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Higher-order compact finite difference method for systems of reaction–diffusion equations[☆]

Yuan-Ming Wang[a,b,∗], Hong-Bo Zhang[a]

[a] Department of Mathematics, East China Normal University, Shanghai 200241, People's Republic of China

[b] Scientific Computing Key Laboratory of Shanghai Universities, Division of Computational Science, E-Institute of Shanghai Universities, Shanghai Normal University, Shanghai 200234, People's Republic of China

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ABSTRACT

This paper is concerned with a compact finite difference method for solving systems of two-dimensional reaction–diffusion equations. This method has the accuracy of fourth-order in both space and time. The existence and uniqueness of the finite difference solution are investigated by the method of upper and lower solutions, without any monotone requirement on the nonlinear term. Three monotone iterative algorithms are provided for solving the resulting discrete system efficiently, and the sequences of iterations converge monotonically to a unique solution of the system. A theoretical comparison result for the various monotone sequences is given. The convergence of the finite difference solution to the continuous solution is proved, and Richardson extrapolation is used to achieve fourth-order accuracy in time. An application is given to an enzyme–substrate reaction–diffusion problem, and some numerical results are presented to demonstrate the high efficiency and advantages of this new approach.

1. Introduction

Many problems in various fields of applied sciences are described by systems of reaction–diffusion equations, and a great deal of work has been done for the qualitative analysis of the systems (see [1] and the references therein). Much work has also been done in relation to numerical methods of such systems (cf. [2–9]). In this paper we give a numerical treatment to a system of reaction–diffusion equations by a higher-order compact finite difference method. This includes the qualitative analysis of the resulting discrete system and several basic monotone iterative algorithms for the computation of the finite difference solution. The reaction–diffusion system under consideration is given in the form

$$\begin{cases} u_t^{(l)} - D_1^{(l)} u_{xx}^{(l)} - D_2^{(l)} u_{yy}^{(l)} = f^{(l)}(x, y, t, \mathbf{u}), & (x, y) \in (0, 1) \times (0, 1),\ t > 0, \\ u^{(l)}(0, y, t) = g_1^{(l)}(y, t), \quad u^{(l)}(1, y, t) = g_2^{(l)}(y, t), & y \in [0, 1],\ t > 0, \\ u^{(l)}(x, 0, t) = h_1^{(l)}(x, t), \quad u^{(l)}(x, 1, t) = h_2^{(l)}(x, t), & x \in [0, 1],\ t > 0, \\ u^{(l)}(x, y, 0) = \phi^{(l)}(x, y), & (x, y) \in [0, 1] \times [0, 1],\ l = 1, 2, \ldots, N, \end{cases} \tag{1.1}$$

where $\mathbf{u} = (u^{(1)}, \ldots, u^{(N)})$ and for each $l = 1, 2, \ldots, N$, $D_1^{(l)}$ and $D_2^{(l)}$ are positive constants. It is assumed that for each $l = 1, 2, \ldots, N$, the functions $f^{(l)}, g_k^{(l)}, h_k^{(l)}$ $(k = 1, 2)$ and $\phi^{(l)}$ are continuous in their respective domains, and $f^{(l)}(\cdot, \mathbf{u})$ is, in general, nonlinear with respect to the components of $\mathbf{u}$.

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∗ Corresponding author at: Department of Mathematics, East China Normal University, Shanghai 200241, People's Republic of China.
E-mail address: ymwang@math.ecnu.edu.cn (Y.-M. Wang).

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There are many ways to formulate a finite difference approximation for the system (1.1). In the usual finite difference method, one approximates the term $u_t^{(l)}$ by Euler backward method and the second-order derivatives $u_{xx}^{(l)}$ and $u_{yy}^{(l)}$ by the second-order central difference quotient (see [10–12,4–6]). However, the resulting difference scheme from this method has only the accuracy of second-order in space and first-order in time (e.g., see [10,11,5,6,13]). In other words, we must take small mesh sizes in order to obtain the desirable accuracy, and thus much computational work is involved. As is well known, by using the Crank–Nicolson technique in the time discretization, the accuracy in time can be improved to second-order without any additional treatment of the initial values (see [14,13]). For the improvement of the accuracy in space, a reasonable approach is to develop higher-order compact finite difference method, which not only provides accurate numerical results and saves computational work, but also is easier to treat boundary conditions (see [15,14]).

Recently, Liao et al. [3] presented a compact finite difference method for (1.1) by using the Crank–Nicolson technique in the time discretization and a fourth-order Padé approximation to $u_{xx}^{(l)}$ and $u_{yy}^{(l)}$. This method requires only a regular five-point difference stencil similar to that used in the standard second-order method, such as the Crank–Nicolson method, and so it possesses the compact property. Moreover, this method has the truncation error $O(\tau^2+h_x^4+h_y^4)$, where τ is the mesh size in time, and h_x and h_y are the mesh sizes in x- and y-directions, respectively. To eliminate the lower-order term in the truncation error, as discussed in [3], Richardson extrapolation can be used on the numerical solution. This makes the final computed solution fourth-order accurate in both space and time. However, to the best of our knowledge, no qualitative analysis, such as the existence–uniqueness problem and the convergence of the numerical solution, was given to this method. On the other hand, since the function $f^{(l)}(\cdot,\mathbf{u})$ is nonlinear in $\mathbf{u}$ the corresponding discrete problem becomes a system of nonlinear algebraic equations. For such a system, it is necessary to develop some kind of iterative algorithm for computing solutions. In this paper, we give a further investigation to the compact method in [3], and develop a number of monotone iterative algorithms for the computation of the solutions of the corresponding discrete system. Our approach to the problem is by the method of upper and lower solutions and its associated monotone iteration, which has been extensively used to various nonlinear problems (see [16–19,4,1,5–7,20–22]).

Firstly, we give some qualitative analyses for the compact finite difference method in [3]. This includes existence and uniqueness of a finite difference solution and the convergence of the numerical solution to the corresponding continuous solution with the accuracy of fourth-order in both space and time. Secondly, we present three basic monotone iterative algorithms for the computation of the finite difference solution using upper and lower solutions as the initial iterations, including a theoretical comparison result for the various monotone sequences. The monotone convergence of the corresponding sequences gives concurrently improved upper and lower bounds of the solution in each iteration. Thereby, from the computational point of view, the monotone convergence has superiority over the ordinary convergence. The definition of upper and lower solutions and the corresponding monotone iterations do not require any monotonicity of the function $f^{(l)}(\cdot,\mathbf{u})$. This enlarges their applications essentially.

The outline of the paper is as follows. In the next section, we discretize problem (1.1) into a system of nonlinear algebraic equation by using the compact method in [3]. In Section 3, we give some auxiliary results which play an important role in our discussions. In Section 4, we deal with the existence and uniqueness problem by the method of upper and lower solutions. Three basic monotone iterative algorithms for the computation of the solution using upper and lower solutions as the initial iterations are presented in Section 5, where the monotone convergence of the sequence of iterations and a theoretical comparison result for the various monotone sequences are proven. In Sections 6 and 7, we investigate the convergence of the method. It is shown that the finite difference solution is fourth-order accurate in space, and after Richardson extrapolation, it also achieve fourth-order accuracy in time. In Section 8, we give an application to an enzyme–substrate reaction–diffusion problem, and present some numerical results to demonstrate the monotone convergence of iterations and the higher-order accuracy of the numerical solution. The Section 9 is for some concluding remarks.

2. Compact finite difference scheme

Let $\Omega=(0,1)\times(0,1)$. We partition Ω with non-isotropic uniform mesh sizes h_x and h_y in the x- and y-directions, respectively. The integers $M_x=1/h_x$ and $M_y=1/h_y$. The mesh points are denoted by $(x_i,y_j)=(ih_x,jh_y)$ $(0\le i\le M_x,\ 0\le j\le M_y)$. For convenience, we also use the index pair (i,j) to represent the mesh point (x_i,y_j). Let $\tau\equiv t_n-t_{n-1}$ be the time increment. For each $l=1,2,\ldots,N$, we define

$$\begin{aligned}&u_{i,j,n}^{(l)}=u^{(l)}(x_i,y_j,t_n),\qquad \mathbf{u}_{i,j,n}=(u_{i,j,n}^{(1)},\ldots,u_{i,j,n}^{(N)}),\qquad f_{i,j,n}^{(l)}(\mathbf{u}_{i,j,n})=f^{(l)}(x_i,y_j,t_n,\mathbf{u}_{i,j,n}),\\&g_{k,j,n}^{(l)}=g_k^{(l)}(y_j,t_n),\qquad h_{k,i,n}^{(l)}=h_k^{(l)}(x_i,t_n)\quad(k=1,2),\qquad \phi_{i,j}^{(l)}=\phi^{(l)}(x_i,y_j).\end{aligned}\tag{2.1}$$

We now discretize problem (1.1) by the compact method in [3] but using a different derivation. We start from the following Crank–Nicolson technique in the time discretization (see [13]):

$$\begin{aligned}&\frac{1}{\tau}(u_{i,j,n+1}^{(l)}-u_{i,j,n}^{(l)})-\frac{D_1^{(l)}}{2}((u_{xx}^{(l)})_{i,j,n+1}+(u_{xx}^{(l)})_{i,j,n})-\frac{D_2^{(l)}}{2}((u_{yy}^{(l)})_{i,j,n+1}+(u_{yy}^{(l)})_{i,j,n})\\&\quad=\frac{1}{2}(f_{i,j,n+1}^{(l)}(\mathbf{u}_{i,j,n+1})+f_{i,j,n}^{(l)}(\mathbf{u}_{i,j,n}))+O(\tau^2),\quad (i,j)\in\Omega,\ n\ge 0.\end{aligned}\tag{2.2}$$

Let

$$\delta_x^2 u_{i,j} = h_x^{-2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}), \qquad \delta_y^2 u_{i,j} = h_y^{-2}(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}),$$

and introduce the finite difference operators

$$\overline{\delta}_\alpha^2 u_{i,j} = \left(1 + \frac{h_\alpha^2}{12}\delta_\alpha^2\right) u_{i,j}, \quad \alpha = x, y. \tag{2.3}$$

According to Numerov's formula (cf. [23]),

$$\delta_\alpha^2 u_{i,j} = \overline{\delta}_\alpha^2 (u_{\alpha\alpha})_{i,j} + O(h_\alpha^4), \quad \alpha = x, y, \tag{2.4}$$

or symbolically,

$$\overline{\delta}_\alpha^{-2} \delta_\alpha^2 u_{i,j} = (u_{\alpha\alpha})_{i,j} + O(h_\alpha^4), \quad \alpha = x, y, \tag{2.5}$$

where $\overline{\delta}_\alpha^{-2} \equiv (\overline{\delta}_\alpha^2)^{-1}$ denotes the inverse of $\overline{\delta}_\alpha^2$.

We now apply the above fourth-order compact approximations to the second-order derivatives involved in (2.2). This yields symbolically that

$$\begin{aligned}&\left(1 - \frac{\tau D_1^{(l)}}{2}\overline{\delta}_x^{-2}\delta_x^2 - \frac{\tau D_2^{(l)}}{2}\overline{\delta}_y^{-2}\delta_y^2\right) u_{i,j,n+1}^{(l)}\\ &\quad = \left(1 + \frac{\tau D_1^{(l)}}{2}\overline{\delta}_x^{-2}\delta_x^2 + \frac{\tau D_2^{(l)}}{2}\overline{\delta}_y^{-2}\delta_y^2\right) u_{i,j,n}^{(l)} + \frac{\tau}{2}(f_{i,j,n+1}^{(l)}(\mathbf{u}_{i,j,n+1}) + f_{i,j,n}^{(l)}(\mathbf{u}_{i,j,n})) + O(\tau^3 + \tau h^4),\end{aligned} \tag{2.6}$$

where $O(h^4)$ denotes the truncated term of the order $O(h_x^4 + h_y^4)$. Multiplying the above equations by the finite difference operator $\overline{\delta}_x^2\overline{\delta}_y^2$, we reach that

$$\begin{aligned}&\left(\overline{\delta}_x^2\overline{\delta}_y^2 - \frac{\tau D_1^{(l)}}{2}\overline{\delta}_y^2\delta_x^2 - \frac{\tau D_2^{(l)}}{2}\overline{\delta}_x^2\delta_y^2\right) u_{i,j,n+1}^{(l)}\\ &\quad = \left(\overline{\delta}_x^2\overline{\delta}_y^2 + \frac{\tau D_1^{(l)}}{2}\overline{\delta}_y^2\delta_x^2 + \frac{\tau D_2^{(l)}}{2}\overline{\delta}_x^2\delta_y^2\right) u_{i,j,n}^{(l)} + \frac{\tau}{2}\overline{\delta}_x^2\overline{\delta}_y^2(f_{i,j,n+1}^{(l)}(\mathbf{u}_{i,j,n+1}) + f_{i,j,n}^{(l)}(\mathbf{u}_{i,j,n})) + O(\tau^3 + \tau h^4).\end{aligned} \tag{2.7}$$

After dropping the $O(\tau^3 + \tau h^4)$ term, we derive a finite difference scheme as follows,

$$\begin{aligned}&\left(\overline{\delta}_x^2\overline{\delta}_y^2 - \frac{\tau D_1^{(l)}}{2}\overline{\delta}_y^2\delta_x^2 - \frac{\tau D_2^{(l)}}{2}\overline{\delta}_x^2\delta_y^2\right) u_{i,j,n+1}^{(l),h}\\ &\quad = \left(\overline{\delta}_x^2\overline{\delta}_y^2 + \frac{\tau D_1^{(l)}}{2}\overline{\delta}_y^2\delta_x^2 + \frac{\tau D_2^{(l)}}{2}\overline{\delta}_x^2\delta_y^2\right) u_{i,j,n}^{(l),h} + \frac{\tau}{2}\overline{\delta}_x^2\overline{\delta}_y^2(f_{i,j,n+1}^{(l)}(\mathbf{u}_{i,j,n+1}^h) + f_{i,j,n}^{(l)}(\mathbf{u}_{i,j,n}^h)), \quad l = 1, 2, \ldots, N,\end{aligned} \tag{2.8}$$

where $\mathbf{u}_{i,j,n}^h = (u_{i,j,n}^{(1),h}, \ldots, u_{i,j,n}^{(N),h})$, and $u_{i,j,n}^{(l),h}$ represents the approximation to $u^{(l)}$ at the point (x_i, y_j, t_n). Define $r_x = \tau/h_x^2$ and $r_y = \tau/h_y^2$, and introduce the discrete operators

$$\mathcal{L}_h^{(l)} = \overline{\delta}_x^2\overline{\delta}_y^2 - \frac{\tau D_1^{(l)}}{2}\overline{\delta}_y^2\delta_x^2 - \frac{\tau D_2^{(l)}}{2}\overline{\delta}_x^2\delta_y^2, \qquad \mathcal{P}_h^{(l)} = \overline{\delta}_x^2\overline{\delta}_y^2 + \frac{\tau D_1^{(l)}}{2}\overline{\delta}_y^2\delta_x^2 + \frac{\tau D_2^{(l)}}{2}\overline{\delta}_x^2\delta_y^2, \qquad \mathcal{H}_h = \frac{\tau}{2}\overline{\delta}_x^2\overline{\delta}_y^2.$$

Then a direct calculation shows that

$$\begin{aligned}\mathcal{L}_h^{(l)} u_{i,j}^h \;&=\; (1 - 2a^{(l)} - 2b^{(l)} + 4c^{(l)})u_{i,j}^h + (a^{(l)} - 2c^{(l)})(u_{i+1,j}^h + u_{i-1,j}^h)\\ &\quad + (b^{(l)} - 2c^{(l)})(u_{i,j+1}^h + u_{i,j-1}^h) + c^{(l)}(u_{i+1,j+1}^h + u_{i+1,j-1}^h + u_{i-1,j+1}^h + u_{i-1,j-1}^h),\\ \mathcal{P}_h^{(l)} u_{i,j}^h \;&=\; (1 - 2\alpha^{(l)} - 2\beta^{(l)} + 4\gamma^{(l)})u_{i,j}^h + (\alpha^{(l)} - 2\gamma^{(l)})(u_{i+1,j}^h + u_{i-1,j}^h)\\ &\quad + (\beta^{(l)} - 2\gamma^{(l)})(u_{i,j+1}^h + u_{i,j-1}^h) + \gamma^{(l)}(u_{i+1,j+1}^h + u_{i+1,j-1}^h + u_{i-1,j+1}^h + u_{i-1,j-1}^h),\\ \mathcal{H}_h u_{i,j}^h &= \tau(50u_{i,j}^h + 5(u_{i+1,j}^h + u_{i-1,j}^h + u_{i,j+1}^h + u_{i,j-1}^h))/144 + \tau(u_{i+1,j+1}^h + u_{i+1,j-1}^h + u_{i-1,j+1}^h + u_{i-1,j-1}^h)/288,\end{aligned} \tag{2.9}$$

where

$$
\begin{aligned}
a^{(l)} &= \frac{1}{2}\left(\frac{1}{6} - r_x D_1^{(l)}\right), \qquad b^{(l)} = \frac{1}{2}\left(\frac{1}{6} - r_y D_2^{(l)}\right), \qquad c^{(l)} = \frac{1}{24}\left(\frac{1}{6} - r_x D_1^{(l)} - r_y D_2^{(l)}\right), \\
\alpha^{(l)} &= \frac{1}{2}\left(\frac{1}{6} + r_x D_1^{(l)}\right), \qquad \beta^{(l)} = \frac{1}{2}\left(\frac{1}{6} + r_y D_2^{(l)}\right), \qquad \gamma^{(l)} = \frac{1}{24}\left(\frac{1}{6} + r_x D_1^{(l)} + r_y D_2^{(l)}\right).
\end{aligned} \tag{2.10}
$$

Accordingly, we can rewrite (2.8) as the following alternative form,

$$
\begin{cases}
\mathcal{L}_h^{(l)} u_{i,j,n+1}^{(l),h} = \mathcal{P}_h^{(l)} u_{i,j,n}^{(l),h} + \mathcal{H}_h \left(f_{i,j,n+1}^{(l)}(\mathbf{u}_{i,j,n+1}^h) + f_{i,j,n}^{(l)}(\mathbf{u}_{i,j,n}^h) \right), \quad (i,j) \in \Omega, n \geq 0, \\
u_{0,j,n+1}^{(l),h} = g_{1,j,n+1}^{(l)}, \qquad u_{M_x,j,n+1}^{(l),h} = g_{2,j,n+1}^{(l)}, \quad j = 0, 1, \ldots, M_y, n \geq 0, \\
u_{i,0,n+1}^{(l),h} = h_{1,i,n+1}^{(l)}, \qquad u_{i,M_y,n+1}^{(l),h} = h_{2,i,n+1}^{(l)}, \quad i = 0, 1, \ldots, M_x, n \geq 0, \\
u_{i,j,0}^{(l),h} = \phi_{i,j}^{(l)}, \quad (i,j) \in \Omega \cup \partial\Omega, \ l = 1, 2, \ldots, N.
\end{cases} \tag{2.11}
$$

For analyzing the above scheme, it is more convenient to consider its matrix form. To do this, we order the mesh points lexicographically. More precisely, we first arrange them from the left to the right in the x-direction and then from the bottom to the top in the y-direction. Corresponding to this ordering, we define the following column vectors:

$$
\begin{aligned}
&U_{h,j,n}^{(l)} = (u_{1,j,n}^{(l),h}, u_{2,j,n}^{(l),h}, \ldots, u_{M_x-1,j,n}^{(l),h})^T, \qquad \mathbf{U}_{h,j,n} = (U_{h,j,n}^{(1)}, U_{h,j,n}^{(2)}, \ldots, U_{h,j,n}^{(N)})^T, \\
&F_{j,n}^{(l)}(\mathbf{U}_{h,j,n}) = (f_{1,j,n}^{(l)}(\mathbf{u}_{1,j,n}^h), f_{2,j,n}^{(l)}(\mathbf{u}_{2,j,n}^h), \ldots, f_{M_x-1,j,n}(\mathbf{u}_{M_x-1,j,n}^h))^T, \\
&\Phi_j^{(l)} = (\phi_{1,j}^{(l)}, \phi_{2,j}^{(l)}, \ldots, \phi_{M_x-1,j}^{(l)})^T, \quad j = 1, 2, \ldots, M_y - 1.
\end{aligned} \tag{2.12}
$$

We also define the following $(M_x - 1)$-order symmetric tridiagonal matrices:

$$
\begin{aligned}
A_0^{(l)} &= \text{tridiag}(a^{(l)} - 2c^{(l)}, 1 - 2a^{(l)} - 2b^{(l)} + 4c^{(l)}, a^{(l)} - 2c^{(l)}), \\
B_0^{(l)} &= \text{tridiag}(\alpha^{(l)} - 2\gamma^{(l)}, 1 - 2\alpha^{(l)} - 2\beta^{(l)} + 4\gamma^{(l)}, \alpha^{(l)} - 2\gamma^{(l)}), \\
A_1^{(l)} &= \text{tridiag}(c^{(l)}, b^{(l)} - 2c^{(l)}, c^{(l)}), \qquad B_1^{(l)} = \text{tridiag}(\gamma^{(l)}, \beta^{(l)} - 2\gamma^{(l)}, \gamma^{(l)}), \\
Q_0 &= \text{tridiag}(5/144, 25/72, 5/144), \qquad Q_1 = \text{tridiag}(1/288, 5/144, 1/288).
\end{aligned} \tag{2.13}
$$

Then system (2.11) can be expressed in the matrix form as

$$
\begin{cases}
A_1^{(l)} U_{h,j-1,n+1}^{(l)} + A_0^{(l)} U_{h,j,n+1}^{(l)} + A_1^{(l)} U_{h,j+1,n+1}^{(l)} = B_1^{(l)} U_{h,j-1,n}^{(l)} + B_0^{(l)} U_{h,j,n}^{(l)} + B_1^{(l)} U_{h,j+1,n}^{(l)} \\
\quad + \tau (Q_1 F_{j-1,n+1}^{(l)}(\mathbf{U}_{h,j-1,n+1}) + Q_0 F_{j,n+1}^{(l)}(\mathbf{U}_{h,j,n+1}) + Q_1 F_{j+1,n+1}^{(l)}(\mathbf{U}_{h,j+1,n+1})) \\
\quad + \tau (Q_1 F_{j-1,n}^{(l)}(\mathbf{U}_{h,j-1,n}) + Q_0 F_{j,n}^{(l)}(\mathbf{U}_{h,j,n}) + Q_1 F_{j+1,n}^{(l)}(\mathbf{U}_{h,j+1,n})) + G_{j,n}^{(l)}, \\
U_{h,j,0}^{(l)} = \Phi_j^{(l)}, \quad j = 1, 2, \ldots, M_y - 1, l = 1, 2, \ldots, N,
\end{cases} \tag{2.14}
$$

where for every l, n and j, $U_{h,0,n}^{(l)} = U_{h,M_y,n}^{(l)} = F_{0,n}^{(l)}(\mathbf{U}_{h,0,n}) = F_{M_y,n}^{(l)}(\mathbf{U}_{h,M_y,n}) = 0$ and $G_{j,n}^{(l)}$ is an $(M_x - 1)$-dimensional vector associated with the boundary functions.

To rewrite (2.14) in a more compact form, we set $\mathcal{M} = (M_x - 1) \times (M_y - 1)$ and define the vectors:

$$
\begin{aligned}
&U_{h,n}^{(l)} = (U_{h,1,n}^{(l)}, U_{h,2,n}^{(l)}, \ldots, U_{h,M_y-1,n}^{(l)})^{\mathrm{T}}, \qquad \mathbf{U}_{h,n} = (U_{h,n}^{(1)}, U_{h,n}^{(2)}, \ldots, U_{h,n}^{(N)})^{\mathrm{T}}, \\
&F_n^{(l)}(\mathbf{U}_{h,n}) = (F_{1,n}^{(l)}(\mathbf{U}_{h,1,n}), \ldots, F_{M_y-1,n}^{(l)}(\mathbf{U}_{h,M_y-1,n}))^{\mathrm{T}}, \\
&G_n^{(l)} = (G_{1,n}^{(l)}, G_{2,n}^{(l)}, \ldots, G_{M_y-1,n}^{(l)})^{\mathrm{T}}, \qquad \Phi^{(l)} = (\Phi_1^{(l)}, \Phi_2^{(l)}, \ldots, \Phi_{M_y-1}^{(l)})^{\mathrm{T}}.
\end{aligned} \tag{2.15}
$$

We also introduce the $\mathcal{M}$-order block matrices $A^{(l)}$, $B^{(l)}$ and Q as

$$
A^{(l)} = \text{tridiag}(A_1^{(l)}, A_0^{(l)}, A_1^{(l)}), \qquad B^{(l)} = \text{tridiag}(B_1^{(l)}, B_0^{(l)}, B_1^{(l)}), \qquad Q = \text{tridiag}(Q_1, Q_0, Q_1). \tag{2.16}
$$

Then, (2.14) reads

$$
\begin{cases}
A^{(l)} U_{h,n+1}^{(l)} = B^{(l)} U_{h,n}^{(l)} + \tau Q \left(F_{n+1}^{(l)}(\mathbf{U}_{h,n+1}) + F_n^{(l)}(\mathbf{U}_{h,n}) \right) + G_n^{(l)}, \\
U_{h,0}^{(l)} = \Phi^{(l)}, \quad l = 1, 2, \ldots, N, n = 0, 1, 2, \ldots.
\end{cases} \tag{2.17}
$$

Remark 2.1. The derivation of scheme (2.8) (or (2.11)) here is slightly different from that in [3] where a fourth-order Padé approximation to $u_{xx}^{(l)}$ and $u_{yy}^{(l)}$ was used (see (2.4) in [3]). In [3], scheme (2.8) was further approximated by another scheme. However, the latter leads to an additional truncation error.

3. Some auxiliary results

In this section, we give some results about the matrices $A^{(l)}$, $B^{(l)}$ and Q in (2.16). These results will play an important role in the forthcoming discussions. If all the entries of a matrix S are positive (or nonnegative), then we say that S is positive (or nonnegative), also denoted by $S > 0$ (or $S \geq 0$) for simplicity. We define positive (or nonnegative) vectors similarly.

Throughout the paper we impose the following hypothesis on the mesh ratios r_x and r_y:

$$\begin{aligned} &\Delta_1^{(l)} \equiv 5r_xD_1^{(l)} - r_yD_2^{(l)} - \frac{5}{6} > 0, \qquad \Delta_2^{(l)} \equiv 5r_yD_2^{(l)} - r_xD_1^{(l)} - \frac{5}{6} > 0, \\ &\Delta_3^{(l)} \equiv \frac{5}{6} - r_xD_1^{(l)} - r_yD_2^{(l)} > 0, \quad l = 1, 2, \ldots, N. \end{aligned} \tag{3.1}$$

Theorem 3.1. *Let condition (3.1) be satisfied. Then for each $l = 1, 2, \ldots .N$,*

(i) *the inverse $(A^{(l)})^{-1}$ exists and is positive, and moreover, $\|(A^{(l)})^{-1}\|_\infty \leq 1$;*
(ii) *the matrix $B^{(l)}$ is nonnegative and $\|B^{(l)}\|_\infty \leq 1$.*

Proof. By (2.16) and (2.13),

$$\begin{aligned} &A^{(l)} = \text{tridiag}(A_1^{(l)}, A_0^{(l)}, A_1^{(l)}), \qquad A_1^{(l)} = \text{tridiag}(c^{(l)}, b^{(l)} - 2c^{(l)}, c^{(l)}), \\ &A_0^{(l)} = \text{tridiag}(a^{(l)} - 2c^{(l)}, 1 - 2a^{(l)} - 2b^{(l)} + 4c^{(l)}, a^{(l)} - 2c^{(l)}). \end{aligned}$$

Thanks to condition (3.1), we have

$$1 - 2a^{(l)} - 2b^{(l)} + 4c^{(l)} > 0, \qquad a^{(l)} - 2c^{(l)} < 0, \qquad c^{(l)} < 0, \qquad b^{(l)} - 2c^{(l)} < 0.$$

This implies that the matrix $A^{(l)}$ is irreducibly diagonally dominant. We have from Corollary 1 of [24] (pp. 85) (also see [25]) that the inverse $(A^{(l)})^{-1}$ exists and is positive.

Let $E = (1, 1, \ldots, 1) \in \mathbf{R}^{\mathcal{M}}$ is an $\mathcal{M}$-vector whose components are all one, and let $(A^{(l)})^{-1}E = S^{(l)}$. By using condition (3.1) and a simple calculation, we see that $A^{(l)}E \geq E$. Denote by $S_i^{(l)}$ the ith-component of $S^{(l)}$ and assume that $S_{i_0}^{(l)} = \max_i S_i^{(l)}$ for some i_0. Then by $A^{(l)}S^{(l)} = E$ and $A^{(l)}E \geq E$, we get $S_{i_0}^{(l)} \leq 1$. This proves $\|(A^{(l)})^{-1}\|_\infty \leq 1$ and so the conclusion in (i).

To prove the conclusion in (ii) we observe from (2.16) and (2.13) that

$$\begin{aligned} &B^{(l)} = \text{tridiag}(B_1^{(l)}, B_0^{(l)}, B_1^{(l)}), \qquad B_1^{(l)} = \text{tridiag}(\gamma^{(l)}, \beta^{(l)} - 2\gamma^{(l)}, \gamma^{(l)}), \\ &B_0^{(l)} = \text{tridiag}(\alpha^{(l)} - 2\gamma^{(l)}, 1 - 2\alpha^{(l)} - 2\beta^{(l)} + 4\gamma^{(l)}, \alpha^{(l)} - 2\gamma^{(l)}). \end{aligned}$$

By condition (3.1),

$$1 - 2\alpha^{(l)} - 2\beta^{(l)} + 4\gamma^{(l)} \geq 0, \qquad \alpha^{(l)} - 2\gamma^{(l)} \geq 0, \qquad \beta^{(l)} - 2\gamma^{(l)} \geq 0, \qquad \gamma^{(l)} \geq 0.$$

This proves $B^{(l)} \geq 0$. It is clear that $B^{(l)}E \leq E$, where E is the same as before, which implies $\|B^{(l)}\|_\infty \leq 1$. The proof of the theorem is completed. □

Using the same argument as above we can obtain more general result as follows.

Theorem 3.2. *Let condition (3.1) be satisfied, and let $M^{(l)}$ be a nonnegative constant. Assume that*

$$\tau M^{(l)} < \frac{12}{5} \min\{\Delta_1^{(l)}, \Delta_2^{(l)}, \Delta_3^{(l)}\}, \quad l = 1, 2, \ldots, N. \tag{3.2}$$

Then for each $l = 1, 2, \ldots, N$, (i) *the inverse $(A^{(l)} + \tau M^{(l)}Q)^{-1}$ exists and is positive; and* (ii) *the matrix $B^{(l)} - \tau M^{(l)}Q$ is nonnegative.*

Define

$$\begin{aligned} &\mathcal{D}^{(l)} = \text{tridiag}(0, A_0^{(l)}, 0), \qquad \mathcal{L}^{(l)} = \text{tridiag}(-A_1^{(l)}, 0, 0), \qquad \mathcal{U}^{(l)} = \text{tridiag}(0, 0, -A_1^{(l)}), \\ &\mathcal{D} = \text{tridiag}(0, Q_0, 0), \qquad \mathcal{L} = \text{tridiag}(Q_1, 0, 0), \qquad \mathcal{U} = \text{tridiag}(0, 0, Q_1). \end{aligned} \tag{3.3}$$

Then we can split the matrices $A^{(l)}$ and Q as

$$A^{(l)} = \mathcal{D}^{(l)} - \mathcal{L}^{(l)} - \mathcal{U}^{(l)}, \qquad Q = \mathcal{D} + \mathcal{L} + \mathcal{U}. \tag{3.4}$$

In analogy to Theorem 3.2 we have the following theorem.

Theorem 3.3. *Let $M^{(l)}$ be a nonnegative constant, and let conditions (3.1) and (3.2) be satisfied. Then for each $l = 1, 2, \ldots, N$,* (i) *the inverses $(\mathcal{D}^{(l)} + \tau M^{(l)}\mathcal{D})^{-1}$ and $(\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + \tau M^{(l)}(\mathcal{D} + \mathcal{L}))^{-1}$ exist and are positive; and* (ii) *the matrices $\mathcal{L}^{(l)} + \mathcal{U}^{(l)} - \tau M^{(l)}(\mathcal{L} + \mathcal{U})$ and $\mathcal{U}^{(l)} - \tau M^{(l)}\mathcal{U}$ are nonnegative.*

4. Qualitative analysis of the compact scheme

To investigate the existence and uniqueness of the solution and derive an efficient algorithm for (2.17), we use the method of upper and lower solutions. Let $q = N\mathcal{M}$. For the vector $\mathbf{U} = (U^{(1)}, \dots, U^{(N)})^{\mathrm{T}}$ in $\mathbf{R}^q$, we define

$$[\mathbf{U}]_{l,N-1} \equiv (U^{(1)}, \dots, U^{(l-1)}, U^{(l+1)}, \dots, U^{(N)})^{\mathrm{T}}. \tag{4.1}$$

Then we can write, e.g.,

$$F_n^{(l)}(\mathbf{U}_{h,n}) = F_n^{(l)}(U_{h,n}^{(l)}, [\mathbf{U}_{h,n}]_{l,N-1}).$$

The definition of upper and lower solutions of (2.17) is given as follows.

Definition 4.1. Two vectors $\widetilde{\mathbf{U}}_{h,n} = (\widetilde{U}_{h,n}^{(1)}, \dots, \widetilde{U}_{h,n}^{(N)})^{\mathrm{T}}$, $\widehat{\mathbf{U}}_{h,n} = (\widehat{U}_{h,n}^{(1)}, \dots, \widehat{U}_{h,n}^{(N)})^{\mathrm{T}}$ in $\mathbf{R}^q$ are called coupled upper and lower solutions of (2.17) if for each $l = 1, 2, \dots, N$ and $n = 0, 1, 2, \dots$, $\widetilde{\mathbf{U}}_{h,n} \geq \widehat{\mathbf{U}}_{h,n}$ and

$$\begin{cases} A^{(l)}\widetilde{U}_{h,n+1}^{(l)} \geq B^{(l)}\widetilde{U}_{h,n}^{(l)} + \tau Q\left(F_{n+1}^{(l)}(\widetilde{U}_{h,n+1}^{(l)}, [\mathbf{V}]_{l,N-1}) + F_n^{(l)}(\widetilde{U}_{h,n}^{(l)}, [\mathbf{V}']_{l,N-1})\right) + G_n^{(l)}, \\ A^{(l)}\widehat{U}_{h,n+1}^{(l)} \leq B^{(l)}\widehat{U}_{h,n}^{(l)} + \tau Q\left(F_{n+1}^{(l)}(\widehat{U}_{h,n+1}^{(l)}, [\mathbf{V}]_{l,N-1}) + F_n^{(l)}(\widehat{U}_{h,n}^{(l)}, [\mathbf{V}']_{l,N-1})\right) + G_n^{(l)}, \\ \qquad \text{for all } \mathbf{V} \in \langle \widehat{\mathbf{U}}_{h,n+1}, \widetilde{\mathbf{U}}_{h,n+1}\rangle, \mathbf{V}' \in \langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n}\rangle, \\ \widetilde{U}_{h,0}^{(l)} \geq \Phi^{(l)} \geq \widehat{U}_{h,0}^{(l)}. \end{cases} \tag{4.2}$$

In the above definition, inequalities between vectors are in the sense of componentwise, and the sector $\langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n}\rangle$ is given by

$$\langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n}\rangle = \{\mathbf{V} \in \mathbf{R}^q : \widehat{\mathbf{U}}_{h,n} \leq \mathbf{V} \leq \widetilde{\mathbf{U}}_{h,n}\}. \tag{4.3}$$

For notational convenience we define, for any $\mathbf{U} = (U^{(1)}, \dots, U^{(N)})^{\mathrm{T}}$ in $\mathbf{R}^q$ with $U^{(l)} = (U_1^{(l)}, \dots, U_{M_y-1}^{(l)})^{\mathrm{T}} \in \mathbf{R}^{\mathcal{M}}$ and $U_j^{(l)} = (u_{1,j}^{(l)}, \dots, u_{M_x-1,j}^{(l)})^{\mathrm{T}} \in \mathbf{R}^{M_x-1}$, the nonnegative vectors

$$|\mathbf{U}|_0 = |U^{(1)}| + \cdots + |U^{(N)}|, \quad |U^{(l)}| = (|U_1^{(l)}|, \dots, |U_{M_y-1}^{(l)}|)^{\mathrm{T}}, \quad |U_j^{(l)}| = (|u_{1,j}^{(l)}|, \dots, |u_{M_x-1,j}^{(l)}|)^{\mathrm{T}}. \tag{4.4}$$

Throughout the paper we make the following basic hypothesis on $F_n^{(l)}$:

(H) For each $l = 1, 2, \dots, N$ and $n = 0, 1, 2, \dots$, there exists a positive constant $M_n^{(l)}$ such that

$$|F_n^{(l)}(\mathbf{U}_{h,n}) - F_n^{(l)}(\mathbf{V}_{h,n})| \leq M_n^{(l)}|\mathbf{U}_{h,n} - \mathbf{V}_{h,n}|_0, \quad \text{for all } \mathbf{U}_{h,n}, \mathbf{V}_{h,n} \in \langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n}\rangle, \tag{4.5}$$

where $\widetilde{\mathbf{U}}_{h,n}$ and $\widehat{\mathbf{U}}_{h,n}$ are coupled upper and lower solutions of (2.17).

The existence of the constant $M_n^{(l)}$ in (4.5) is trivial, if $F_n^{(l)}(\mathbf{U}_{h,n})$ is a C^1-function of $\mathbf{U}_{h,n}$ in $\langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n}\rangle$. Our first theorem is concerned with the existence problem.

Theorem 4.1. *Let $\widetilde{\mathbf{U}}_{h,n}$ and $\widehat{\mathbf{U}}_{h,n}$ be coupled upper and lower solutions of (2.17), and let hypothesis (H) hold. Also let the conditions (3.1) and (3.2) be satisfied with respect to the constant $M_n^{(l)}$ in (4.5). Then system (2.17) has at least one solution $\mathbf{U}_{h,n}^*$ in $\langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n}\rangle$.*

Proof. Given any $\mathbf{V}_{h,1} = (V_{h,1}^{(1)}, \dots, V_{h,1}^{(N)})^{\mathrm{T}} \in \langle \widehat{\mathbf{U}}_{h,1}, \widetilde{\mathbf{U}}_{h,1}\rangle$, we consider the linear problem

$$\begin{cases} (A^{(l)} + \tau M_1^{(l)} Q)U_{h,1}^{(l)} = B^{(l)}U_{h,0}^{*(l)} + \tau Q\left(F_1^{(l)}(\mathbf{V}_{h,1}) + M_1^{(l)}V_{h,1}^{(l)} + F_0^{(l)}(\mathbf{U}_{h,0}^*)\right) + G_0^{(l)}, \\ U_{h,0}^{*(l)} = \Phi^{(l)}, \quad l = 1, 2, \dots, N, \end{cases} \tag{4.6}$$

where $\mathbf{U}_{h,0}^* = (U_{h,0}^{*(1)}, \dots, U_{h,0}^{*(N)})^{\mathrm{T}}$. Since by Theorem 3.1, the inverse $(A^{(l)} + \tau M_1^{(l)} Q)^{-1}$ exists, the above problem has a unique solution $\mathbf{U}_{h,1} \equiv (U_{h,1}^{(1)}, \dots, U_{h,1}^{(N)})^{\mathrm{T}}$. Define a mapping $\mathcal{T}_1 : \langle \widehat{\mathbf{U}}_{h,1}, \widetilde{\mathbf{U}}_{h,1}\rangle \longrightarrow \mathbf{R}^q$ by

$$\mathcal{T}_1\mathbf{V}_{h,1} \equiv \mathbf{U}_{h,1}. \tag{4.7}$$

It is clear from hypothesis (H) that $\mathcal{T}_1$ is a continuous map on $\langle \widehat{\mathbf{U}}_{h,1}, \widetilde{\mathbf{U}}_{h,1}\rangle$. We show that $\mathcal{T}_1$ maps $\langle \widehat{\mathbf{U}}_{h,1}, \widetilde{\mathbf{U}}_{h,1}\rangle$ into itself.

It is easily seen from (4.2), (4.5) and (4.6) that for any $\mathbf{V}_{h,1} \in \langle \widehat{\mathbf{U}}_{h,1}, \widetilde{\mathbf{U}}_{h,1} \rangle$,

$$\begin{aligned}(A^{(l)} + \tau M_1^{(l)} Q)(\widetilde{U}_{h,1}^{(l)} - U_{h,1}^{(l)}) &\geq B^{(l)} \left(\widetilde{U}_{h,0}^{(l)} - U_{h,0}^{*(l)} \right) + \tau Q \left(F_1^{(l)}(\widetilde{U}_{h,1}^{(l)}, [\mathbf{V}_{h,1}]_{l,N-1}) - F_1^{(l)}(\mathbf{V}_{h,1}) + M_1^{(l)}(\widetilde{U}_{h,1}^{(l)} - V_{h,1}^{(l)}) \right) \\ &\quad + \tau Q \left(F_0^{(l)}(\widetilde{U}_{h,0}^{(l)}, [\mathbf{U}_{h,0}^*]_{l,N-1}) - F_0^{(l)}(\mathbf{U}_{h,0}^*) \right) \\ &\geq (B^{(l)} - \tau M_0^{(l)} Q) \left(\widetilde{U}_{h,0}^{(l)} - U_{h,0}^{*(l)} \right).\end{aligned}$$

Since $\widetilde{U}_{h,0}^{(l)} - U_{h,0}^{*(l)} = \widetilde{U}_{h,0}^{(l)} - \Phi^{(l)} \geq 0$ and by Theorem 3.2, $B^{(l)} - \tau M_0^{(l)} Q \geq 0$, the positivity of $(A^{(l)} + \tau M_1^{(l)} Q)^{-1}$ ensures that $\widetilde{U}_{h,1}^{(l)} - U_{h,1}^{(l)} \geq 0$, i.e., $\widetilde{U}_{h,1}^{(l)} \geq U_{h,1}^{(l)}$ for each $l = 1, 2, \ldots, N$. A similar argument using the property of lower solution gives $U_{h,1}^{(l)} \geq \widehat{U}_{h,1}^{(l)}$ for each $l = 1, 2, \ldots, N$. This proves $\mathbf{U}_{h,1} \in \langle \widehat{\mathbf{U}}_{h,1}, \widetilde{\mathbf{U}}_{h,1} \rangle$. By Brower's fixed point theorem there exists $\mathbf{U}_{h,1}^* \in \langle \widehat{\mathbf{U}}_{h,1}, \widetilde{\mathbf{U}}_{h,1} \rangle$ such that $\mathcal{T}_1 \mathbf{U}_{h,1}^* = \mathbf{U}_{h,1}^*$, or equivalently,

$$\begin{cases} A^{(l)} U_{h,1}^{*(l)} = B^{(l)} U_{h,0}^{*(l)} + \tau Q \left(F_1^{(l)}(\mathbf{U}_{h,1}^*) + F_0^{(l)}(\mathbf{U}_{h,0}^*) \right) + G_0^{(l)}, \\ U_{h,0}^{*(l)} = \Phi^{(l)}, \quad l = 1, 2, \ldots, N. \end{cases} \tag{4.8}$$

Using $\mathbf{U}_{h,1}^* = (U_{h,1}^{*(1)}, \ldots, U_{h,1}^{*(N)})^{\mathrm{T}}$ we define a mapping $\mathcal{T}_2 : \langle \widehat{\mathbf{U}}_{h,2}, \widetilde{\mathbf{U}}_{h,2} \rangle \longrightarrow \mathbf{R}^q$ by

$$\mathcal{T}_2 \mathbf{V}_{h,2} \equiv \mathbf{U}_{h,2}, \quad \forall\, \mathbf{V}_{h,2} \in \langle \widehat{\mathbf{U}}_{h,2}, \widetilde{\mathbf{U}}_{h,2} \rangle,$$

where $\mathbf{U}_{h,2} = (U_{h,2}^{(1)}, \ldots, U_{h,2}^{(N)})^{\mathrm{T}}$ is the unique solution of the linear problem

$$(A^{(l)} + \tau M_2^{(l)} Q) U_{h,2}^{(l)} = B^{(l)} U_{h,1}^{*(l)} + \tau Q \left(F_2^{(l)}(\mathbf{V}_{h,2}) + M_2^{(l)} V_{h,2}^{(l)} + F_1^{(l)}(\mathbf{U}_{h,1}^*) \right) + G_1^{(l)}. \tag{4.9}$$

By the similar argument as that for $\mathcal{T}_1$, we conclude that there exists $\mathbf{U}_{h,2}^* \in \langle \widehat{\mathbf{U}}_{h,2}, \widetilde{\mathbf{U}}_{h,2} \rangle$ such that $\mathcal{T}_2 \mathbf{U}_{h,2}^* = \mathbf{U}_{h,2}^*$, i.e.,

$$A^{(l)} U_{h,2}^{*(l)} = B^{(l)} U_{h,1}^{*(l)} + \tau Q \left(F_2^{(l)}(\mathbf{U}_{h,2}^*) + F_1^{(l)}(\mathbf{U}_{h,1}^*) \right) + G_1^{(l)}. \tag{4.10}$$

A continuation of this process shows that there exists $\mathbf{U}_{h,n}^* \in \langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n} \rangle$ such that

$$\begin{cases} A^{(l)} U_{h,n+1}^{*(l)} = B^{(l)} U_{h,n}^{*(l)} + \tau Q \left(F_{n+1}^{(l)}(\mathbf{U}_{h,n+1}^*) + F_n^{(l)}(\mathbf{U}_{h,n}^*) \right) + G_n^{(l)}, \\ U_{h,0}^{*(l)} = \Phi^{(l)}, \quad l = 1, 2, \ldots, N, n = 0, 1, 2, \ldots. \end{cases} \tag{4.11}$$

This shows that $\mathbf{U}_{h,n}^*$ is a solution of (2.17) in $\langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n} \rangle$. □

By Theorem 4.1, (2.17) has at least one solution, provided that it possesses a pair of coupled upper and lower solutions, which also serve as the upper and lower bounds of this solution. To guarantee the uniqueness of the solution we assume that

$$\tau \sum_{l=1}^{N} M_n^{(l)} < 1, \quad n = 1, 2, \ldots, \tag{4.12}$$

where $M_n^{(l)}$ are the Lipschitz constants in (4.5).

Theorem 4.2. *Let the conditions in Theorem 4.1 hold. If, in addition, condition (4.12) be satisfied, then system (2.17) has a unique solution $\mathbf{U}_{h,n}^*$ in $\langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n} \rangle$.*

Proof. Let $\mathbf{U}_{h,n} = (U_{h,n}^{(1)}, \ldots, U_{h,n}^{(N)})^{\mathrm{T}}$ and $\mathbf{U}'_{h,n} = (U_{h,n}^{\prime(1)}, \ldots, U_{h,n}^{\prime(N)})^{\mathrm{T}}$ be any two solutions of (2.17) in $\langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n} \rangle$, and let $\mathbf{W}_{h,n} = \mathbf{U}_{h,n} - \mathbf{U}'_{h,n}$ with its components $W_{h,n}^{(l)} = U_{h,n}^{(l)} - U_{h,n}^{\prime(l)}$ $(l = 1, 2, \ldots, N)$. By (2.17),

$$\begin{cases} A^{(l)} W_{h,n+1}^{(l)} = B^{(l)} W_{h,n}^{(l)} + \tau Q \left(F_{n+1}^{(l)}(\mathbf{U}_{h,n+1}) - F_{n+1}^{(l)}(\mathbf{U}'_{h,n+1}) + F_n^{(l)}(\mathbf{U}_{h,n}) - F_n^{(l)}(\mathbf{U}'_{h,n}) \right), \\ W_{h,0}^{(l)} = 0, \quad l = 1, 2, \ldots, N, n = 0, 1, 2, \ldots. \end{cases} \tag{4.13}$$

Using the positivity of $(A^{(l)})^{-1}$, the nonnegativity of $B^{(l)}$ and Q and the Lipschitz condition (4.5), we obtain from (4.13) that

$$|W_{h,n+1}^{(l)}| \leq (A^{(l)})^{-1} B^{(l)} |W_{h,n}^{(l)}| + \tau (A^{(l)})^{-1} Q \left(M_{n+1}^{(l)} |\mathbf{W}_{h,n+1}|_0 + M_n^{(l)} |\mathbf{W}_{h,n}|_0 \right), \quad l = 1, 2, \ldots, N.$$

Addition of the above inequalities over l yields

$$|\mathbf{W}_{h,n+1}|_0 \leq \sum_{l=1}^{N}(A^{(l)})^{-1}B^{(l)}|W_{h,n}^{(l)}| + \tau\sum_{l=1}^{N}(A^{(l)})^{-1}Q\left(M_{n+1}^{(l)}|\mathbf{W}_{h,n+1}|_0 + M_n^{(l)}|\mathbf{W}_{h,n}|_0\right). \tag{4.14}$$

Consider the case $n = 0$. Since $W_{h,0}^{(l)} = 0$ for every l, the above inequality for $n = 0$ becomes

$$|\mathbf{W}_{h,1}|_0 \leq \tau\left(\sum_{l=1}^{N}M_1^{(l)}(A^{(l)})^{-1}\right)Q|\mathbf{W}_{h,1}|_0.$$

By Theorem 3.1, $\|(A^{(l)})^{-1}\|_\infty \leq 1$. This together with $\|Q\|_\infty \leq 1$ yields

$$\||\mathbf{W}_{h,1}|_0\|_\infty \leq \tau\left(\sum_{l=1}^{N}M_1^{(l)}\right)\||\mathbf{W}_{h,1}|_0\|_\infty.$$

Thus by condition (4.12), $|\mathbf{W}_{h,1}|_0 = 0$.

Using $|\mathbf{W}_{h,1}|_0 = 0$ in (4.14) with $n = 1$ leads to

$$\||\mathbf{W}_{h,2}|_0\|_\infty \leq \tau\left(\sum_{l=1}^{N}M_2^{(l)}\right)\||\mathbf{W}_{h,2}|_0\|_\infty.$$

Again by condition (4.12), $|\mathbf{W}_{h,2}|_0 = 0$. An induction argument yields $|\mathbf{W}_{h,n}|_0 = 0$ for every n. This proves $\mathbf{U}_{h,n} = \mathbf{U}'_{h,n}$ and thus the uniqueness of the solution. □

5. Monotone iterative algorithms

Theorem 4.2 shows that if $\widetilde{\mathbf{U}}_{h,n}$ and $\widehat{\mathbf{U}}_{h,n}$ are a pair of coupled upper and lower solutions of (2.17) then it has a unique solution $\mathbf{U}^*_{h,n} = (U_{h,n}^{*(1)}, \ldots, U_{h,n}^{*(N)})^{\mathrm{T}}$ in $\langle\widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n}\rangle$. To compute the solution $\mathbf{U}^*_{h,n}$ we develop here three monotone iterative algorithms using $\widetilde{\mathbf{U}}_{h,n}$ and $\widehat{\mathbf{U}}_{h,n}$ as a pair of initial iterations. The corresponding sequences $\{\overline{\mathbf{U}}_{h,n}^{(m)}\} = \{((\overline{U}_{h,n}^{(1)})^{(m)}, \ldots, (\overline{U}_{h,n}^{(N)})^{(m)})^{\mathrm{T}}\}$ and $\{\underline{\mathbf{U}}_{h,n}^{(m)}\} = \{((\underline{U}_{h,n}^{(1)})^{(m)}, \ldots, (\underline{U}_{h,n}^{(N)})^{(m)})^{\mathrm{T}}\}$ not only converge monotonically to $\mathbf{U}^*_{h,n}$ but also improve the upper and lower bounds of the solution, step by step.

Our first iterative algorithm is of Picard type and is given by

$$\begin{cases} (A^{(l)} + \tau M_{n+1}^{(l)}Q)(\overline{U}_{h,n+1}^{(l)})^{(m+1)} = B^{(l)}U_{h,n}^{*(l)} + \tau Q\max\limits_{\mathbf{V}\in\mathcal{S}_{n+1}^{(m)}}\left(M_{n+1}^{(l)}V^{(l)} + F_{n+1}^{(l)}(\mathbf{V})\right) + \tau QF_n^{(l)}(\mathbf{U}^*_{h,n}) + G_n^{(l)}, \\ (A^{(l)} + \tau M_{n+1}^{(l)}Q)(\underline{U}_{h,n+1}^{(l)})^{(m+1)} = B^{(l)}U_{h,n}^{*(l)} + \tau Q\min\limits_{\mathbf{V}\in\mathcal{S}_{n+1}^{(m)}}\left(M_{n+1}^{(l)}V^{(l)} + F_{n+1}^{(l)}(\mathbf{V})\right) + \tau QF_n^{(l)}(\mathbf{U}^*_{h,n}) + G_n^{(l)}, \\ (\overline{U}_{h,0}^{(l)})^{(m+1)} = (\underline{U}_{h,0}^{(l)})^{(m+1)} = \Phi^{(l)}, \quad l = 1, 2, \ldots, N, n = 0, 1, 2, \ldots, \end{cases} \tag{5.1}$$

where $M_{n+1}^{(l)}$ is the Lipschitz constant in (4.5), and

$$\mathcal{S}_{n+1}^{(m)} = \{\mathbf{V}\in\mathbf{R}^q : \underline{\mathbf{U}}_{h,n+1}^{(m)} \leq \mathbf{V} \leq \overline{\mathbf{U}}_{h,n+1}^{(m)}\}, \qquad \overline{\mathbf{U}}_{h,n+1}^{(0)} = \widetilde{\mathbf{U}}_{h,n+1}, \qquad \underline{\mathbf{U}}_{h,n+1}^{(0)} = \widehat{\mathbf{U}}_{h,n+1}. \tag{5.2}$$

In the above iterative algorithm, the maximum and the minimum of a vector function are in the sense of componentwise. To show that the sequences given by (5.1) are well defined it is crucial that the sequences $\{\overline{\mathbf{U}}_{h,n}^{(m)}\}$, $\{\underline{\mathbf{U}}_{h,n}^{(m)}\}$ possess the property $\overline{\mathbf{U}}_{h,n}^{(m)} \geq \underline{\mathbf{U}}_{h,n}^{(m)}$ for every m and n.

Lemma 5.1. *Let the conditions in Theorem 4.1 be satisfied. Then the sequences $\{\overline{\mathbf{U}}_{h,n}^{(m)}\}$ and $\{\underline{\mathbf{U}}_{h,n}^{(m)}\}$ and the set $\mathcal{S}_{n+1}^{(m)}$ given by (5.1) and (5.2) are all well defined and possess the property*

$$\widehat{\mathbf{U}}_{h,n} \leq \underline{\mathbf{U}}_{h,n}^{(m-1)} \leq \underline{\mathbf{U}}_{h,n}^{(m)} \leq \overline{\mathbf{U}}_{h,n}^{(m)} \leq \overline{\mathbf{U}}_{h,n}^{(m-1)} \leq \widetilde{\mathbf{U}}_{h,n} \quad (m, n = 1, 2, \ldots). \tag{5.3}$$

Proof. Let $m = 0$ in (5.1) with any fixed $n = 0, 1, 2, \ldots$. Since $\overline{\mathbf{U}}_{h,n+1}^{(0)} = \widetilde{\mathbf{U}}_{h,n+1}$, $\underline{\mathbf{U}}_{h,n+1}^{(0)} = \widehat{\mathbf{U}}_{h,n+1}$ and $\widetilde{\mathbf{U}}_{h,n+1} \geq \widehat{\mathbf{U}}_{h,n+1}$, the set $\mathcal{S}_{n+1}^{(0)}$ is well defined, and thus the right-hand side of (5.1) is known when $m = 0$. By Theorem 3.2, the inverse $(A^{(l)} + \tau M_{n+1}^{(l)}Q)^{-1}$ exists and is positive. Hence the first iterations $\overline{\mathbf{U}}_{h,n+1}^{(1)}$, $\underline{\mathbf{U}}_{h,n+1}^{(1)}$ exist, and

$$(A^{(l)} + \tau M_{n+1}^{(l)}Q)((\overline{U}_{h,n+1}^{(l)})^{(1)} - (\underline{U}_{h,n+1}^{(l)})^{(1)}) \geq 0.$$

It follows from the positivity of $(A^{(l)} + \tau M_{n+1}^{(l)} Q)^{-1}$ that $(\overline{U}_{h,n+1}^{(l)})^{(1)} \geq (\underline{U}_{h,n+1}^{(l)})^{(1)}$ for every l. This proves $\overline{\mathbf{U}}_{h,n+1}^{(1)} \geq \underline{\mathbf{U}}_{h,n+1}^{(1)}$. Since by hypothesis (H), the function $M_{n+1}^{(l)} V^{(l)} + F_{n+1}^{(l)}(\mathbf{V})$ is nondecreasing in $V^{(l)}$ for all $\mathbf{V} \in \langle \widehat{\mathbf{U}}_{h,n+1}, \widetilde{\mathbf{U}}_{h,n+1} \rangle$, the inequalities in (4.2) imply

$$\begin{cases} (A^{(l)} + \tau M_{n+1}^{(l)} Q)\widetilde{U}_{h,n+1}^{(l)} \geq B^{(l)} \widetilde{U}_{h,n}^{(l)} + \tau Q \max\limits_{\mathbf{V} \in \mathcal{S}_{n+1}^{(0)}} \left(M_{n+1}^{(l)} V^{(l)} + F_{n+1}^{(l)}(\mathbf{V}) \right) + \tau Q F_n^{(l)}(\widetilde{U}_{h,n}^{(l)}, [\mathbf{U}_{h,n}^*]_{l,N-1}) + G_n^{(l)}, \\ (A^{(l)} + \tau M_{n+1}^{(l)} Q)\widehat{U}_{h,n+1}^{(l)} \leq B^{(l)} \widehat{U}_{h,n}^{(l)} + \tau Q \min\limits_{\mathbf{V} \in \mathcal{S}_{n+1}^{(0)}} \left(M_{n+1}^{(l)} V^{(l)} + F_{n+1}^{(l)}(\mathbf{V}) \right) + \tau Q F_n^{(l)}(\widehat{U}_{h,n}^{(l)}, [\mathbf{U}_{h,n}^*]_{l,N-1}) + G_n^{(l)}, \\ \quad l = 1, 2, \ldots, N. \end{cases} \tag{5.4}$$

By (5.4), (5.1) and (4.5) with $m = 0$, we have for each $l = 1, 2, \ldots, N$,

$$(A^{(l)} + \tau M_{n+1}^{(l)} Q)(\widetilde{U}_{h,n+1}^{(l)} - (\overline{U}_{h,n+1}^{(l)})^{(1)}) \geq (B^{(l)} - \tau M_n^{(l)} Q) \left(\widetilde{U}_{h,n}^{(l)} - U_{h,n}^{*(l)} \right).$$

Since $\widetilde{U}_{h,n}^{(l)} - U_{h,n}^{*(l)} \geq 0$ and $B^{(l)} - \tau M_n^{(l)} Q \geq 0$, we have from $(A^{(l)} + \tau M_{n+1}^{(l)} Q)^{-1} > 0$ that $\widetilde{U}_{h,n+1}^{(l)} - (\overline{U}_{h,n+1}^{(l)})^{(1)} \geq 0$ which implies $\overline{\mathbf{U}}_{h,n+1}^{(1)} \leq \widetilde{\mathbf{U}}_{h,n+1}$. A similar argument using the property of a lower solution gives $\widehat{\mathbf{U}}_{h,n+1} \leq \underline{\mathbf{U}}_{h,n+1}^{(1)}$. This proves (5.3) for $m = 1$. Finally, the conclusion of the lemma follows from the principle of induction. □

In view of the monotone property (5.3) the limits

$$\lim_{m \to \infty} \overline{\mathbf{U}}_{h,n}^{(m)} = \overline{\mathbf{U}}_{h,n}, \qquad \lim_{m \to \infty} \underline{\mathbf{U}}_{h,n}^{(m)} = \underline{\mathbf{U}}_{h,n} \tag{5.5}$$

exist and

$$\widehat{\mathbf{U}}_{h,n} \leq \underline{\mathbf{U}}_{h,n}^{(m-1)} \leq \underline{\mathbf{U}}_{h,n}^{(m)} \leq \underline{\mathbf{U}}_{h,n} \leq \overline{\mathbf{U}}_{h,n} \leq \overline{\mathbf{U}}_{h,n}^{(m)} \leq \overline{\mathbf{U}}_{h,n}^{(m-1)} \leq \widetilde{\mathbf{U}}_{h,n} \quad (m, n = 1, 2, \ldots). \tag{5.6}$$

Letting $m \to \infty$ in (5.1) and using the exactly same argument as that in proving Lemma A of Appendix in [9], we know that the limits $\overline{\mathbf{U}}_{h,n}$ and $\underline{\mathbf{U}}_{h,n}$ satisfy

$$\begin{cases} A^{(l)} \overline{U}_{h,n+1}^{(l)} = B^{(l)} U_{h,n}^{*(l)} + \tau Q \max\limits_{\mathbf{V} \in \mathcal{S}_{n+1}} \left(F_{n+1}^{(l)}(\overline{U}_{h,n+1}^{(l)}, [\mathbf{V}]_{l,N-1}) \right) + \tau Q F_n^{(l)}(\mathbf{U}_{h,n}^*) + G_n^{(l)}, \\ A^{(l)} \underline{U}_{h,n+1}^{(l)} = B^{(l)} U_{h,n}^{*(l)} + \tau Q \min\limits_{\mathbf{V} \in \mathcal{S}_{n+1}} \left(F_{n+1}^{(l)}(\underline{U}_{h,n+1}^{(l)}, [\mathbf{V}]_{l,N-1}) \right) + \tau Q F_n^{(l)}(\mathbf{U}_{h,n}^*) + G_n^{(l)}, \\ \overline{U}_{h,0}^{(l)} = \underline{U}_{h,0}^{(l)} = \Phi^{(l)}, \quad l = 1, 2, \ldots, N, n = 0, 1, 2, \ldots, \end{cases} \tag{5.7}$$

where

$$\mathcal{S}_{n+1} = \{\mathbf{V} \in \mathbf{R}^q : \underline{\mathbf{U}}_{h,n+1} \leq \mathbf{V} \leq \overline{\mathbf{U}}_{h,n+1}\}. \tag{5.8}$$

By the maximum–minimum theorem,

$$\begin{cases} A^{(l)} \overline{U}_{h,n+1}^{(l)} = B^{(l)} U_{h,n}^{*(l)} + \tau Q \left(F_{n+1}^{(l)}(\overline{U}_{h,n+1}^{(l)}, [\boldsymbol{\Xi}]_{l,N-1}) + F_n^{(l)}(\mathbf{U}_{h,n}^*) \right) + G_n^{(l)}, \\ A^{(l)} \underline{U}_{h,n+1}^{(l)} = B^{(l)} U_{h,n}^{*(l)} + \tau Q \left(F_{n+1}^{(l)}(\underline{U}_{h,n+1}^{(l)}, [\boldsymbol{\Theta}]_{l,N-1}) + F_n^{(l)}(\mathbf{U}_{h,n}^*) \right) + G_n^{(l)}, \\ \overline{U}_{h,0}^{(l)} = \underline{U}_{h,0}^{(l)} = \Phi^{(l)}, \quad l = 1, 2, \ldots, N, n = 0, 1, 2, \ldots, \end{cases} \tag{5.9}$$

where $\boldsymbol{\Xi}$ and $\boldsymbol{\Theta}$ are intermediate vectors in $\mathcal{S}_{n+1}$. Based on this relation we have the following monotone convergence of Picard iteration (5.1) to the unique solution $\mathbf{U}_{h,n}^*$.

Theorem 5.1. *Let the conditions in Theorem 4.2 be satisfied. Then the sequences $\{\overline{\mathbf{U}}_{h,n}^{(m)}\}$, $\{\underline{\mathbf{U}}_{h,n}^{(m)}\}$ given by (5.1) converge monotonically from above and below, respectively, to the unique solution $\mathbf{U}_{h,n}^*$ of (2.17) in $\langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n} \rangle$. Moreover,*

$$\widehat{\mathbf{U}}_{h,n} \leq \underline{\mathbf{U}}_{h,n}^{(m-1)} \leq \underline{\mathbf{U}}_{h,n}^{(m)} \leq \mathbf{U}_{h,n}^* \leq \overline{\mathbf{U}}_{h,n}^{(m)} \leq \overline{\mathbf{U}}_{h,n}^{(m-1)} \leq \widetilde{\mathbf{U}}_{h,n} \quad (m, n = 1, 2, \ldots). \tag{5.10}$$

Proof. It suffices to show $\overline{\mathbf{U}}_{h,n} = \underline{\mathbf{U}}_{h,n} = \mathbf{U}_{h,n}^*$ for every n. But this follows by applying the argument in the proof of Theorem 4.2 to the relation (5.9). □

Picard iteration (5.1) leads to a nine-diagonal linear system at each step of iterations (for each n). To maintain the monotone convergence of the iterations and simplify the computations essentially, we now propose two new iterations, called block Jacobi iteration and block Gauss–Seidel iteration, respectively. The two new iterations are based on the decomposition (3.4) of the matrices $A^{(l)}$ and Q, and are described as follows:

(a) *Block Jacobi iteration.*

Let $\widetilde{\mathbf{U}}_{h,n}$ and $\widehat{\mathbf{U}}_{h,n}$ be a pair of coupled upper and lower solutions of (2.17). Using $\overline{\mathbf{U}}^{(0)}_{J,h,n} = \widetilde{\mathbf{U}}_{h,n}$ and $\underline{\mathbf{U}}^{(0)}_{J,h,n} = \widehat{\mathbf{U}}_{h,n}$ we construct sequences $\{\overline{\mathbf{U}}^{(m)}_{J,h,n}\} = \{((\overline{U}^{(1)}_{J,h,n})^{(m)}, \ldots, (\overline{U}^{(N)}_{J,h,n})^{(m)})^{\mathrm{T}}\}$ and $\{\underline{\mathbf{U}}^{(m)}_{J,h,n}\} = \{((\underline{U}^{(1)}_{J,h,n})^{(m)}, \ldots, (\underline{U}^{(N)}_{J,h,n})^{(m)})^{\mathrm{T}}\}$ by

$$\begin{cases} (\mathcal{D}^{(l)} + \tau M^{(l)}_{n+1}\mathcal{D})(\overline{U}^{(l)}_{J,h,n+1})^{(m+1)} = B^{(l)}U^{*(l)}_{h,n} + (\mathcal{L}^{(l)} + \mathcal{U}^{(l)} - \tau M^{(l)}_{n+1}(\mathcal{L}+\mathcal{U}))(\overline{U}^{(l)}_{J,h,n+1})^{(m)} \\ \quad + \tau Q \max\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right) + \tau Q F^{(l)}_n(\mathbf{U}^*_{h,n}) + G^{(l)}_n, \\ (\mathcal{D}^{(l)} + \tau M^{(l)}_{n+1}\mathcal{D})(\underline{U}^{(l)}_{J,h,n+1})^{(m+1)} = B^{(l)}U^{*(l)}_{h,n} + (\mathcal{L}^{(l)} + \mathcal{U}^{(l)} - \tau M^{(l)}_{n+1}(\mathcal{L}+\mathcal{U}))(\underline{U}^{(l)}_{J,h,n+1})^{(m)} \\ \quad + \tau Q \min\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right) + \tau Q F^{(l)}_n(\mathbf{U}^*_{h,n}) + G^{(l)}_n, \\ (\overline{U}^{(l)}_{J,h,0})^{(m+1)} = (\underline{U}^{(l)}_{J,h,0})^{(m+1)} = \Phi^{(l)}, \quad l = 1,2,\ldots,N,\ n = 0,1,2,\ldots, \end{cases} \tag{5.11}$$

where $M^{(l)}_{n+1}$ is the Lipschitz constant in (4.5), and $\mathcal{S}^{(m)}_{n+1}$ is defined by (5.2) with respect to $\overline{\mathbf{U}}^{(m)}_{J,h,n+1}$ and $\underline{\mathbf{U}}^{(m)}_{J,h,n+1}$.

(b) *Block Gauss–Seidel iteration.*

The block Gauss–Seidel iteration is designed by replacing the matrices $\mathcal{D}^{(l)}$, $\mathcal{D}$, $\mathcal{L}^{(l)} + \mathcal{U}^{(l)}$ and $\mathcal{L} + \mathcal{U}$ in (5.11) by the matrices $\mathcal{D}^{(l)} - \mathcal{L}^{(l)}$, $\mathcal{D} + \mathcal{L}$, $\mathcal{U}^{(l)}$ and $\mathcal{U}$, respectively. The produced sequences are denoted by $\{\overline{\mathbf{U}}^{(m)}_{G,h,n}\}$ and $\{\underline{\mathbf{U}}^{(m)}_{G,h,n}\}$.

Since the matrices $\mathcal{D}^{(l)} + M^{(l)}_{n+1}\mathcal{D}$ and $\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + M^{(l)}_{n+1}(\mathcal{D} + \mathcal{L})$ are respectively block diagonal and block lower-tridiagonal, and each block is a tridiagonal matrix, we could use certain explicit and efficient algorithm, such as Thomas algorithm, at each step of the block Jacobi and block Gauss–Seidel iterations (for each n). This simplifies the computations essentially.

Like Picard iteration, we have the following convergence result of the above iterations.

Theorem 5.2. *Let the conditions in Theorem 4.2 be satisfied. Then the conclusions in Lemma 5.1 and Theorem 5.1 are valid for the sequences produced by the block Jacobi and block Gauss–Seidel iterations.*

Proof. By Theorem 3.3, the inverses $(\mathcal{D}^{(l)} + \tau M^{(l)}_n\mathcal{D})^{-1}$ and $(\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + \tau M^{(l)}_n(\mathcal{D}+\mathcal{L}))^{-1}$ exist and are positive. Moreover, the matrices $\mathcal{L}^{(l)} + \mathcal{U}^{(l)} - \tau M^{(l)}_n(\mathcal{L}+\mathcal{U})$ and $\mathcal{U}^{(l)} - \tau M^{(l)}_n\mathcal{U}$ are nonnegative. Accordingly, we follow the same line as in the proofs of Lemma 5.1 and Theorem 5.1 to reach the desired results. □

It is seen from Theorems 5.1 and 5.2 that when upper and lower solutions $\widetilde{\mathbf{U}}_{h,n}, \widehat{\mathbf{U}}_{h,n}$ are used as coupled initial iterations, each of Picard, block Jacobi and block Gauss–Seidel iterations yields two monotone sequences which converge monotonically to the unique solution $\mathbf{U}^*_{h,n}$ of (2.17) in $\langle \widehat{\mathbf{U}}_{h,n}, \widetilde{\mathbf{U}}_{h,n}\rangle$. We now compare these iterations.

Theorem 5.3. *Let the conditions in Theorem 4.1 hold, and let $\{\overline{\mathbf{U}}^{(m)}_{h,n}, \underline{\mathbf{U}}^{(m)}_{h,n}\}$, $\{\overline{\mathbf{U}}^{(m)}_{J,h,n}, \underline{\mathbf{U}}^{(m)}_{J,h,n}\}$ and $\{\overline{\mathbf{U}}^{(m)}_{G,h,n}, \underline{\mathbf{U}}^{(m)}_{G,h,n}\}$ be the sequences produced by Picard, block Jacobi and block Gauss–Seidel iterations, respectively. Then*

$$\underline{\mathbf{U}}^{(m)}_{J,h,n} \le \underline{\mathbf{U}}^{(m)}_{G,h,n} \le \underline{\mathbf{U}}^{(m)}_{h,n} \le \overline{\mathbf{U}}^{(m)}_{h,n} \le \overline{\mathbf{U}}^{(m)}_{G,h,n} \le \overline{\mathbf{U}}^{(m)}_{J,h,n}, \quad m, n = 1,2,\ldots. \tag{5.12}$$

Proof. Let $\overline{\mathbf{W}}^{(m)}_{h,n} = \overline{\mathbf{U}}^{(m)}_{G,h,n} - \overline{\mathbf{U}}^{(m)}_{h,n}$ and $\underline{\mathbf{W}}^{(m)}_{h,n} = \underline{\mathbf{U}}^{(m)}_{h,n} - \underline{\mathbf{U}}^{(m)}_{G,h,n}$, and let $(\overline{W}^{(l)}_{h,n})^{(m)} = (\overline{U}^{(l)}_{G,h,n})^{(m)} - (\overline{U}^{(l)}_{h,n})^{(m)}$ and $(\underline{W}^{(l)}_{h,n})^{(m)} = (\underline{U}^{(l)}_{h,n})^{(m)} - (\underline{U}^{(l)}_{G,h,n})^{(m)}$. Then we have from (5.1) and the corresponding formulas of block Gauss–Seidel iteration that

$$\begin{cases} (\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + \tau M^{(l)}_{n+1}(\mathcal{D}+\mathcal{L}))(\overline{W}^{(l)}_{h,n+1})^{(m+1)} = (\mathcal{U}^{(l)} - \tau M^{(l)}_{n+1}\mathcal{U})\left((\overline{U}^{(l)}_{G,h,n+1})^{(m)} - (\overline{U}^{(l)}_{h,n+1})^{(m+1)}\right) \\ \quad + \tau Q \max\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{G,n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right) - \tau Q \max\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right), \\ (\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + \tau M^{(l)}_{n+1}(\mathcal{D}+\mathcal{L}))(\underline{W}^{(l)}_{h,n+1})^{(m+1)} = (\mathcal{U}^{(l)} - \tau M^{(l)}_{n+1}\mathcal{U})\left((\underline{U}^{(l)}_{h,n+1})^{(m+1)} - (\underline{U}^{(l)}_{G,h,n+1})^{(m)}\right) \\ \quad + \tau Q \min\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right) - \tau Q \min\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{G,n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right), \end{cases} \tag{5.13}$$

where $\mathcal{S}^{(m)}_{G,n+1}$ stands for $\mathcal{S}^{(m)}_{n+1}$ in (5.2) but with respect to the block Gauss–Seidel iteration. Since $\mathcal{U}^{(l)} - \tau M^{(l)}_{n+1}\mathcal{U} \ge 0$, the monotone property of the sequences implies that

$$\begin{cases} (\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + \tau M^{(l)}_{n+1}(\mathcal{D}+\mathcal{L}))(\overline{W}^{(l)}_{h,n+1})^{(m+1)} \ge (\mathcal{U}^{(l)} - \tau M^{(l)}_{n+1}\mathcal{U})(\overline{W}^{(l)}_{h,n+1})^{(m)} \\ \quad + \tau Q \max\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{G,n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right) - \tau Q \max\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right), \\ (\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + \tau M^{(l)}_{n+1}(\mathcal{D}+\mathcal{L}))(\underline{W}^{(l)}_{h,n+1})^{(m+1)} \ge (\mathcal{U}^{(l)} - \tau M^{(l)}_{n+1}\mathcal{U})(\underline{W}^{(l)}_{h,n+1})^{(m)} \\ \quad + \tau Q \min\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right) - \tau Q \min\limits_{\mathbf{V}\in\mathcal{S}^{(m)}_{G,n+1}} \left(M^{(l)}_{n+1}V^{(l)} + F^{(l)}_{n+1}(\mathbf{V})\right). \end{cases} \tag{5.14}$$

We now use induction. Consider the case $m = 0$. Since the considered iterations possess the same initial data, the relation (5.14) for $m = 0$ is reduced to

$$(\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + \tau M^{(l)}_{n+1}(\mathcal{D} + \mathcal{L}))(\overline{W}^{(l)}_{h,n+1})^{(1)} \ge 0, \qquad (\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + \tau M^{(l)}_{n+1}(\mathcal{D} + \mathcal{L}))(\underline{W}^{(l)}_{h,n+1})^{(1)} \ge 0.$$

The above with the positivity of $(\mathcal{D}^{(l)} - \mathcal{L}^{(l)} + \tau M^{(l)}_{n+1}(\mathcal{D} + \mathcal{L}))^{-1}$ leads to that $(\overline{W}^{(l)}_{h,n})^{(1)} \ge 0$ and $(\underline{W}^{(l)}_{h,n})^{(1)} \ge 0$ for every l and n. Finally, we show inductively that $(\overline{W}^{(l)}_{h,n})^{(m)} \ge 0$ and $(\underline{W}^{(l)}_{h,n})^{(m)} \ge 0$ for all $m \ge 1$, i.e.,

$$\underline{\mathbf{U}}^{(m)}_{G,h,n} \le \underline{\mathbf{U}}^{(m)}_{h,n} \le \overline{\mathbf{U}}^{(m)}_{h,n} \le \overline{\mathbf{U}}^{(m)}_{G,h,n}, \quad m, n = 1, 2, \ldots.$$

We can prove the other inequalities in (5.12) in the same manner. □

Remark 5.1. Since we adopt the locally extreme values on the right-hand sides of the above proposed iterations, the monotone convergence of the corresponding sequences follows without any requirement on the monotonicity of $F^{(l)}_{n+1}$. This enlarges their applications essentially. If the function $F^{(l)}_{n+1}(U^{(l)}_{h,n+1}, [\mathbf{U}_{h,n+1}]_{l,N-1})$ is monotone in $[\mathbf{U}_{h,n+1}]_{l,N-1}$ for every l and n, then the computation of maximum and minimum values in the iterations is trivial. Otherwise, the maximum and minimum values can be determined by $(f^{(l)}_{u^{(k)}})_{i,j,n+1} = 0$.

Remark 5.2. Newton's method (or its variation) is a well-known iterative method for solving nonlinear systems. However, in general, it does not possess the monotone convergence (5.10). Obviously, the monotone convergence (5.10) gives concurrently improved upper and lower bounds of the solution in each iteration. This exhibits its superiority over the ordinary convergence.

Remark 5.3. According to (5.12), Picard iteration may converge faster than the block Gauss–Seidel iteration. The latter in turn may converge faster than the block Jacobi iteration. However, the implementation of the block Jacobi and block Gauss–Seidel iterations is more easy since they can be computed only by solving $(M_x - 1)$-order tridiagonal linear systems.

6. Convergence of the compact scheme

In this section, we deal with the convergence of the compact scheme (2.11) (or (2.17)). For this purpose, we assume that $t \in (0, T]$ for an arbitrary finite $T > 0$, and $\tau = T/M_t$.

Lemma 6.1 (*See [8]*). *Let $\{\zeta_i\}$ be a sequence of real numbers such that for certain $0 < \gamma < 1$ and $\delta > 0$,*

$$|\zeta_i| \le \gamma|\zeta_i| + (1+\gamma)|\zeta_{i-1}| + \delta, \quad i = 1, 2, \ldots. \tag{6.1}$$

Then

$$|\zeta_i| \le \mathrm{e}^{\frac{2i\gamma}{1-\gamma}}|\zeta_0| + \frac{\delta}{2\gamma}\left(\mathrm{e}^{\frac{2i\gamma}{1-\gamma}} - 1\right), \quad i = 0, 1, 2, \ldots. \tag{6.2}$$

Assume that the solution $\mathbf{u}(x, y, t)$ of (1.1) is sufficiently smooth. Let $\mathbf{u}_{i,j,n} = (u^{(1)}_{i,j,n}, \ldots, u^{(N)}_{i,j,n})$ be the value of $\mathbf{u}(x, y, t)$ at the mesh point (x_i, y_j, t_n), and let $\mathbf{u}^h_{i,j,n} = (u^{(1),h}_{i,j,n}, \ldots, u^{(N),h}_{i,j,n})$ stand for the solution of (2.11). We now consider the errors $e^{(l),h}_{i,j,n} = u^{(l)}_{i,j,n} - u^{(l),h}_{i,j,n}$. In fact, we have from (2.7) and (2.11) that

$$\begin{cases} \mathcal{L}^{(l)}_h e^{(l),h}_{i,j,n+1} = \mathcal{P}^{(l)}_h e^{(l),h}_{i,j,n} + \mathcal{H}_h\left(f^{(l)}_{i,j,n+1}(\mathbf{u}_{i,j,n+1}) + f^{(l)}_{i,j,n}(\mathbf{u}_{i,j,n}) - f^{(l)}_{i,j,n+1}(\mathbf{u}^h_{i,j,n+1}) - f^{(l)}_{i,j,n}(\mathbf{u}^h_{i,j,n})\right) + \varepsilon^{(l)}_{i,j,n}, \\ \quad (i,j) \in \Omega, \quad n = 0, 1, 2, \ldots, M_t - 1, \\ e^{(l),h}_{0,j,n+1} = e^{(l),h}_{M_x,j,n+1} = 0, \quad j = 0, 1, \ldots, M_y, n = 0, 1, 2, \ldots, M_t - 1, \\ e^{(l),h}_{i,0,n+1} = e^{(l),h}_{i,M_y,n+1} = 0, \quad i = 0, 1, \ldots, M_x, n = 0, 1, 2, \ldots, M_t - 1, \\ e^{(l),h}_{i,j,0} = 0, \quad (i,j) \in \Omega \cup \partial\Omega, \ l = 1, 2, \ldots, N, \end{cases} \tag{6.3}$$

where $\varepsilon^{(l)}_{i,j,n}$ is the truncation error satisfying

$$|\varepsilon^{(l)}_{i,j,n}| \le C_1(\tau^3 + \tau h^4), \quad (i,j) \in \Omega, n = 0, 1, \ldots, M_t, l = 1, 2, \ldots, N \tag{6.4}$$

with C_1 being a positive constant independent of τ and h. Let

$$E^{(l)}_{h,j,n} = (e^{(l),h}_{1,j,n}, e^{(l),h}_{2,j,n}, \ldots, e^{(l),h}_{M_x-1,j,n})^{\mathrm{T}}, \qquad E^{(l)}_{h,n} = (E^{(l)}_{h,1,n}, E^{(l)}_{h,2,n}, \ldots, E^{(l)}_{h,M_y-1,n})^{\mathrm{T}},$$
$$\varepsilon^{(l)}_{j,n} = (\varepsilon^{(l)}_{1,j,n}, \varepsilon^{(l)}_{2,j,n}, \ldots, \varepsilon^{(l)}_{M_x-1,j,n})^{\mathrm{T}}, \qquad \mathcal{E}^{(l)}_{n} = (\mathcal{E}^{(l)}_{1,n}, \mathcal{E}^{(l)}_{2,n}, \ldots, \mathcal{E}^{(l)}_{M_y-1,n})^{\mathrm{T}},$$
$$U^{(l)}_{j,n} = (u^{(l)}_{1,j,n}, u^{(l)}_{2,j,n}, \ldots, u^{(l)}_{M_x-1,j,n})^{\mathrm{T}}, \qquad U^{(l)}_{n} = (U^{(l)}_{1,n}, U^{(l)}_{2,n}, \ldots, U^{(l)}_{M_y-1,n})^{\mathrm{T}},$$
$$\mathbf{U}_n = (U^{(1)}_n, U^{(2)}_n, \ldots, U^{(N)}_n)^{\mathrm{T}}, \qquad \mathbf{E}_{h,n} = (E^{(1)}_{h,n}, E^{(2)}_{h,n}, \ldots, E^{(N)}_{h,n})^{\mathrm{T}}.$$

In terms of the matrices in (2.16) and the vectors in (2.15), we can write the relation (6.3) as

$$\begin{cases} A^{(l)}E^{(l)}_{h,n+1} = B^{(l)}E^{(l)}_{h,n} + \tau Q\left(F^{(l)}_{n+1}(\mathbf{U}_{n+1}) + F^{(l)}_{n}(\mathbf{U}_{n}) - F^{(l)}_{n+1}(\mathbf{U}_{h,n+1}) - F^{(l)}_{n}(\mathbf{U}_{h,n})\right) + \mathcal{E}^{(l)}_n, \\ E^{(l)}_{h,0} = 0, \quad l = 1, 2, \ldots, N, n = 0, 1, 2, \ldots, M_t - 1. \end{cases} \tag{6.5}$$

Theorem 6.1. *Let $\mathcal{S}^{(l)}_{i,j,n}$ be the set such that $u^{(l)}_{i,j,n}, u^{(l),h}_{i,j,n} \in \mathcal{S}^{(l)}_{i,j,n}$, and let M^* be the constant such that $\tau NM^* < \frac{1}{2}$, and for $(i,j) \in \Omega$, $n = 0, 1, \ldots, M_t$ and $k, l = 1, 2, \ldots, N$,*

$$\left|(f^{(l)}_{v^{(k)}})_{i,j,n}(\mathbf{v}_{i,j,n})\right| \le M^*, \quad \mathbf{v}_{i,j,n} = (v^{(1)}_{i,j,n}, \ldots, v^{(N)}_{i,j,n}),\ v^{(l)}_{i,j,n} \in \mathcal{S}^{(l)}_{i,j,n}. \tag{6.6}$$

Also let condition (3.1) be satisfied. Then

$$\max_{(i,j)\in\Omega}\left|u^{(l)}_{i,j,n} - u^{(l),h}_{i,j,n}\right| \le C^*(\tau^2 + h^4), \quad l = 1, 2, \ldots, N;\ n = 0, 1, 2, \ldots, M_t, \tag{6.7}$$

where C^* is a positive constant independent of τ and h.

Proof. Using the positivity of $(A^{(l)})^{-1}$ and the nonnegativity of $B^{(l)}$ and Q, we have from (6.5) and (6.6) that

$$|E^{(l)}_{h,n+1}| \le (A^{(l)})^{-1}B^{(l)}|E^{(l)}_{h,n}| + \tau M^*(A^{(l)})^{-1}Q\left(|\mathbf{E}_{h,n+1}|_0 + |\mathbf{E}_{h,n}|_0\right) + (A^{(l)})^{-1}\mathcal{E}^{(l)}_n.$$

Since $\|(A^{(l)})^{-1}\|_\infty \le 1$, $\|B^{(l)}\|_\infty \le 1$ and $\|Q\|_\infty \le 1$, the above inequality implies that

$$\|E^{(l)}_{h,n+1}\|_\infty \le \|E^{(l)}_{h,n}\|_\infty + \tau M^* \sum_{l=1}^{N}\left(\|E^{(l)}_{h,n+1}\|_\infty + \|E^{(l)}_{h,n}\|_\infty\right) + C_1(\tau^3 + \tau h^4).$$

This leads to

$$\sum_{l=1}^{N}\|E^{(l)}_{h,n+1}\|_\infty \le \left(1 + \tau NM^*\right)\sum_{l=1}^{N}\|E^{(l)}_{h,n}\|_\infty + \tau NM^*\sum_{l=1}^{N}\|E^{(l)}_{h,n+1}\|_\infty + NC_1(\tau^3 + \tau h^4).$$

By Lemma 6.1, we arrive at

$$\sum_{l=1}^{N}\|E^{(l)}_{h,n}\|_\infty \le \left(\mathrm{e}^{\frac{2TNM^*}{1-\tau NM^*}} - 1\right)\frac{C_1}{2M^*}(\tau^2 + h^4) \le \left(\mathrm{e}^{4TNM^*} - 1\right)\frac{C_1}{2M^*}(\tau^2 + h^4).$$

This proves (6.7). □

The estimate (6.7) implies that the solution of scheme (2.11) (or (2.17)) converges to the solution of (1.1) with the accuracy of $O(\tau^2 + h^4)$ as $(\tau, h) \to (0, 0)$.

7. Richardson extrapolation algorithm

Theorem 6.1 shows that scheme (2.11) (or (2.17)) is fourth-order accurate in space, but only second-order accurate in time. In order to make the numerical solution fourth-order accurate in both space and time, Richardson extrapolation can be applied (e.g., see [3]). We now give a mathematical justification for such application.

Theorem 7.1. *Let the conditions in Theorem 6.1 be satisfied. Then for each $l = 1, 2, \ldots, N$, there exists a function $v^{(l)}(x, y, t)$, which does not depend on the mesh sizes, such that*

$$u^{(l),h}_{i,j,n} = u^{(l)}_{i,j,n} + \tau^2 v^{(l)}_{i,j,n} + O(\tau^4 + h^4), \quad (i,j) \in \Omega, n = 0, 1, 2 \ldots, M_t. \tag{7.1}$$

Proof. Crank–Nicolson time discretization (2.2) can be written as

$$\frac{1}{\tau}(u^{(l)}_{i,j,n+1} - u^{(l)}_{i,j,n}) - \frac{D^{(l)}_1}{2}((u^{(l)}_{xx})_{i,j,n+1} + (u^{(l)}_{xx})_{i,j,n}) - \frac{D^{(l)}_2}{2}((u^{(l)}_{yy})_{i,j,n+1} + (u^{(l)}_{yy})_{i,j,n})$$
$$= \frac{1}{2}(f^{(l)}_{i,j,n+1}(\mathbf{u}_{i,j,n+1}) + f^{(l)}_{i,j,n}(\mathbf{u}_{i,j,n})) - \frac{\tau^2}{24}((u^{(l)}_{ttt})_{i,j,n+1} + (u^{(l)}_{ttt})_{i,j,n}) + O(\tau^4).$$

Following the derivation of (2.7) we get

$$\mathcal{L}^{(l)}_h u^{(l)}_{i,j,n+1} = \mathcal{P}^{(l)}_h u^{(l)}_{i,j,n} + \mathcal{H}_h\left(f^{(l)}_{i,j,n+1}(\mathbf{u}_{i,j,n+1}) + f^{(l)}_{i,j,n}(\mathbf{u}_{i,j,n})\right) - \frac{\tau^2}{12}\mathcal{H}_h\left((u^{(l)}_{ttt})_{i,j,n+1} + (u^{(l)}_{ttt})_{i,j,n}\right) + O(\tau^5 + \tau h^4). \quad (7.2)$$

Let $v^{(l)}$ be the solution of following linear problem:

$$\begin{cases} v^{(l)}_t - D^{(l)}_1 v^{(l)}_{xx} - D^{(l)}_2 v^{(l)}_{yy} = \sum_{k=1}^{N} f^{(l)}_{u^{(k)}}(x,y,t,\mathbf{u})v^{(k)} + \frac{1}{12}u^{(l)}_{ttt}, & (x,y)\in\Omega,\ 0<t\le T,\\ v^{(l)}(0,y,t) = v^{(l)}(1,y,t) = 0, & y\in[0,1],\ 0<t\le T,\\ v^{(l)}(x,0,t) = v^{(l)}(x,1,t) = 0, & x\in[0,1],\ 0<t\le T,\\ v^{(l)}(x,y,0) = 0, & (x,y)\in\overline{\Omega},\ l=1,2,\ldots,N. \end{cases} \quad (7.3)$$

By the same argument for (2.7) we see that $v^{(l)}$ satisfies

$$\mathcal{L}^{(l)}_h v^{(l)}_{i,j,n+1} = \mathcal{P}^{(l)}_h v^{(l)}_{i,j,n} + \mathcal{H}_h \sum_{k=1}^{N}\left((f^{(l)}_{u^{(k)}})_{i,j,n+1}(\mathbf{u}_{i,j,n+1})(v^{(k)})_{i,j,n+1} + (f^{(l)}_{u^{(k)}})_{i,j,n}(\mathbf{u}_{i,j,n})(v^{(k)})_{i,j,n}\right)$$
$$+ \frac{1}{12}\mathcal{H}_h\left((u^{(l)}_{ttt})_{i,j,n+1} + (u^{(l)}_{ttt})_{i,j,n}\right) + O(\tau^3 + \tau h^4). \quad (7.4)$$

Multiplying τ^2 in (7.4) and then adding the resulting relation to (7.2) lead to that the function $w^{(l)} = u^{(l)} + \tau^2 v^{(l)}$ satisfies

$$\mathcal{L}^{(l)}_h w^{(l)}_{i,j,n+1} = \mathcal{P}^{(l)}_h w^{(l)}_{i,j,n} + \mathcal{H}_h\left(f^{(l)}_{i,j,n+1}(\mathbf{u}_{i,j,n+1}) + \tau^2\sum_{k=1}^{N}(f^{(l)}_{u^{(k)}})_{i,j,n+1}(\mathbf{u}_{i,j,n+1})(v^{(k)})_{i,j,n+1}\right)$$
$$+ \mathcal{H}_h\left(f^{(l)}_{i,j,n}(\mathbf{u}_{i,j,n}) + \tau^2\sum_{k=1}^{N}(f^{(l)}_{u^{(k)}})_{i,j,n}(\mathbf{u}_{i,j,n})(v^{(k)})_{i,j,n}\right) + O(\tau^5 + \tau h^4). \quad (7.5)$$

Let $\mathbf{w}_{i,j,q} = (w^{(1)}_{i,j,q}, \ldots, w^{(N)}_{i,j,q})$, and by Taylor expansion,

$$f^{(l)}_{i,j,q}(\mathbf{w}_{i,j,q}) = f^{(l)}_{i,j,q}(\mathbf{u}_{i,j,q}) + \tau^2\sum_{k=1}^{N}(f^{(l)}_{u^{(k)}})_{i,j,q}(\mathbf{u}_{i,j,q})(v^{(k)})_{i,j,q} + O(\tau^4), \quad q = n, n+1.$$

Substituting this relation into (7.5) we obtain

$$\mathcal{L}^{(l)}_h w^{(l)}_{i,j,n+1} = \mathcal{P}^{(l)}_h w^{(l)}_{i,j,n} + \mathcal{H}_h\left(f^{(l)}_{i,j,n+1}(\mathbf{w}_{i,j,n+1}) + f^{(l)}_{i,j,n}(\mathbf{w}_{i,j,n})\right) + O(\tau^5 + \tau h^4). \quad (7.6)$$

Finally, relation (7.1) follows from the argument for (6.7) by replacing (2.7) by (7.6). □

An important application of the error expansion (7.1) is to construct Richardson extrapolation algorithm for (2.11). To describe this algorithm, we denote $u^{(l),h}_{i,j,n}(\tau)(l = 1, 2, \ldots, N)$ the solution of (2.11) with time mesh size τ, and let $u^{(l)}_{i,j,n}(\tau)$ and $v^{(l)}_{i,j,n}(\tau)$ be the values of the solutions of (1.1) and (7.3) at (x_i, y_j, t_n) using the time mesh size τ.

Richardson extrapolation algorithm:

Step 1. Compute $u^{(l),h}_{i,j,n}(\tau)$ and $u^{(l),h}_{i,j,n}(\tau/2)$ $(l = 1, 2, \ldots, N)$;

Step 2. Compute the extrapolation solution $w^{(l),h}_{i,j,n}(\tau)$ by

$$w^{(l),h}_{i,j,n}(\tau) = \left(4u^{(l),h}_{i,j,2n}(\tau/2) - u^{(l),h}_{i,j,n}(\tau)\right)/3, \quad l = 1, 2, \ldots, N. \quad (7.7)$$

Theorem 7.2. *Let the conditions in Theorem 6.1 be satisfied. Then*

$$\max_{(i,j)\in\Omega}\left|u^{(l)}_{i,j,n}(\tau) - w^{(l),h}_{i,j,n}(\tau)\right| \le C^{**}(\tau^4 + h^4), \quad l = 1, 2, \ldots, N;\ n = 0, 1, 2, \ldots, M_t, \quad (7.8)$$

where C^{**} is a positive constant independent of τ and h.

Proof. By Theorem 7.1, we have the error expansions

$$u^{(l),h}_{i,j,n}(\tau) = u^{(l)}_{i,j,n}(\tau) + \tau^2 v^{(l)}_{i,j,n}(\tau) + O(\tau^4 + h^4),$$
$$u^{(l),h}_{i,j,2n}(\tau/2) = u^{(l)}_{i,j,2n}(\tau/2) + \tau^2 v^{(l)}_{i,j,2n}(\tau/2)/4 + O(\tau^4 + h^4).$$

Since $u^{(l)}_{i,j,n}(\tau) = u^{(l)}_{i,j,2n}(\tau/2)$ and $v^{(l)}_{i,j,n}(\tau) = v^{(l)}_{i,j,2n}(\tau/2)$, we deduce

$$w^{(l),h}_{i,j,n}(\tau) = u^{(l)}_{i,j,n}(\tau) + O(\tau^4 + h^4),$$

and thus the relation (7.8). □

Remark 7.1. The Richardson extrapolation algorithm requires more arithmetic operations than the scheme (2.11) itself. But its fourth-order accuracy in time allows the use of much larger time mesh size in order to obtain satisfactory numerical results (see the numerical results in the next section).

8. An application and numerical results

In this section, we give an application of the results in the previous sections to an enzyme–substrate reaction–diffusion problem. In the meantime, we present some numerical results to demonstrate the monotone convergence of iterations and the higher-order accuracy of the numerical solution, as predicted in the analysis. To do this, it is necessary to find a pair of coupled upper and lower solutions of (2.17) (or (2.11)). The construction of this pair depends mainly on the nonlinear function $F^{(l)}_n(\mathbf{U})$. Our application also illustrates some technique for constructing such pairs.

In the enzyme–substrate reaction–diffusion problem, the equations for two substrates u and v are given by (1.1) with $N = 2$, $(u^{(1)}, u^{(2)}) \equiv (u, v)$ and

$$\begin{aligned} f^{(1)}(x, y, t, u, v) &= a_1(\rho_1 - u) - \sigma_1 uv(1 + u + b_1 u^2)^{-1} + q_1(x, y, t), \\ f^{(2)}(x, y, t, u, v) &= a_2(\rho_2 - v) - \sigma_2 uv(1 + u + b_2 u^2)^{-1} + q_2(x, y, t). \end{aligned} \tag{8.1}$$

where a_i, ρ_i, σ_i and b_i $(i = 1, 2)$ are positive constants, and q_i $(i = 1, 2)$ are nonnegative continuous functions (see [26,1]). In this problem, the boundary and initial functions $g^{(l)}_i$, $h^{(l)}_i$, $\phi^{(l)}$ $(i = 1, 2;\ l = 1, 2)$ are nonnegative. The introduction of the functions q_i $(i = 1, 2)$ in (8.1) is to construct a continuous solution which is used to compare with our numerical solution.

For this problem the finite difference approximation (2.17) is reduced to

$$\begin{cases} A^{(1)}U_{h,n+1} = B^{(1)}U_{h,n} + \tau Q\left(F^{(1)}_{n+1}(U_{h,n+1}, V_{h,n+1}) + F^{(1)}_n(U_{h,n}, V_{h,n})\right) + G^{(1)}_n, \\ A^{(2)}V_{h,n+1} = B^{(2)}V_{h,n} + \tau Q\left(F^{(2)}_{n+1}(U_{h,n+1}, V_{h,n+1}) + F^{(2)}_n(U_{h,n}, V_{h,n})\right) + G^{(2)}_n, \\ U_{h,0} = \Phi^{(1)}, \qquad V_{h,0} = \Phi^{(2)}, \quad n = 0, 1, 2, \ldots, \end{cases} \tag{8.2}$$

where for each $l = 1, 2$ and $j = 1, 2, \ldots, M_y - 1$,

$$\begin{aligned} F^{(l)}_n(U_{h,n}, V_{h,n}) &= (F^{(l)}_{1,n}(U_{h,1,n}, V_{h,1,n}), \ldots, F^{(l)}_{M_y-1,n}(U_{h,M_y-1,n}, V_{h,M_y-1,n}))^{\mathrm{T}}, \\ F^{(l)}_{j,n}(U_{h,j,n}, V_{h,j,n}) &= (f^{(l)}(x_1, y_j, t_n, u^h_{1,j,n}, v^h_{1,j,n}), \ldots, f^{(l)}(x_{M_x-1}, y_j, t_n, u^h_{M_x-1,j,n}, v^h_{M_x-1,j,n}))^{\mathrm{T}}. \end{aligned} \tag{8.3}$$

The requirements of coupled upper and lower solutions $(\widetilde{U}_{h,n}, \widetilde{V}_{h,n})^{\mathrm{T}}$, $(\widehat{U}_{h,n}, \widehat{V}_{h,n})^{\mathrm{T}}$ for problem (8.2) become

$$\begin{cases} A^{(1)}\widetilde{U}_{h,n+1} \geq B^{(1)}\widetilde{U}_{h,n} + \tau Q\left(F^{(1)}_{n+1}(\widetilde{U}_{h,n+1}, V) + F^{(1)}_n(\widetilde{U}_{h,n}, V')\right) + G^{(1)}_n, \\ A^{(2)}\widetilde{V}_{h,n+1} \geq B^{(2)}\widetilde{V}_{h,n} + \tau Q\left(F^{(2)}_{n+1}(U, \widetilde{V}_{h,n+1}) + F^{(2)}_n(U', \widetilde{V}_{h,n})\right) + G^{(2)}_n, \\ A^{(1)}\widehat{U}_{h,n+1} \leq B^{(1)}\widehat{U}_{h,n} + \tau Q\left(F^{(1)}_{n+1}(\widehat{U}_{h,n+1}, V) + F^{(1)}_n(\widehat{U}_{h,n}, V')\right) + G^{(1)}_n, \\ A^{(2)}\widehat{V}_{h,n+1} \leq B^{(2)}\widehat{V}_{h,n} + \tau Q\left(F^{(2)}_{n+1}(U, \widehat{V}_{h,n+1}) + F^{(2)}_n(U', \widehat{V}_{h,n})\right) + G^{(2)}_n, \\ \qquad \text{for all } U \in \langle \widehat{U}_{h,n+1}, \widetilde{U}_{h,n+1}\rangle, U' \in \langle \widehat{U}_{h,n}, \widetilde{U}_{h,n}\rangle, V \in \langle \widehat{V}_{h,n+1}, \widetilde{V}_{h,n+1}\rangle, V' \in \langle \widehat{V}_{h,n}, \widetilde{V}_{h,n}\rangle, \\ \widetilde{U}_{h,0} \geq \Phi^{(1)} \geq \widehat{U}_{h,0}, \qquad \widetilde{V}_{h,0} \geq \Phi^{(2)} \geq \widehat{V}_{h,0}, \quad n = 0, 1, 2, \ldots. \end{cases} \tag{8.4}$$

Let $W^{(1)}_{h,n}$, $W^{(2)}_{h,n}$ be the respective positive solutions of the linear systems

$$\begin{cases} A^{(l)}W^{(l)}_{h,n+1} = B^{(l)}W^{(l)}_{h,n} + 2\tau(a_l\rho_l + \overline{q}_l)QE + G^{(l)}_n, \quad n = 0, 1, 2, \ldots, \\ W^{(l)}_{h,0} = \Phi^{(l)}, \quad l = 1, 2, \end{cases} \tag{8.5}$$

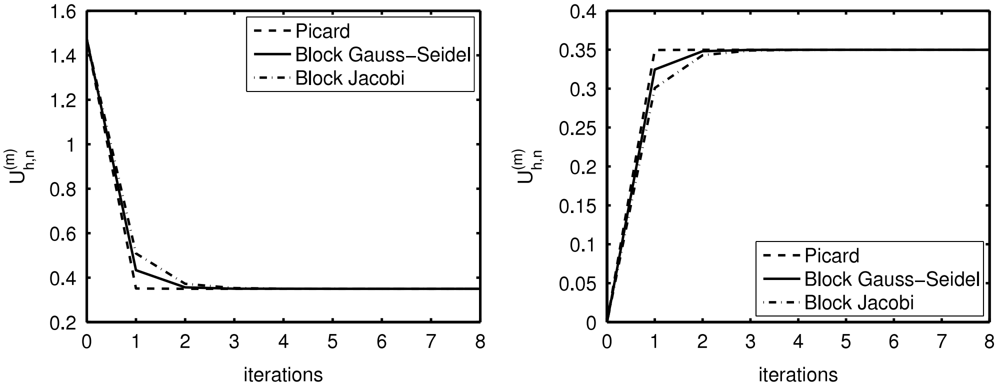

Fig. 8.1. The monotone property of $\{\overline{U}^{(m)}_{h,n}, \underline{U}^{(m)}_{h,n}\}$ at (0.5, 0.6, 1) by different iterations (left: $\{\overline{U}^{(m)}_{h,n}\}$; right: $\{\underline{U}^{(m)}_{h,n}\}$).

where the constant $\overline{q}_l$ is a nonnegative upper bound of the function q_l $(l = 1, 2)$, and $E = (1, 1, \ldots, 1)^T \in \mathbf{R}^{\mathcal{M}}$ is a vector whose components are all one. It is easy to verify that the pair $(\widetilde{U}_{h,n}, \widetilde{V}_{h,n})^T = (W^{(1)}_{h,n}, W^{(2)}_{h,n})^T$, $(\widehat{U}_{h,n}, \widehat{V}_{h,n})^T = (0, 0)^T$ satisfy the relations in (8.4), and therefore they are coupled upper and lower solutions of (8.2).

Let $M^*_n = \max_{l=1,2} \|W^{(l)}_{h,n}\|_\infty$. Since

$$\begin{aligned} &\partial f^{(1)}/\partial u = -a_1 - \sigma_1 v(1 - b_1u^2)(1 + u + b_1u^2)^{-2}, \qquad \partial f^{(1)}/\partial v = -\sigma_1 u(1 + u + b_1u^2)^{-1}, \\ &\partial f^{(2)}/\partial u = -\sigma_2 v(1 - b_2u^2)(1 + u + b_2u^2)^{-2}, \qquad \partial f^{(2)}/\partial v = -a_2 - \sigma_2 u(1 + u + b_2u^2)^{-1}, \end{aligned} \tag{8.6}$$

the Lipschitz constants $M^{(l)}_n$ in (4.5) may be taken as

$$M^{(l)}_n = \sigma_l M^*_n + a_l, \quad l = 1, 2. \tag{8.7}$$

Let $\mathbf{W}_{h,n} = (W^{(1)}_{h,n}, W^{(2)}_{h,n})^T$ and $\mathbf{0} = (0, 0)^T$, and let the mesh sizes satisfy the conditions (3.1), (3.2) and (4.12). Then by Theorem 4.2, problem (8.2) has a unique solution $(U^*_{h,n}, V^*_{h,n})^T$ in $\langle \mathbf{0}, \mathbf{W}_{h,n} \rangle$, and by Theorems 5.1 and 5.2, the sequences $\{(\overline{U}^{(m)}_{h,n}, \overline{V}^{(m)}_{h,n})^T\}$ and $\{(\underline{U}^{(m)}_{h,n}, \underline{V}^{(m)}_{h,n})^T\}$ from Picard iteration, block Jacobi iteration and block Gauss–Seidel iteration for (8.2) with $(\overline{U}^{(0)}_{h,n}, \overline{V}^{(0)}_{h,n})^T = (W^{(1)}_{h,n}, W^{(2)}_{h,n})^T$ and $(\underline{U}^{(0)}_{h,n}, \underline{V}^{(0)}_{h,n})^T = (0, 0)^T$ converge monotonically to $(U^*_{h,n}, V^*_{h,n})^T$.

To give some numerical results, we take the boundary functions $g^{(l)}_i(y, t) = h^{(l)}_i(x, t) \equiv 0$, and choose the physical parameters $D^{(l)}_i = 1 (i = 1, 2; l = 1, 2)$, $a_1 = \sigma_1 = b_1 = 1$, $\rho_1 = 10$, $a_2 = 5$ and $\rho_2 = \sigma_2 = b_2 = 2$. The initial functions $\phi^{(l)}$ are taken as $\phi^{(l)} = \sin \pi x \sin \pi y$ $(l = 1, 2)$. It is easy to check that when

$$\begin{cases} q_1(x, y, t) = (2\pi^2 - 1)z_1 - a_1(\rho_1 - z_1) + \sigma_1 z_1 z_2 (1 + z_1 + b_1 z_1^2)^{-1}, \\ q_2(x, y, t) = (2\pi^2 - (1 + t)^{-1})z_2 - a_2(\rho_2 - z_2) + \sigma_2 z_1 z_2 (1 + z_1 + b_2 z_1^2)^{-1}, \\ z_1 = e^{-t} \sin \pi x \sin \pi y, \qquad z_2 = (1 + t)^{-1} \sin \pi x \sin \pi y, \end{cases} \tag{8.8}$$

the solution of the model problem is given by $(u, v) = (z_1, z_2)$. In our computations, we take the equal mesh size in space, i.e., $h_x = h_y = h$. All computations are carried out by using a MATLAB subroutine on a Pentium-4 computer with 2G memory.

8.1. The monotone convergence of the iterations

Let $h = 0.05$ and $\tau = h^2/3$. Using $(\overline{U}^{(0)}_{h,n}, \overline{V}^{(0)}_{h,n})^T = (W^{(1)}_{h,n}, W^{(2)}_{h,n})^T$ and $(\underline{U}^{(0)}_{h,n}, \underline{V}^{(0)}_{h,n})^T = (0, 0)^T$, we compute the corresponding sequences $\{(\overline{U}^{(m)}_{h,n}, \overline{V}^{(m)}_{h,n})^T\}$ and $\{(\underline{U}^{(m)}_{h,n}, \underline{V}^{(m)}_{h,n})^T\}$ from Picard iteration, block Jacobi iteration and block Gauss–Seidel iteration. The termination criterion of iterations is given by

$$\|\overline{U}^{(m)}_{h,n} - \underline{U}^{(m)}_{h,n}\|_\infty + \|\overline{V}^{(m)}_{h,n} - \underline{V}^{(m)}_{h,n}\|_\infty < \varepsilon \tag{8.9}$$

for various ε.

In Fig. 8.1, we plot the values of sequences $\{\overline{U}^{(m)}_{h,n}\}$ and $\{\underline{U}^{(m)}_{h,n}\}$ at the point $(x_i, y_j, t_n) = (0.5, 0.6, 1)$, where the tolerance $\varepsilon = 10^{-15}$. As expected from our analysis, the sequence $\{\overline{U}^{(m)}_{h,n}\}$ is monotone nonincreasing, while the sequence $\{\underline{U}^{(m)}_{h,n}\}$ is monotone nondecreasing. Besides, the comparison result (5.12) is also confirmed.

To compare Picard iteration with block Jacobi and block Gauss–Seidel iterations, the required number of iterations (No. of iter.) and CPU time (in seconds) at $t_n = 1$ for different iterations with the tolerance $\varepsilon = 10^{-12}$ are given in Table 8.1. We see that with the same mesh size h, Picard iteration converges faster than block Gauss–Seidel and block Jacobi iterations, but Picard iteration costs more computational time, especially for small mesh size h. The comparison justifies our efforts to develop block iterations for this application.

Table 8.1
The number of iterations and CPU time at $t_n = 1$ for different iterations.

h	Picard		Block Gauss–Seidel		Block Jacobi	
	No. of iter.	CPU time (s)	No. of iter.	CPU time (s)	No. of iter.	CPU time (s)
1/50	4	1208.2121	12	1197.1829	15	1489.2635
1/60	4	2951.9913	12	2429.4816	15	2970.6958
1/70	4	5774.7514	12	4370.1625	15	5359.6328
1/80	4	9971.7243	12	7368.3041	15	8931.3693

Table 8.2
The accuracy of the numerical solution $(U^*_{h,n}, V^*_{h,n})^{\mathrm{T}}$ at $t_n = 1$ by scheme (8.2).

h	τ	$\mathrm{error}_u(h, n)$	$\mathrm{order}_u(h, n)$	$\mathrm{error}_v(h, n)$	$\mathrm{order}_v(h, n)$
1/4	1/16	5.79622736e−04	4.02667	6.38843794e−04	4.02618
1/8	1/64	3.55627762e−05	4.00669	3.92097296e−05	4.00664
1/16	1/256	2.21239780e−06	4.00167	2.43934882e−06	4.00167
1/32	1/1024	1.38114653e−07	4.00042	1.52283213e−07	4.00042
1/64	1/4096	8.62963290e−09	4.00044	9.51491674e−09	4.00010
1/128	1/16384	5.39188583e−10		5.94642002e−10	

Table 8.3
The accuracy of the numerical solution $(U^*_{h,n}, V^*_{h,n})^{\mathrm{T}}$ at $t_n = 1$ by SFD.

h	τ	$\mathrm{error}_u(h, n)$	$\mathrm{order}_u(h, n)$	$\mathrm{error}_v(h, n)$	$\mathrm{order}_v(h, n)$
1/4	1/16	1.97334981e−02	2.03526	2.11564107e−02	2.02307
1/8	1/64	4.81425340e−03	2.00877	5.20518174e−03	2.00580
1/16	1/256	1.19627162e−03	2.00219	1.29607658e−03	2.00145
1/32	1/1024	2.98614504e−04	2.00055	3.23693309e−04	2.00036
1/64	1/4096	7.46253248e−05	2.00014	8.09029679e−05	2.00009
1/128	1/16384	1.86545629e−05		2.02244696e−05	

8.2. The accuracy of the scheme

To demonstrate the accuracy of scheme (8.2), we calculate the order of maximum error of numerical solution $(U^*_{h,n}, V^*_{h,n})^{\mathrm{T}}$, which is defined by

$$\begin{aligned} &\mathrm{order}_\alpha(h, n) = \log_2\left(\frac{\mathrm{error}_\alpha(h, n)}{\mathrm{error}_\alpha(h/2, n)}\right), \quad \alpha = u, v, \\ &\mathrm{error}_u(h, n) = \|U^*_{h,n} - U_n\|_\infty, \qquad \mathrm{error}_v(h, n) = \|V^*_{h,n} - V_n\|_\infty, \end{aligned} \tag{8.10}$$

where $(U_n, V_n)^{\mathrm{T}}$ denotes the true solution vector. In Table 8.2, we list the maximum errors $\mathrm{error}_u(h, n)$ and $\mathrm{error}_v(h, n)$ as well as the order of them at $t_n = 1$ for different mesh sizes, where the numerical solution is calculated by Picard iteration with the tolerance $\varepsilon = 10^{-15}$. The data in this table demonstrate that the numerical solution $(U^*_{h,n}, V^*_{h,n})^{\mathrm{T}}$ has the fourth-order accuracy. This coincides well with the analysis.

For comparison, we also solve the model problem by the standard finite difference method (SFD) as in [4,6,7]. This method leads to a system of nonlinear algebraic equations in the form (8.2) with the matrices

$$A = \mathrm{tridiag}(-I, A_1, -I), \qquad A_1 = \mathrm{tridiag}(-1, 4, -1), \qquad B = Q = I.$$

Thus, a similar Picard iteration can be used in the actual computations. The corresponding maximum errors $\mathrm{error}_\alpha(h, n)$ and the orders $\mathrm{order}_\alpha(h, n)$ $(\alpha = u, v)$ at $t_n = 1$ are given in Table 8.3, where the tolerance $\varepsilon = 10^{-15}$. It is seen that the standard method possesses only the second-order accuracy.

To further improve the accuracy of scheme (8.2) we use Richardson extrapolation algorithm for the numerical solution $(U^*_{h,n}, V^*_{h,n})^{\mathrm{T}}$. The corresponding maximum errors $\mathrm{error}_\alpha(h, n)$ and the orders $\mathrm{order}_\alpha(h, n)$ $(\alpha = u, v)$ at $t_n = 1$ using $\tau = h$ are presented in Table 8.4.

Comparing Table 8.4 with Table 8.2, we find that the fourth-order accuracy of extrapolation algorithm is still attained even if we use the larger τ than that used for scheme (8.2).

9. Concluding remarks

In this paper, we gave some numerical analyses for a system of two-dimensional nonlinear reaction–diffusion equations by a compact finite difference method. This method has the accuracy of fourth-order in space and time, and so the numerical solution meets the true solution accurately. We obtained the existence and uniqueness of the numerical solution, and provided three monotone iterative algorithms for solving the resulting nonlinear discrete systems. All procedures do not

Table 8.4
The accuracy of the extrapolation algorithm at $t_n = 1$.

h	τ	$\text{error}_u(h, n)$	$\text{order}_u(h, n)$	$\text{error}_v(h, n)$	$\text{order}_v(h, n)$
1/4	1/4	6.03162477e−04	4.06949	6.44254866e−04	4.02817
1/8	1/8	3.59249119e−05	4.00658	3.94874333e−05	4.00658
1/16	1/16	2.23508640e−06	4.00166	2.45673416e−06	4.00167
1/32	1/32	1.39532550e−07	4.00041	1.53368726e−07	4.00041
1/64	1/64	8.71829076e−09	4.00037	9.58279400e−09	4.00028
1/128	1/128	5.44753354e−10		5.98808669e−10	

require any monotonicity of the involved nonlinear function and so enlarge their applications essentially. The numerical results coincide with the analyses very well and demonstrate the high efficiency of the proposed method.

In this work, we developed a technique for analyzing higher-order compact finite difference methods. We also extended the method of upper and lower solutions to higher-order compact scheme for two-dimensional partial differential equations. The proposed methodology can be generalized to three-dimensional problems straightforwardly.

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