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HIGH-ORDER COMPACT DIFFERENCE METHODS FOR SIMULATING WAVE PROPAGATIONS IN EXCITABLE MEDIA

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Abstract. In this paper, we present a study of some high-order compact difference schemes for solving the Fitzhugh-Nagumo equations governed by two coupled time-dependent nonlinear reaction diffusion equations in two variables. Solving the Fitzhugh-Nagumo equations is quite challenging, since the equations involve spatial and temporal dynamics in two different scales and the solutions exhibit shock-like waves. The numerical schemes employed have sixth order accuracy in space, and fourth order in time if the fourth order Runge-Kutta method is adopted for time marching. To improve efficiency, we also propose an ADI scheme (for two dimensional problems), which has second order accuracy in time. Numerical results are presented for plane wave propagation in one dimension and spiral waves for two dimensions.

Key words. Spiral waves, excitable medium, FitzHugh-Nagumo equations, compact difference methods.

1. Introduction

In this work, we consider the following two-dimensional (2D) Fitzhugh–Nagumo type model (cf. [1, 2]) for the description of waves in excitable media given by

$$\frac{\partial u}{\partial t} = \nabla^2 u + f(u,v), \quad \frac{\partial v}{\partial t} = g(u,v), \tag{1}$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ denotes the Laplace operator, $u = u(x,y,t)$ and $v = v(x,y,t)$ are the so-called excitation variable and recovery variable, respectively. The functions $f(u,v)$ and $g(u,v)$ represent the local reaction kinetics of the species. Here we adopt the simplified Barkley model given by [3]

$$f = \frac{1}{\epsilon}u(1-u)(u - \frac{v+b}{a}), \quad g = u - v, \tag{2}$$

where the constants a and b control the excitability threshold and duration, and ϵ determines the time scale of the fast variable u. Usually, ϵ is selected quite small such that the time scale of u is several orders of magnitude faster than that of v. A larger value of a would increase the excitation variable duration, whereas a larger ratio b/a increases the excitation threshold.

To make the problem (1) complete, we assume that (1) hold true for $(x,y,t) \in \Omega \times [0,T]$, where $\Omega \subset R^2$ is an open, bounded, connected polygonal domain with boundary $\partial\Omega$, along with zero-flux boundary conditions

$$\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0 \quad \text{on } \partial\Omega \times (0,T), \tag{3}$$

where n is the unit outer normal vector of $\partial\Omega$, and appropriate initial conditions

$$u(x,y,0) = u_0(x,y), \quad v(x,y,0) = v_0(x,y) \quad \text{in } \Omega. \tag{4}$$

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The FitzhughNagumo model (1)–(4) is the most widely used mathematical model of excitation and propagation of impulse in excitable media such as nerve membranes. Over the years, there have been many studies devoted to this model and its many variations (e.g., [4] and references therein). Due to the complexity of the problem, numerical simulation plays a very important role in studing the FitzhughNagumo model. For example, Barkley [3] presented a simple and efficient finite difference algorithm (attached with a complete subroutine) for solving the 2D FitzhughNagumo equations. Later, Olmos and Shizgal [5] proposed a Chebyshev multidomain method, and a new finite difference method for solving both 1D and 2D FitzhughNagumo equations. Ramos [6] numerically studied the propagation of spiral waves in 2D reactivediffusive media. In [7], Amdjadi proposed a numerical method for testing the dynamics and stability of spiral waves in excitable media. Bürger, Ruiz-Baier and Schneider [8] presented some fully space-time adaptive multiresolution methods based on the finite volume method and Barkley's method for simulating the complex dynamics of waves in excitable media. In [9], Dehghan and Fakhar-Izadi developed two pseudospectral methods based on Fourier series and rational Chebyshev functions to solve the 1D Nagumo equation.

The main objective of the present paper is to introduce the high-order compact difference method ([10, Ch.5] and references) to simulate the wave propagation problem in excitable media. Previous studies (cf. [10, Ch.5] and references therein) have shown that the high-order compact difference method is a very efficient algorithm and has a much smaller dispersive error compared to the standard same order finite difference method.

The rest of the paper is organized as follows. In Sect. 2, we demonstrate that how the high-order compact difference scheme can be constructed for both 1D and 2D problems. Numerical results are presented in Sect. 3 to show the efficiency of our scheme. We conclude the paper in Sect. 4.

2. Derivation of the compact difference scheme

In the high-order compact difference methods (cf. [11, 12, 13, 14] and references therein) , the spatial derivatives in the governing PDEs are not approximated directly by the traditional explicit finite differences, but are evaluated through solving a system of linear equations. More specifically, given scalar pointwise values u, the derivatives of u are obtained by solving a tridiagonal or pentadiagonal system. Below we will show how to develop 1D and 2D high-order compact difference schemes for solving the FitzhughNagumo equation.

2.1. 1D compact difference scheme. First, let us construct a sixth-order compact difference scheme to evaluate the second derivatives. Consider a uniform 1D mesh consisting of N points:

$$x_1 < x_2 < \cdots < x_{i-1} < x_i < x_{i+1} < \cdots < x_N$$

with mesh size $h = x_{i+1} - x_i$. Given the function values $u_i = u(x_i), 1 \le i \le N$, the approximate second derivatives $u_i^{''}$ at interior points can be reconstructed by the following three point formula:

(5)

$$\alpha u_{i-1}^{''} + u_i^{''} + \alpha u_{i+1}^{''} = \frac{a}{h^2}(u_{i+1} - 2u_i + u_{i-1}) + \frac{b}{4h^2}(u_{i+2} - 2u_i + u_{i-2}), \quad 2 \le i \le N-2,$$

where $\alpha = \frac{2}{11}, a = \frac{4}{3}(1-\alpha), b = \frac{1}{3}(-1+10\alpha)$.

At the most left boundary point x_1, a sixth-order formula can be given as [10, Ch.5]:

$$u_1^{''} + \alpha u_2^{''} = (c_1 u_1 + c_2 u_2 + c_3 u_3 + c_4 u_4 + c_5 u_5 + c_6 u_6 + c_7 u_7)/h^2, \tag{6}$$

where $\alpha = \frac{126}{11}, c_1 = \frac{2077}{157}, c_2 = -\frac{2943}{110}, c_3 = \frac{573}{44}, c_4 = \frac{167}{99}, c_5 = -\frac{18}{11}, c_6 = \frac{57}{110}, c_7 = -\frac{131}{1980}$.

At the second left boundary point x_2, the sixth-order formula is given as [10, Ch.5]:

$$\alpha u_1^{''} + u_2^{''} + \alpha u_3^{''} = (c_1 u_1 + c_2 u_2 + c_3 u_3 + c_4 u_4 + c_5 u_5 + c_6 u_6 + c_7 u_7)/h^2, \tag{7}$$

where $\alpha = \frac{11}{128}, c_1 = \frac{585}{512}, c_2 = -\frac{141}{64}, c_3 = \frac{459}{512}, c_4 = \frac{9}{32}, c_5 = -\frac{81}{512}, c_6 = \frac{3}{64}, c_7 = -\frac{3}{512}$.

By symmetry, at the second right boundary point x_{N-1}, the sixth-order formula is given as [10, Ch.5]:

$$\begin{aligned} &\alpha u_{N-2}^{''} + u_{N-1}^{''} + \alpha u_N^{''} \\ = \; &(c_1 u_N + c_2 u_{N-1} + c_3 u_{N-2} + c_4 u_{N-3} + c_5 u_{N-4} + c_6 u_{N-5} + c_7 u_{N-6})/h^2, \end{aligned} \tag{8}$$

where the coefficients α and c_i $(1 \le i \le 7)$ are the same as (7).

Similarly, at the most right boundary point x_N, a sixth-order formula can be given as [10, Ch.5]:

$$\alpha u_{N-1}^{''} + u_N^{''} = (c_1 u_N + c_2 u_{N-1} + c_3 u_{N-2} + c_4 u_{N-3} + c_5 u_{N-4} + c_6 u_{N-5} + c_7 u_{N-6})/h^2, \tag{9}$$

where the coefficients α and c_i $(1 \le i \le 7)$ are the same as (6).

Note that the scheme (5)-(9) can be written as $Au^{''} = \frac{1}{h^2} Bu$, i.e., the second derivatives at all grid points can be obtained by solving a tridiagonal linear system, since the matrix A is a $N \times N$ tridiagonal matrix.

After the spatial discretization, the time-dependent governing PDEs can be integrated by various time marching schemes.

First, let us consider the 1D case of (1):

$$\frac{\partial u}{\partial t} = R(u) := \frac{\partial^2 u}{\partial x^2} + f(u), \tag{10}$$

with properly imposed boundary and initial conditions.

A fully sixth-order compact difference scheme with the classical fourth-order four-stage Runge-Kutta (RK4) method for solving (10) can be given as follows: Given the approximate solution U^n at t_n, the solution U^{n+1} at $t_{n+1} = t_n + \tau$ is obtained through the operations

$$\begin{aligned} &U_0 := U^n, \quad k_0 = \tau \cdot R(U_0), \\ &U_1 = U_0 + k_0/2, \quad k_1 = \tau \cdot R(U_1), \\ &U_2 = U_0 + k_1/2, \quad k_2 = \tau \cdot R(U_2), \\ &U_3 = U_0 + k_2, \quad k_3 = \tau \cdot R(U_3), \\ &U^{n+1} = U_0 + \frac{1}{6}(k_0 + 2k_1 + 2k_2 + k_3), \end{aligned}$$

where the second derivative involved in the residual $R(U_i)$ at each stage is calculated by using the sixth-order compact difference scheme presented above. Here τ denotes the time step size.

For a 1D system of equations, the above compact difference scheme coupled with RK4 method can be applied as a vector form.

2.2. 2D compact difference scheme. For a 2D system of (1), to avoid the explicit time step constraint caused by the RK4 method, we adopt the Alternating Direction Implicit (ADI) method developed in [12].

First, we divide the physical domain $\Omega = [x_l, x_r] \times [y_l, y_r]$ by a uniform mesh in each direction:

$$x_i = x_l + (i-1)h_x,\ 1 \le i \le N_x, \quad y_j = y_l + (j-1)h_y,\ 1 \le j \le N_y,$$

where $h_x = \frac{x_r - x_l}{N_x - 1}, h_y = \frac{y_r - y_l}{N_y - 1}$, and N_x and N_y denote the total numbers of points in the x- and y-direction, respectively.

Denote u_{xx} (or u_{yy}) for the second derivative of u with respect to x (or y). Applying the ADI method to the u equation of (1), we have

$$\frac{u_{ij}^{n+\frac{1}{2}} - u_{ij}^n}{0.5\tau} = (u_{xx})_{ij}^{n+\frac{1}{2}} + (u_{yy})_{ij}^n + f(u_{ij}^n, v_{ij}^n), \tag{11}$$

$$\frac{u_{ij}^{n+1} - u_{ij}^{n+\frac{1}{2}}}{0.5\tau} = (u_{xx})_{ij}^{n+\frac{1}{2}} + (u_{yy})_{ij}^{n+1} + f(u_{ij}^n, v_{ij}^n), \tag{12}$$

The second derivative u_{xx} in (11) can be reconstructed row-by-row by using the sixth-order compact difference method developed above, i.e., $(u_{xx})_{,j} = \frac{1}{h_x^2} A^{-1} B u_{,j}$. Substituting this into (11), we obtain: For any $1 \le j \le N_y$, solve

$$(I_{N_x} - \frac{\tau}{2h_x^2} A^{-1} B) u_{,j}^{n+\frac{1}{2}} = u_{,j}^n + \frac{\tau}{2}[(u_{yy})_{,j}^n + f(u_{ij}^n, v_{ij}^n)], \tag{13}$$

where I_{N_x} is the $N_x \times N_x$ identity matrix, and A is a $N_x \times N_x$ tridiagonal matrix.

By symmetry, (12) can be solved as follows: For any $1 \le i \le N_x$, solve

$$(I_{N_y} - \frac{\tau}{2h_y^2} C^{-1} D) u_{i,}^{n+1} = u_{i,}^{n+\frac{1}{2}} + \frac{\tau}{2}[(u_{xx})_{i,}^{n+\frac{1}{2}} + f(u_{ij}^n, v_{ij}^n)], \tag{14}$$

where I_{N_y} is the $N_y \times N_y$ identity matrix, C is a $N_y \times N_y$ tridiagonal matrix and comes from the compact difference reconstruction for u_{yy} via $(u_{yy})_{i,} = \frac{1}{h_y^2} C^{-1} D u_{i,}$.

Since there is no second derivative involved, the v equation of (1) can be simply solved as: For any $1 \le i \le N_x, 1 \le j \le N_y$, solve

$$v_{ij}^{n+1} = v_{ij}^n + \tau g(u_{ij}^n, v_{ij}^n). \tag{15}$$

We like to remark that this ADI method is more efficient than the high-order compact RK4 method, because during each marching time step, our ADI method only needs two second-derivative reconstructions; while the RK4 method needs eight second-derivative reconstructions (each stage needs two reconstructions).

3. Numerical results

3.1. Example 1. We first test our high-order compact scheme with an analytical solution for the 1D Fitzhugh-Nagumo equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - u(1-u)(a-u), \quad 0 < x < 1,\ 0 < t < 1, \tag{16}$$

TABLE 1. Example 1. Convergence results obtained with uniform mesh points.

Mesh points	Time step sizes	Total time steps	Errors	Rates
$N = 11$	$\tau = 0.0025$	Nstep=400	$e_h = 1.4198e - 08$	-
$N = 21$	$\tau = 6.2500e - 4$	Nstep=1600	$e_h = 2.2139e - 10$	$r = 6.0030$
$N = 41$	$\tau = 1.5625e - 4$	Nstep=6400	$e_h = 3.4124e - 12$	$r = 6.0197$
$N = 81$	$\tau = 3.9063e - 5$	Nstep=25600	$e_h = 5.2514e - 14$	$r = 6.0219$

with Dirichlet boundary conditions $u(0,t)$ and $u(1,t)$, and initial condition $u(x,0)$ imposed properly such that the problem has an exact solution

$$u(x,t) = 1/[1 + \exp(x/\sqrt{2} + (a - 0.5)t)].$$

In our tests, we choose the constant $a = 1$ and $\tau = 0.25h^2$.

We performed the calculations using different numbers of uniform mesh points. The obtained pointwise errors e_h, and the convergence rates $r = \log(e_h/e_{h/2})/\log 2$, are presented in Table 1, which clearly shows the convergence rate $O(h^6)$. This is consistent with the theoretical convergence rates $O(h^6 + \tau^4)$ of our scheme, since the time error $O(\tau^4) = O(h^8)$ is much smaller than the spatial error $O(h^6)$ due to the time step constraint. The solutions and errors obtained with 11 and 21 points are presented in Figure 1.

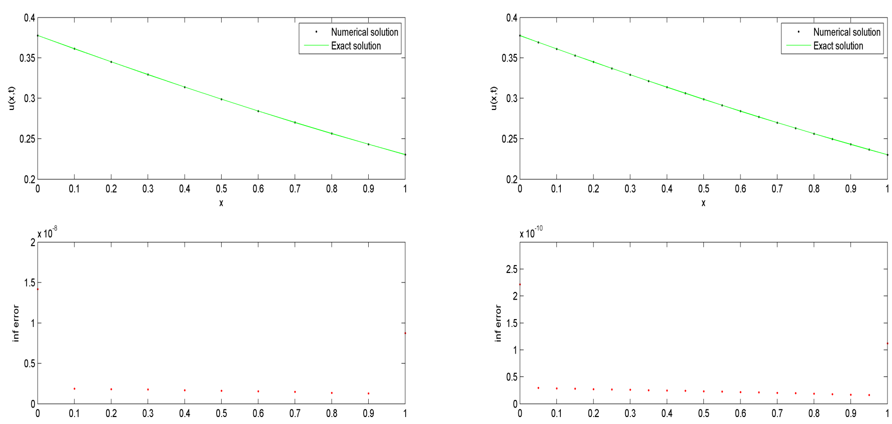

FIGURE 1. Example 1. The analytical and numerical solutions, and the pointwise errors obtained with N=11 points (Left), and N=21 points (Right).

3.2. Example 2. We now consider the 1D case of (1)-(4) with unknown analytical solutions (cf. [5, Sec. 3.1]). The physical domain is $\Omega = [-30, 30]$. The parameters considered are $\epsilon = 0.005, a = 0.3, b = 0.01$ and the total integration time $T = 5$. The initial conditions for u and v are given by

$$(17) \quad u(x,0) = \begin{cases} u_0(x) & x < 0 \\ 0 & x \geq 0 \end{cases}, \qquad v(x,0) = \begin{cases} 0.3 & x < -25 \\ 0 & x \geq -25 \end{cases}$$

where $u_0(x)$ has the general form

$$u_0(x) = (1 + \exp(4|x| - c_1)))^{-2} - (1 + \exp(4(|x| - c_2)))^{-2}, \tag{18}$$

with $c_1 = 25$ and $c_2 = 21$.

Fig. 2 shows several snapshots of the pulses $u(x, t)$ at times $t = 0, 1.66, 3.33$ and 5 obtained by a sixth-order compact difference scheme in space coupled with the RK4 method in time (i.e., the method is the same as Example 1, but in vector form). Here we used 121 and 512 uniformly distributed points in Ω, and the time step size is $\tau = 0.25h^2$, where h is the mesh size. From Fig. 2, we can see that 121 points can produce a solution which is indistinct from that obtained with 512 points. Note that [5] used 512 points to obtain the similar solution.

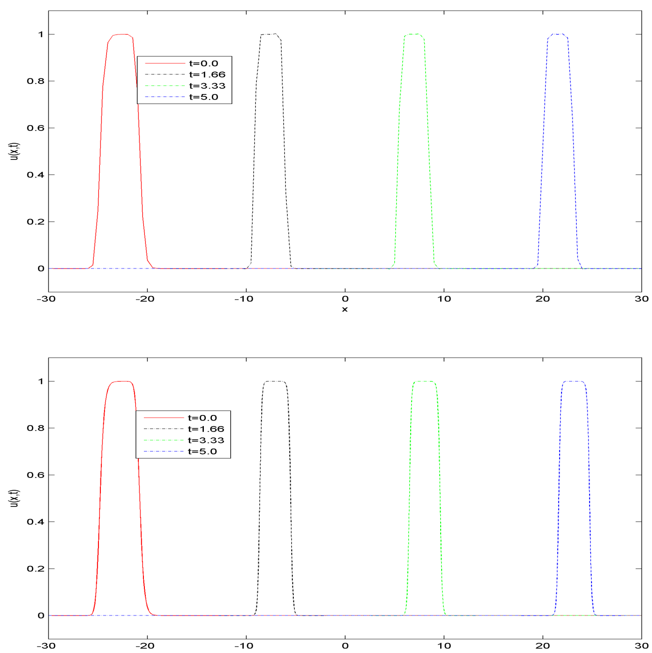

FIGURE 2. Example 2. The solution u obtained at different times with N=121 points (Top), and N=512 points (Bottom).

3.3. Example 3. Now we solve the 2D model (1)-(4) with $\Omega = [0, 50]^2, T = 150$, and the time step size $\tau = 0.01$, which leads to the total time step $Nstep = 15000$. The parameters for function f of (2) are chosen as $\epsilon = 0.02, b = 0.001$, with a variable constant a. Numerical results show that the dynamics of the solutions of (1)-(4) change quite drastically with different constant a. Here we are only interested in obtaining the periodic spiral wave.

Figures 3 and 4 show the spiral waves obtained on uniform rectangular grids of $N_x = N_y = 101$ and $N_x = N_y = 201$ for $a = 0.33$ and 0.36, respectively. The initial

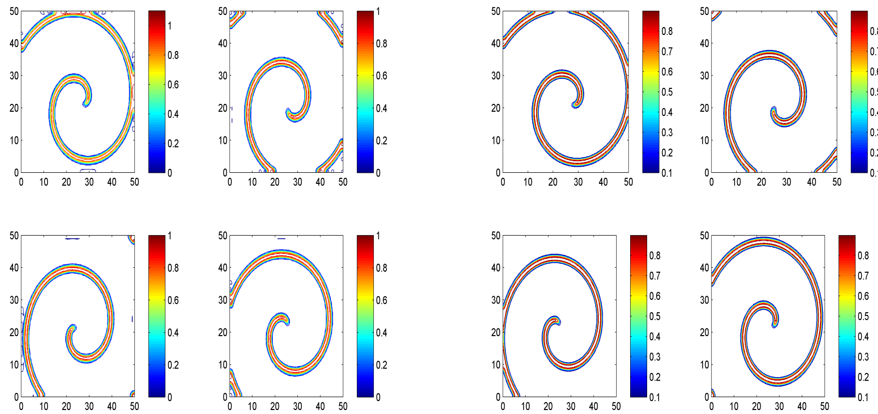

FIGURE 3. Example 3. The solution u obtained for $a = 0.33$ at $t = 40, 80, 120, 150$ (rotated clockwise) with $N_x = N_y = 101$ points (Left group), and $N_x = N_y = 201$ points (Right group).

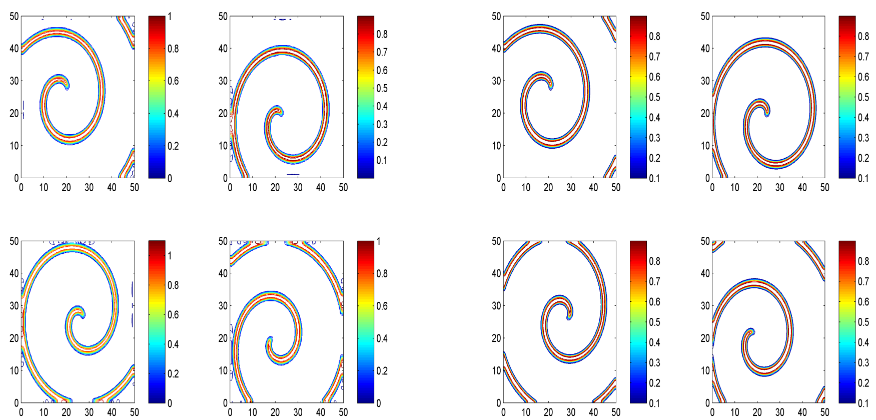

FIGURE 4. Example 3. The solution u obtained for $a = 0.36$ at $t = 40, 80, 120, 150$ (rotated clockwise) with $N_x = N_y = 101$ points (Left group), and $N_x = N_y = 201$ points (Right group).

conditions we used are

(19)
$$u(x,0) = \begin{cases} 0 & x < 25 \text{ or } y > 30 \\ u_0(x) & \text{otherwise} \end{cases}, \quad v(x,0) = \begin{cases} 0.1 & x < 25 \text{ and } y < 30 \\ 0 & \text{otherwise} \end{cases},$$

where $u_0(x)$ has the same form as (18), but with $c_1 = 28$ and $c_2 = 25$.

With many numerical tests, we find that the numerical solution converges when $N_x = N_y \geq 201$. Figs. 3 and 4 show that $N_x = N_y = 201$ gives a more smooth solution than that obtained with $N_x = N_y = 101$, since the fine mesh removes the noises caused by the coarse mesh. The CPU times used for $N_x = N_y = 101$, $N_x = N_y = 201$ and $N_x = N_y = 201$ are approximately 326s, 1322s and 3682s, respectively. Our algorithm is implemented with MATLAB running on a desktop with Intel Core 2 Duo CPU at 2.93 GHz and 1.98 GB memory.

4. Conclusions

In this paper, we developed the sixth-order compact difference methods for solving wave propagation problems in excitable media. Note that higher-order compact difference schemes can be constructed similarly (cf. [10, Ch.5]). Numerical examples are presented to show the efficiency of our algorithm. In the future, we plan to improve our algorithm to solve more complicated spiral waves in two dimensions or scroll waves in three dimensions.

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