary conditions

$$\begin{cases} \dfrac{\partial u}{\partial n} = f(x,y,t), \quad (x,y)\ on\ \partial\Omega, \\ \dfrac{\partial v}{\partial n} = g(x,y,t), \quad (x,y)\ on\ \partial\Omega, \end{cases} \tag{1.3}$$

where $a, \varepsilon, \beta, \gamma$ and δ are constants, $(x,y,t) \in \Omega \times [0,T]$, $\Omega \subset \mathbb{R}^2$, K_u represents the diffusion coefficient of u, u_0, v_0, f and g are sufficiently smooth functions.

In the past few decades, many researchers have done for the numerical solution of the FN equations. Various numerical methods have been announced including the finite difference method [4-6], Haar wavelet method [7], finite element method [8-9], spectral method [2, 10-12] and so on [3]. Recently, Muhammad et al. derived a stochastic explicit scheme to approximate the stochastic FN model. They analyzed the unique existence, consistency and stability of the proposed scheme [13].

In this work, we employ a high order Runge–Kutta algorithm for the coupled system of FN equation. With Chebyshev spectral method, FN equation is approximated to a system of ordinary differential equations which can be decomposed by the fourth-order Runge-Kutta (RK4) method. The constructed scheme is explicit matrices form which has the advantage of processing boundary conditions.

The rest of the article is organized as follows. In Section 2, we give a brief introduction of Chebyshev spectral method with Neumann boundary condition, also the discrete Laplacian is discussed. The full-discrete scheme is presented in Section 3. In Section 4, we test some numerical experiments, including 1D FN equation and 2D FN equation with long period simulation. The conclusion of this article is given in last Section.

2. Chebyshev spectral method for Neumann boundary conditions

In this section, we consider Chebyshev approximation in the space for Neumann boundary value problems.

2.1. Chebyshev spectral method

The spectral method is based on finite-order function expansion and truncation to approximate the original function. In order to normalize the space region $[a,b]$ to $[-1,1]$, we use the linear transformation $x \to \frac{L}{2}(x+1)+a, \quad L=b-a.$ In this work, we consider Chebyshev orthogonal polynomials, the trial function $T_k(x)$ is selected as orthogonal function [15]

$$T_k(x)=\cos(k\arccos(x)), \quad k\in N^*.$$

For any function $u(x)\in C^1[-1,1]$ can be expanded according to this set of basis function as follows:

$$u(x)=\sum_{k=0}^{\infty}H_k(x)u(x),$$

where the kth spectral expansion coefficients $H_k(x)$ are defined as

$$H_k(x)=\frac{2}{\pi C_k}\int_{-1}^{1}\frac{u(x)T_k(x)}{\sqrt{(1-x^2)}}, \quad C_k=\begin{cases}2, & k=0,\\ 1, & k\neq 0.\end{cases} \tag{1.4}$$

To consider the accuracy of the discrete integration in Eq. (1.4) and efficiency of the processing Neumann boundary conditions, Gauss-Chebyshev-Lobatto (GCL) points are considered as collocation points:

$$x_k=\cos(\frac{k\pi}{N}), \quad k=0,1,\ldots,N$$

where N is the number of points, the Lagrange interpolation polynomial at these unequally interpolation are defined as

$$H_k(x) = \frac{(-1)^{(k+1)}(1-x^2)T_N(x)}{C_k N^2 (x-x_k)},\ C_k = \begin{cases} 2, & k = 0, N, \\ 1, & otherwise, \end{cases}$$

and the approximation of $u(x)$ with truncated series is

$$u(x) \simeq \sum_{k=0}^{N} H_k(x) u(x_k),$$

The first derivative of $u(x)$ can be approximated by

$$u'(x) \simeq \sum_{k=0}^{N} H'_k(x) u(x_k). \tag{1.5}$$

Eq. (1.5) can be expressed in the form of matrix and vector

$U' \simeq D_{(N)} U$,

where $U = [u(x_0), u(x_1), \cdots, u(x_N)]^T$, $U' = [u'(x_0), u'(x_1), \cdots, u'(x_N)]^T$, $D_{(N)}$ is an $(N+1) \times (N+1)$ matrix and so-called the first-order Chebyshev differentiation matrix.

Theorem 2.1 ([16]) Chebyshev differentiation matrix

Given an arbitrary integer $N \geq 1$, each element of the first-order Chebyshev differentiation matrix depends on the values of i, j, N. This matrix is defined as following

$$[D_{(N)}]_{ij} = \begin{cases} \dfrac{C_i}{C_j} \dfrac{(-1)^{i+j}}{(x_i - x_j)}, & i \neq j, \\ -\dfrac{x_i}{2(1-x_i^2)}, & (i = j) \neq 0, N, \\ (D_{(N)})_{00} = -(D_{(N)})_{NN} = \dfrac{2N^2+1}{6}. \end{cases}$$

The second derivative of $u(x)$ can be approximated as d matrix form

$$U'' \simeq D_{(N)}(U') \simeq D_{(N)}(D_{(N)} U) = D_{(N)}^2 U',$$

where $D_{(N)}^2$ is the second-order Chebyshev differentiation matrix.

2.2. Discrete Laplacian in 2-dimension

Before discrete processing, we need define two Matrix Operators.

Definition 1 Kronecker product

Given two arbitrary matrices $\mathbf{A} \in \mathbb{R}^{(k \times l)}$ and $\mathbf{B} \in \mathbb{R}^{(m \times n)}$, their Kronecker product $\mathbf{C}$ can be calculated by

$$\mathbf{C} = \mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \cdots & a_{1l}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \cdots & a_{2l}\mathbf{B} \\ \vdots & \vdots & & \vdots \\ a_{k1}\mathbf{B} & a_{k2}\mathbf{B} & \cdots & a_{kl}\mathbf{B} \end{pmatrix} \in \mathbb{R}^{(km)\times(\ln)}, \tag{1.6}$$

Definition 2 Hadamard product

Given two same dimension matrices $\mathbf{A} \in \mathbb{R}^{(m \times n)}$ and $\mathbf{B} \in \mathbb{R}^{(m \times n)}$, their Hadamard product $\mathbf{C} = A \odot B$ is an $m \times n$ matrix with elements defined by

$(\mathbf{C})_{ij} = (\mathbf{A} \odot \mathbf{B})_{ij} = a_{ij} \bullet b_{ij}$.

For an integer $N \geq 1$, any function $u(x)$ in $[a,b]\times[c,d]$ can be discrete on grid points as following:

$$u_{(N+1)\times(N+1)} = \begin{pmatrix} u_{00} & u_{01} & \cdots & u_{0N} \\ u_{10} & u_{11} & \cdots & u_{1N} \\ \vdots & \vdots & & \vdots \\ u_{N0} & u_{N1} & \cdots & u_{NN} \end{pmatrix}, \tag{1.7}$$

or

$$u_{(N+1)^2} = [(u_{00}, u_{01}, \cdots, u_{0N}), (u_{10}, u_{11}, \cdots, u_{1N}), \cdots, (u_{N0}, u_{N1}, \cdots, u_{NN})], \tag{1.8}$$

where the first form (Eq. 1.7) of discrete $u(x)$ is a square matrix of $(N+1)$ -order, and the second form (Eq. 1.8) of discrete $u(x)$ is a $(N+1)^2$ vector.

Now, expending Chebyshev spectral method to 2-dimensional space, we obtain two kinds of discrete Laplacian:

$$\Delta u \simeq (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}) u_{(N+1)\times(N+1)} \simeq D_{(N)}^2 u_{(N+1)\times(N+1)} + u_{(N+1)\times(N+1)} (D_{(N)}^2)^T, \tag{1.9}$$

and

$$\Delta u \simeq (\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2})u_{(N+1)^2} \simeq (D_{(N)}^2 \otimes I_{(N+1)} + I_{(N+1)} \otimes D_{(N)}^2)u_{(N+1)^2}, \tag{1.10}$$

respectively. Fig.1 show the two kinds of discrete Laplacian with $N=10$. It is clear that the first discrete form is less computational amount than the second form. In this manuscript, Eq. 1.9 is selected as discrete Laplacian form to improve computing efficiency.

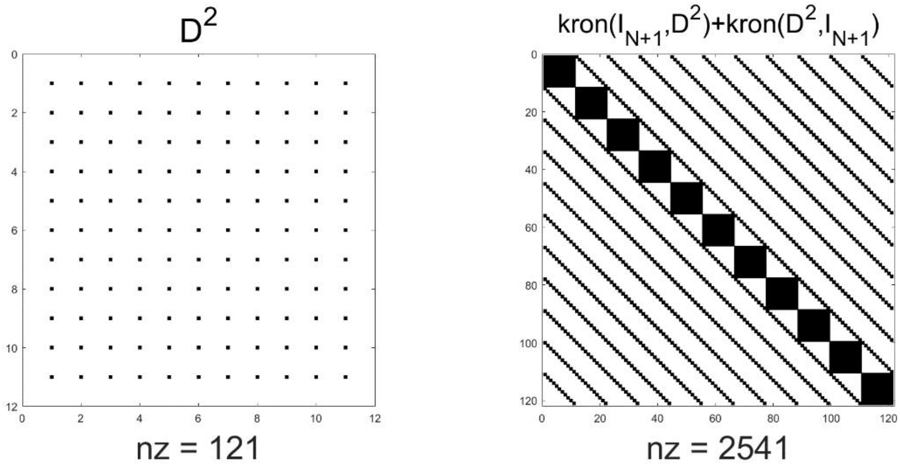

Fig. 1. Sparsity plot of two discrete Laplacian forms. Left, the 11×11 discrete Laplacian (1.9). Right, the 121×121 discrete Laplacian (1.10).

Thus, with the application of Chebyshev spectral method, Eq. (1.1) is given by

$$\begin{cases} \dfrac{dU}{dt} = K_u(D_{(N)}^2 U + U(D_{(N)}^2)^T) + U \odot (1-U)(U-a) - V, \\ \dfrac{dV}{dt} = \varepsilon(\beta U - \gamma V - \delta). \end{cases} \tag{1.11}$$

2.3. Neumann boundary conditions processing

Let the value of the function $u(x)\in C^1[a,b]$ at the GCL points $x=(x_0,x_1,\dots,x_N)^T$ be the vector $U=(u_0,u_1,\dots,u_N)$, where $u_0=u(b), u_N=u(a)$. Neumann boundary conditions

$$\begin{cases} \left.\dfrac{du}{dx}\right|_{x=a} = f(x), \\ \left.\dfrac{du}{dx}\right|_{x=b} = g(x), \end{cases}$$

are implemented by

$$\begin{pmatrix} u'(b) \\ u'(a) \end{pmatrix} = \begin{pmatrix} (D_N)_{00} & (D_N)_{01} & \cdots & (D_N)_{0N} \\ (D_N)_{N0} & (D_N)_{N1} & \cdots & (D_N)_{NN} \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_N \end{pmatrix} = \begin{pmatrix} g(x) \\ f(x) \end{pmatrix},$$

the boundary value problem can be solved by the system

$$\begin{pmatrix} u_0 \\ u_N \end{pmatrix} = \begin{pmatrix} (D_N)_{00} & (D_N)_{0N} \\ (D_N)_{N0} & (D_N)_{NN} \end{pmatrix}^{-1} \left(\begin{pmatrix} g(x) \\ f(x) \end{pmatrix} - \begin{pmatrix} (D_N)_{01} & (D_N)_{02} & \cdots & (D_N)_{0(N-1)} \\ (D_N)_{(N-1)0} & (D_N)_{(N-1)1} & \cdots & (D_N)_{(N-1)(N-1)} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-1} \end{pmatrix} \right),$$

whereas for the homogeneous Neumann boundary problems, the solving system is

$$\begin{pmatrix} u_0 \\ u_N \end{pmatrix} = -\begin{pmatrix} (D_N)_{00} & (D_N)_{0N} \\ (D_N)_{N0} & (D_N)_{NN} \end{pmatrix}^{-1} \begin{pmatrix} (D_N)_{01} & (D_N)_{02} & \cdots & (D_N)_{0(N-1)} \\ (D_N)_{(N-1)0} & (D_N)_{(N-1)1} & \cdots & (D_N)_{(N-1)(N-1)} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N-1} \end{pmatrix}.$$

3. Full-discrete scheme

To integrate the coupled systems (Eq. 1.1) in time direction, a high-order difference method will be used. Rewriting Eq. (1.1 – 1.3) as following:

$$\begin{cases} \dfrac{dU}{dt} = F(U,V), \\ \dfrac{dV}{dt} = G(U,V), \\ U(t=0) = U_{0,} \quad V(t=0) = V_0, \\ \dfrac{\partial U}{\partial n} = f(x,y,t), \dfrac{\partial V}{\partial n} = g(x,y,t). \end{cases} \tag{1.12}$$

where

$$F(U,V) = K_u(D_{(N)}^2 U + U(D_{(N)}^2)^T) + U \odot (1-U)(U-a) - V,$$

and

$$G(U,V) = \varepsilon(\beta U - \gamma V - \delta).$$

We consider explicit Fourth-order Runge-Kutta method (RK4) to discrete the ordinary differential equations (1.12).

Definition 3 Runge-Kutta algorithm [Ref.12]

For nonlinear ODE problem

$y' = f(t, y),\ \ y(t_0) = y_0,$

the Fourth-order Runge-Kutta method is in the form

$y_{n+1} = y_n + \Delta t K(y_n, t_n, \Delta t)$

where $K(y_n, t_n, \Delta t)$ is determined by $f(t, y)$.

Then we can construct the full-discrete scheme:

Chebyshev-Fourth order Runge-Kutta (CRK4) scheme: Given the approximate solution matrices U_n and V_n at the time t_n, the approximate solution U_{n+1} and V_{n+1} at the time t_{n+1} can be calculated via

$$\begin{cases} K_1 U = \Delta t \cdot F(U_n, V_n), & K_1 V = \Delta t \cdot G(U_n, V_n), \\ K_2 U = \Delta t \cdot F(U_n + \frac{\Delta t}{2} K_1 U, V_n + \frac{\Delta t}{2} K_1 V), & K_2 U = \Delta t \cdot G(U_n + \frac{\Delta t}{2} K_1 U, V_n + \frac{\Delta t}{2} K_1 V), \\ K_3 U = \Delta t \cdot F(U_n + \frac{\Delta t}{2} K_2 U, V_n + \frac{\Delta t}{2} K_2 V), & K_3 U = \Delta t \cdot G(U_n + \frac{\Delta t}{2} K_2 U, V_n + \frac{\Delta t}{2} K_2 V), \\ K_4 U = \Delta t \cdot F(U_n + \Delta t K_3 U, V_n + \Delta t K_3 V), & K_4 U = \Delta t \cdot G(U_n + \Delta t K_3 U, V_n + \Delta t K_3 V), \end{cases}$$

$$\begin{cases} U_{n+1} = U_n + \frac{\Delta t}{6}(K_1 U + 2K_2 U + 2K_3 U + K_4 U), \\ V_{n+1} = V_n + \frac{\Delta t}{6}(K_1 V + 2K_2 V + 2K_3 V + K_4 V), \end{cases}$$

where Δt is the step size at time direction. Neumann boundary conditions will be considered after RK iteration.

Remark 1. CRK4 is an explicit scheme. We refer readers to Ref. [12, 14] for the details of the stability analysis and error estimation.

4. Full-discrete scheme

To verify the accuracy and efficiency of the presented scheme in solving the Fitzhugh-Nagumo equations, several examples are performed in this section. L_2 and L_∞ error norms are used to measure the accuracy of the method

$$L_2 = \left[\sum_j \omega_j \left| u(x_j,t) - u_{exact}(u_j,t) \right|^2 \right]^{\frac{1}{2}},$$

$$L_\infty = \max_j \left| u(x_j,t) - u_{exact}(u_j,t) \right|,$$

where ω_j are the GCL weight defined by

$$\omega_j = \begin{cases} \dfrac{\pi}{2N}, & i = 0, N, \\ \dfrac{\pi}{N}, & \mathit{otherwise.} \end{cases}$$

Example 1 Consider the following 1-D Fitzhugh-Nagumo equation

$$u_t = u_{xx} + u(1-u)(u-\rho), \quad (x,t) \in [0,1]\times[0,T]$$

with initial condition

$$u(x,0) = \frac{1}{1+e^{\frac{-x}{\sqrt{2}}}}, \quad x \in [0,1],$$

and the boundary conditions are given as

$$u(0,t) = \frac{1}{1+e^{\frac{-ct}{\sqrt{2}}}}, \; u(1,t) = \frac{1}{1+e^{\frac{-1-ct}{\sqrt{2}}}},$$

where $c = \sqrt{2}(\frac{1}{2} - \rho).$

This example has the exact solution

$$u_{exact}(x,t) = \frac{1}{1+e^{\frac{-s}{\sqrt{2}}}}$$

where the wave speed $s = x + ct$.

We choose parameters as $\rho = 0.75$, $N = 10$. Error norms L_2 and L_∞ are summarized in Table 1. From the comparison, the presented method can achieve higher accuracy than others. Then numerical solutions by the CRK4 scheme are plotted in Fig. 2 for $N = 10, \Delta = 1\times10^{-4}$ which shows the effect of varying ρ.

Table 1. Error norms L_2 and L_∞ for $\rho = 0.75, N = 10$ with different values of Δt.

$\Delta t = 10^{-4}$		$t = 0.01$	$t = 1$
L_2	CRK4	1.0799×10^{-9}	4.1044×10^{-9}
	[12] method	2.17×10^{-9}	1.51×10^{-9}
	[3] method	1×10^{-7}	6×10^{-7}
L_∞	CRK4	1.85×10^{-9}	7.2999×10^{-9}
	[12] method	2.07×10^{-9}	1.47×10^{-9}
	[3] method	2×10^{-7}	9×10^{-7}
$\Delta t = 10^{-5}$		$t = 0.01$	$t = 1$
L_2	CRK4	1.0792×10^{-10}	4.1050×10^{-10}
	[12] method	2.17×10^{-9}	4.08×10^{-9}
	[2] method	1×10^{-7}	6×10^{-7}
L_∞	CRK4	1.8481×10^{-10}	7.3009×10^{-10}
	[12] method	2.07×10^{-9}	3.90×10^{-9}
	[3] method	2×10^{-7}	9×10^{-7}

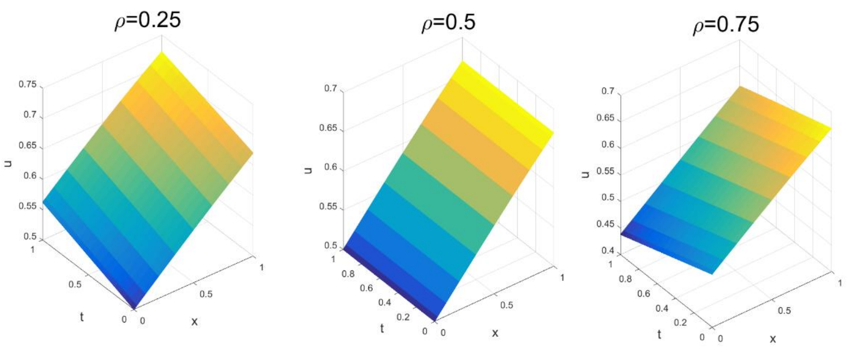

Fig. 2. Numerical solutions for $N = 10, \Delta = 1\times10^{-4}$ and different values of ρ.

Example 2[Long period simulation] Consider the following 2-D Fitzhugh-Nagumo model (1.1) with initial conditions

$$u(x,y,0)=\begin{cases}1, & \text{if } 0\le x,y\le 1.25,\\ 0, & \text{otherwise},\end{cases}$$

$$v(x,y,0)=\begin{cases}0.1, & \text{if } 0\le x\le 2.5,\ 1.25\le y\le 2.5,\\ 0, & \text{otherwise}.\end{cases}$$

over a square domain size $[0,2.5]\times[0,2.5]$ with homogeneous Neumann boundary condition. Parameters in the numerical example are chosen as $a = 0.1,\ \varepsilon = 0.01, \beta = 0.5, \gamma = 1, \delta = 0, K_u = 10^{-4}, N = 50,$ and $\Delta = 0.01$. Fig. 3 displays the stable spiral wave numerical simulations at different time levels $t = 0,150,300,450$.

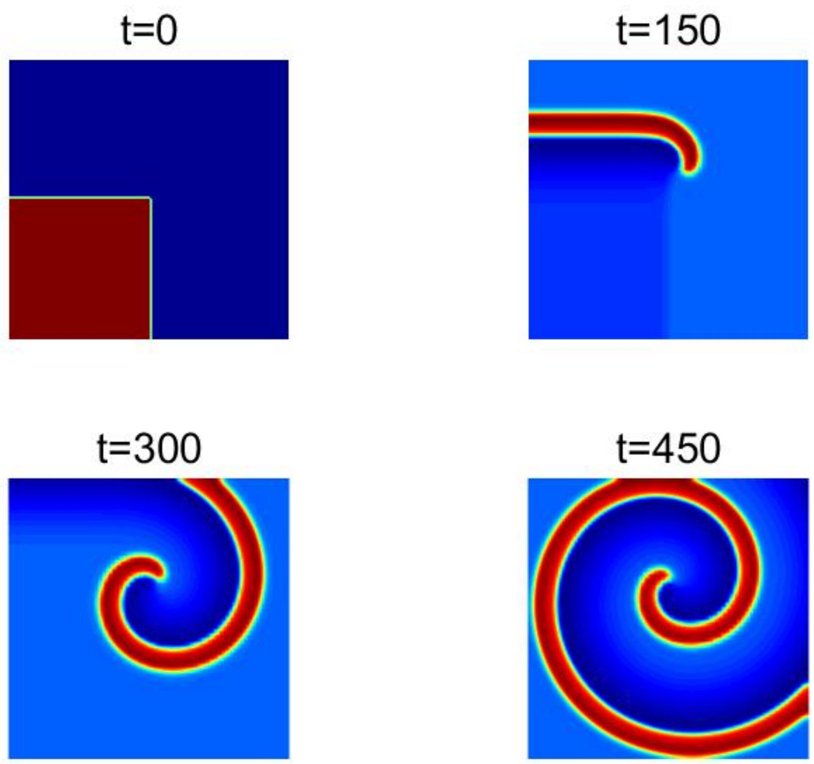

Fig.3 Solutions of the 2D Fitzhugh–Nagumo model at $t = 0,150,300,450$.

5. Conclusions

In this work, we developed Chebyshev spectral method in combination with high-order Runge-Kutta algorithm. The nonlinear Fitzhugh-Nagumo equation can be approximated in an explicit matrix form and become ease to implement the boundary conditions. The presented method was able to offer better numerical solutions in comparison with others. At the same time, the spiral wave simulation in a long period for the FHN model demonstrates that the proposed scheme (CRK4) is efficient and reliable. As a conceivable outgrowth, the presented method is capable for other coupled equations in physics.

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