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A higher-order compact ADI method with monotone iterative procedure for systems of reaction–diffusion equations☆

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ABSTRACT

This paper is concerned with an existing compact finite difference ADI method, published in the paper by Liao et al. (2002) [3], for solving systems of two-dimensional reaction–diffusion equations with nonlinear reaction terms. This method has an accuracy of fourth-order in space and second-order in time. The existence and uniqueness of its solution are investigated by the method of upper and lower solutions, without any monotone requirement on the nonlinear reaction terms. The convergence of the finite difference solution to the continuous solution is proved. An efficient monotone iterative algorithm is presented for solving the resulting discrete system, and some techniques for the construction of upper and lower solutions are discussed. An application using a model problem gives numerical results that demonstrate the high efficiency and advantages of the method.

1. Introduction

Many problems in various fields of applied sciences are described by systems of reaction–diffusion equations. A great deal of work has been devoted to the qualitative analysis of these systems (see [1] and the references therein) and the numerical methods for the computation of their solutions (cf. [2–9]). In this paper, we present a numerical treatment of a system of two-dimensional reaction–diffusion equations with nonlinear reaction terms by a compact finite difference ADI method. This includes the qualitative analysis of the resulting discrete system and a basic monotone iterative algorithm for the computation of numerical solutions. The reaction–diffusion system under consideration is given by

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

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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Finite difference methods have long been used to approximate the solution of ordinary or partial differential equations. 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 [4–6,10–13]). 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 [5,6,10,11,13]). In other words, we must use very fine meshes in order to obtain the desirable accuracy. 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 [13]). For the improvement of the spatial accuracy, it is desirable to develop a class of methods that are both higher-order (higher than second-order) and compact. The higher-order accuracy of these methods allows coarser meshes to be used, thus lowering computational costs. The compact property means that these methods utilize only mesh points directly adjacent to the node about which the differences are taken. This makes the treatment of the boundary conditions easier (see [14,15]).

The study on the higher-order compact methods is extensive, and different forms of the methods have been developed. Hirsh [16] developed a higher-order compact difference technique for some fluid mechanics problems by treating the first and second derivatives as unknowns, and it was numerically exhibited through a variety of test examples. Forester [17] proposed a higher-order difference scheme that allowed the underlying method to remain compact. In the context of fourth-order compact difference discretizations, a class of methods were first proposed by MacKinnon and Carey [14] for material interface discontinuities. The main idea of these methods is to increase the accuracy of the standard central difference approximation from the second-order to the fourth-order by approximating compactly the leading truncation error terms. The extension of these methods to boundary value problems in computational mechanics was discussed in [15]. The similar methods were proposed in [18–20] for convection diffusion equations, in [21] for the Euler equation, in [22] for the stream-function vorticity equation, and in [23,24] for the Poisson equation. These methods are also similar to the so-called Operator Compact Implicit methods developed by several investigators (see [25]) although they were derived in a different manner.

On the other hand, alternating direction implicit (ADI) methods are popular methods for solving two- or three-dimensional parabolic differential equations (see [26–29]). The ADI method reduces two- or three-dimensional problems to a succession of one-dimensional problems. Usually, one needs only to solve a sequence of tridiagonal systems. Hence, the overall computation is simple and fast.

Recently, Liao et al. [3] presented a compact finite difference ADI 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 $u_{yy}^{(l)}$. Since an ADI technique is adopted in this method it reduces the two-dimensional problem to two one-dimensional problems. This reduction gives a practical advantage in the computation of numerical solutions. However, its higher-order convergence was exhibited only numerically through two test examples in [3]. To the best of our knowledge, no theoretical analysis, such as the existence–uniqueness problem and the convergence of numerical solutions, has so far been given to this method. On the other hand, since the function $f^{(l)}(\cdot, \mathbf{u})$ is usually 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 its solutions. In this paper, we give a further theoretical investigation to this method, and develop a *monotone* iterative algorithm for the computation of the solutions of the corresponding discrete system. Our approach is by the method of upper and lower solutions and its associated monotone iteration. This method has been extensively used to various nonlinear problems (see [1,4–9,30–36]).

Firstly, we give some qualitative analyses for the compact finite difference ADI method in [3]. This includes the 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 space and second-order in time. Secondly, by using upper and lower solutions as the initial iterations, we present a basic monotone iterative algorithm for the computation of the numerical solution. Unlike Newton's method, this algorithm maintains the tridiagonal structure of the ADI method. On the other hand, the monotone convergence of the corresponding sequences gives concurrently improving upper and lower bounds for the solution. 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 here do not require any monotonicity of the functions $f^{(l)}(\cdot, \mathbf{u})$. This enlarges the application of the monotone iterative algorithm essentially.

The outline of the paper is as follows. In the next section, we discretize problem (1.1) into a system of nonlinear algebraic equations by using the compact finite difference ADI method in [3]. In Section 3, we give some auxiliary results. These results will play an important role in our discussions. The existence and uniqueness problem is treated in Section 4 by the method of upper and lower solutions, and the convergence of the method is discussed in Section 5. It is shown that the finite difference solution has the accuracy of fourth-order in space and second-order in time. Section 6 is devoted to a basic monotone iterative algorithm for the computation of the numerical solutions. In Section 7, we discuss some techniques for the construction of upper and lower solutions. An application of the method to an enzyme–substrate reaction–diffusion problem is given in Section 8. We use some numerical results to demonstrate the monotone convergence of iterations, the higher-order accuracy of the numerical solution and the corresponding computational cost (CPU time in seconds), and to compare the proposed monotone iterative algorithm with the standard Newton's method. The final section contains some concluding remarks.