Implicit, compact, linearized \( \theta \)-methods with factorization for multidimensional reaction-diffusion equations

J.I. Ramos

Departamento de Lenguajes y Ciencias de la Computación, E.T.S. Ingenieros Industriales, Universidad de Málaga, Plaza El Ejido, s/n, 29013-Málaga, Spain

Abstract

An iterative predictor–corrector technique for the elimination of the approximate factorization errors which result from the factorization of implicit, three-point compact, linearized \( \theta \)-methods in multidimensional reaction-diffusion equations is proposed, and its convergence and linear stability are analyzed. Four compact, approximate factorization techniques which do not account for the approximate factorization errors and which involve three-point stencils for each one-dimensional operator are developed. The first technique uses the full Jacobian matrix of the reaction terms, requires the inversion of, in general, dense matrices, and its approximate factorization errors are second-order accurate in time. The second and third methods approximate the Jacobian matrix by diagonal or triangular ones which are easily inverted but their approximate factorization errors are, however, first-order accurate in time. The fourth approximately factorized, compact, implicit method has approximate factorization errors which are second-order accurate in time and requires the inversion of lower and upper triangular matrices. The techniques are applied to a nonlinear, two-species, two-dimensional system of reaction-diffusion equations in order to determine the approximate factorization errors and those resulting from the approximations to the Jacobian matrix as functions of the allocation of the reaction terms, space and time. © 1998 Elsevier Science Inc. All rights reserved.

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1. Introduction

Recently, there has been a renewed interest in the development and application of compact, high-order accurate, finite difference methods for the numerical solution of the Navier–Stokes equations [1–4]. For example, Rokicki and Floryan [1] employed the vorticity-streamfunction formulation and nine-point stencils in their studies of two-dimensional, incompressible flows and analyzed several types of boundary conditions for the vorticity at the solid walls which employed six-point stencils. A nine-point stencil was also used by Marinos [2] in his studies of the two-dimensional biharmonic equation in rectangles. A fourth-order accurate, compact finite difference method with a nine-point stencil has also been proposed by Spotz and Carey [3] for the vorticity-streamfunction formulation of the two-dimensional Navier–Stokes equations. Lele [4] developed a family of finite difference methods which provide an improved representation of a range of scales, i.e., they have spectral-like resolution, for the evaluation of the first-, second-, and higher-order derivatives. Such a family of schemes was derived from generalizations of the Padé scheme and involve more than three grid points for one-dimensional problems; an analogous comment also applies to the compact, high-order, finite difference methods developed by Carpenter et al. [5,6] in their studies of one-dimensional, initial-boundary value problems by means of compact, fourth- and sixth-order accurate, spatial operators.

As stated above, the compact, finite difference methods presented in Refs. [1–6] result in stencils with at least nine grid points for two-dimensional problems; therefore, their computational solution is very expensive because all the dependent variables are coupled and form a very large system. It must be noted, however, that, in the past, several compact, three-point, finite difference methods which are fourth-order accurate in space were proposed for one-dimensional problems [7–10]. For example, Adam [7] developed a three-point, Hermitian method for one-dimensional, parabolic equations which considers both the dependent variable and its first-order spatial derivative as unknowns. However, he employed second-order difference formula for the boundary conditions, and, therefore, his method is only second-order accurate in space. Hirsh [8] also developed a fourth-order accurate, compact finite difference method with only three grid-points for one-dimensional problems by considering the dependent variable and its first- and second-order spatial derivatives as unknowns; therefore, for a scalar, one-dimensional problem in a grid consisting of \( N \) points, the dimensions of the matrix that has to be inverted to calculate that the unknowns are \( 3N \times 3N \). Christie [9] used a formulation similar to that of Hirsh [8] but eliminated the first- and second-order spatial derivatives so that his scheme results in an \( N \times N \) matrix for one-dimensional problems. Ramos [10] developed a fourth-order accurate, compact finite difference method with only three grid-point for one-dimensional systems of reaction-diffusion...
equations and eliminated the first- and second-order spatial derivatives so that the final matrix had a block tridiagonal structure.

When compact, fourth-order accurate, finite difference methods are employed in the numerical solution of nonlinear multidimensional problems, their computational solution is very expensive because all the dependent variables are coupled and form a very large system, and iterations are required to determine the values of the discrete dependent variables at the grid points.

In this paper, fourth-order accurate, compact, linearized $\theta$-methods with only three-grid point stencils for one-dimensional problems which employ factorization and reduce the solution of multidimensional problems to the iterative solution of one-dimensional ones are presented. Linearized $\theta$-methods which are based on the use of $\theta$-techniques and the linearization of the nonlinear terms are used to analyze multidimensional reaction-diffusion equations such as those occurring in combustion. These techniques are actually methods of lines in space because only the time variable is discretized while the spatial coordinates are kept continuous. However, upon the discretization of the spatial derivatives by means of three-point, compact finite difference methods, linearized $\theta$-methods provide large systems of linear, algebraic equations as shown in Section 2 which may be easily solved either directly or by various global iteration techniques; unfortunately, their computational solution is very expensive because all the dependent variables are coupled and form a very large system. In order to alleviate this, approximate factorization methods may be developed.

Approximate factorization methods which replace the solution of multidimensional problems by sequences of one-dimensional ones are operator-splitting techniques which have received much attention in the recent past [11–13]. For example, Strang [11] developed a symmetric, alternating-direction implicit (ADI) technique for multidimensional, time-dependent inviscid flows in two dimensions with the half steps ordered for maximum accuracy. Briley and McDonald [12] developed linearized block implicit methods for the Navier–Stokes equations, while Beam and Warming [13] used an implicit factorization for the compressible Navier–Stokes equations. The formulations of Strang [11] and Briley and McDonald [12] provide the values of the discretized dependent variables, whereas Beam and Warming [13] used a delta formulation which provides the difference between the values of the discrete dependent variables at two subsequent time steps. Other approximate factorization techniques have been developed by Dukowicz and Dvinsky [14] for the incompressible Navier–Stokes equations; these techniques yield a second-order accurate splitting of the governing equations.

Although the approximate factorization methods considered in Refs. [11–14] provide second-order accuracy in time, the approximate factorization of multidimensional operators introduces approximate factorization errors. These approximate factorization errors have been studied by Steinthorsson and Shih

In this paper, an iterative predictor–corrector method is proposed to eliminate the approximate factorization errors which occur in the factorization of compact, implicit, linearized \( \theta \)-methods in multidimensional reaction-diffusion equations. This method only involves three grid points for each one-dimensional operator and provides fourth-order spatial accuracy. The convergence and the linear or Fourier–von Neumann stability of the predictor–corrector method is analyzed in Section 3.

In Sections 4 and 5, a family of approximate factorization techniques which do not account for the approximate factorization errors and which involves three-point stencils for each one-dimensional operator is considered. The first or fully-linearized technique usually requires the inversion of dense matrices if the Jacobian matrix of the reaction or source terms is dense. Such an inversion may be very demanding for large systems of reaction-diffusion equations such as those which occur in chemical kinetics, combustion, ecology, biology, etc. Therefore, approximate factorization methods which do not require the inversion of dense matrices and which approximate the Jacobian matrix by either diagonal or triangular ones are presented in Sections 5.1 and 5.2, respectively. These diagonal and triangular approximations are shown to result in approximate factorization errors which are first-order accurate in time. A second-order accurate, approximate factorization technique which requires the inversion of lower and upper triangular matrices is developed in Section 5.3. Although, only two-dimensional reaction-diffusion problems are considered, the approach proposed here can easily be extended to three-dimensional systems of convection–diffusion-reaction equations.

2. \( \theta \)-methods of lines for multidimensional reaction-diffusion equations

Consider the following system of two-dimensional reaction-diffusion equations

\[
\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + S(U, t, x, y),
\]

where \( S \) is a function in \( C^1(\mathbb{R}^N \times \mathbb{R} \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}^N) \), \( U \in \mathbb{R}^N, x \in \mathbb{R}, y \in \mathbb{R}, \) and \( t \in \mathbb{R} \) where the diffusion coefficients in the \( x \)- and \( y \)-directions have been set equal to unity. The independent variables \( t \ (0 \leq t < \infty) \), and \( x \ (0 \leq x \leq l_x) \) and \( y \ (0 \leq y \leq l_y) \) are the time and spatial coordinates, respectively, and \( l_x \) and \( l_y \) denote the domain’s dimensions in the \( x \)- and \( y \)-directions, respectively. Although the methods presented here can be easily generalized to the case that the diffusion coefficient is a nonlinear tensor, we have adopted Eq. (1) to illustrate them because of its simplicity.
2.1. Implicit, iterative $h$-methods of lines

Spatial $h$-methods of lines for Eq. (1) may be obtained by discretizing the time derivative while keeping continuous the (independent) spatial variables and can be expressed as

\[
\frac{U^{n+1} - U^n}{k} = \theta \frac{\partial^2 U^{n+1}}{\partial x^2} + (1 - \theta) \frac{\partial^2 U^n}{\partial x^2} + 0 \frac{\partial^2 U^{n+1}}{\partial y^2} + (1 - \theta) \frac{\partial^2 U^n}{\partial y^2} + \theta S^{n+1} + (1 - \theta) S^n,
\]

where $k = t^{n+1} - t^n$ is the time step, $U^n = U(t^n, x, y)$, and $S^n = S(U^n, t^n, x, y)$. The values $\theta = 0$ and $\theta = 1$ correspond to first-order accurate in space, explicit and implicit, respectively, methods of lines, while $\theta = 0.5$ corresponds to a second-order accurate method of lines in time. In this paper, we shall be interested on implicit techniques, and especially on $0 \leq \theta \leq 1$.

**Remark 1.** Instead of using a single parameter $\theta$ to define the implicitness of the reaction and diffusion processes in Eq. (2), it is possible to use three parameters, $0 \leq \theta_x \leq 1$, $0 \leq \theta_y \leq 1$ and $0 \leq \theta_R \leq 1$ for the diffusion terms in the $x$- and $y$-directions and the reaction terms, respectively. However, Eq. (2) is only $O(k^2)$ accurate for $\theta_x = \theta_y = \theta_R = 0.5$.

Eq. (2) is, in general, nonlinear due to the nonlinearity of $S$; therefore, its solution requires an iterative technique. Iterations may, however, be eliminated by linearizing the nonlinear terms which appear in this equation with respect to time as indicated in the next section.

2.2. Fully-linearized, implicit $h$-methods of lines

If the nonlinear term $S^{n+1}$ is approximated by means of its Taylor polynomial of first degree around $(U^n, t^n, x, y)$, Eq. (2) becomes

\[
\frac{U^{n+1} - U^n}{k} = \theta \frac{\partial^2 U^{n+1}}{\partial x^2} + (1 - \theta) \frac{\partial^2 U^n}{\partial x^2} + S^n + \theta T^n k + \theta \frac{\partial^2 U^{n+1}}{\partial y^2} + (1 - \theta) \frac{\partial^2 U^n}{\partial y^2} + \theta J^n (U^{n+1} - U^n),
\]

where

\[
T^n = \frac{\partial F}{\partial t} (U^n, t^n, x, y), \quad J^n = \frac{\partial F}{\partial U} (U^n, t^n, x, y).
\]

Eq. (3) may also be written as

\[
\frac{\Delta U}{k} = \theta \frac{\partial^2 \Delta U}{\partial x^2} + \frac{\partial^2 U^n}{\partial x^2} + S^n + \theta T^n k + \theta \frac{\partial^2 \Delta U}{\partial y^2} + \frac{\partial^2 U^n}{\partial y^2} + \theta J^n \Delta U,
\]

where $\Delta U = U^{n+1} - U^n$. 

Eq. (5) corresponds to a delta formulation, and both Eqs. (3) and (5) correspond to large systems of linear algebraic equations and couple all the dependent variables at \((r^{n+1}, x, y)\). This two-dimensional system may be reduced to sequences of one-dimensional equations by means of the factorization techniques presented in the next sections.

3. Factorization of fully-linearized, implicit \(\theta\)-methods of lines

The two-dimensional differential operator which appears in Eq. (5) may be written in the following exact factorization form

\[
\begin{pmatrix}
I - k\theta \frac{\partial^2}{\partial x^2} & I - k\delta\theta J
\end{pmatrix}
\begin{pmatrix}
I - k\theta \frac{\partial^2}{\partial y^2} & I - k\epsilon\theta J
\end{pmatrix}
\Delta U = \text{RHS} + E_{AF},
\]

where \(I\) denotes the unit or identity matrix,

\[\delta + \epsilon = 1,\]

\[L(\Delta U) = \text{RHS} = k \left( \frac{\partial^2 U^n}{\partial x^2} + \frac{\partial^2 U^n}{\partial y^2} + S^n + k\theta T^n \right),\]

and \(E_{AF}\) denotes the approximate factorization errors, i.e.,

\[E_{AF} = k^2\theta^2 \left( \frac{\partial^4}{\partial x^2 \partial y^2} I + \epsilon \frac{\partial^2}{\partial x^2} J + \delta J \frac{\partial^2}{\partial y^2} I + \delta\epsilon J^2 \right) \Delta U.\]

Eq. (6) can also be written as

\[L_x(\Delta U^x) = \begin{pmatrix} I - k\theta \frac{\partial^2}{\partial x^2} & & \\
\end{pmatrix} \Delta U^x = \text{RHS} + E_{AF},\]

\[L_y(\Delta U) = \begin{pmatrix} I - k\theta \frac{\partial^2}{\partial y^2} & \end{pmatrix} \Delta U = \Delta U^y,\]

which represent linear systems of one-dimensional operators in the \(x\)- and \(y\)-directions, respectively. However, since \(E_{AF}\) depends on \(\Delta U\) (cf. Eq. (9)), Eqs. (10) and (11) are coupled. Moreover, Eq. (10) contains a mixed fourth-order derivative which was not present in Eq. (1) (cf. Eq. (9)); this mixed derivative may be eliminated as follows. From Eq. (11), one can easily obtain

\[\Delta G \equiv \frac{\partial^2 \Delta U}{\partial y^2} = \frac{1}{k\theta} [(I - k\epsilon\theta J)\Delta U - \Delta U^y],\]

which substituted into Eq. (10) yields

\[L_x(\Delta U^{xk}) = \text{RHS} + k\theta \frac{\partial^2}{\partial x^2}(\Delta U - \Delta U^x) + k^2\theta^2 \left( \delta J \frac{\partial^2}{\partial y^2} I + \delta\epsilon J^2 \right) \Delta U,\]

which only contains second-order spatial derivatives.
In order to solve Eqs. (10) and (13) and thus account for the approximate factorization errors, the following iterative predictor–corrector strategy is proposed.

3.1. Predictor–corrector technique

In the predictor step, the following one-dimensional operators are solved

\[ L_x(\Delta U^{*P}) = \text{RHS}, \quad L_y(\Delta U^P) = \Delta U^{*P}, \]

where the superscript P denotes the predictor step, and the factorization errors have not been considered.

In the corrector step, the following one-dimensional operators are solved

\[ L_x(\Delta U^{*m}) = \text{RHS} + E_{AF}^{m-1}, \quad L_y(\Delta U^m) = \Delta U^{*m}, \]

where \( m = 1, 2, \ldots \), denotes the \( m \)th iteration within the time step and the values corresponding to \( m = 0 \) are those of the predictor step. Eq. (15) is to be solved until a user-specified convergence criterion is satisfied.

The factorized method of lines and the predictor–corrector technique presented above are general since no reference was made to the discretization of the second-order spatial derivatives; in fact, the one-dimensional operators in the \( x \)- and \( y \)-directions might be solved analytically since they are linear. However, due to the spatial dependence of, for example, \( \text{RHS} \) and \( \text{J} \), the coefficients of the differential operators are functions of the spatial coordinates; therefore, it is, in general, impossible to obtain their analytical solutions.

If the spatial derivatives are discretized by means of second-order accurate finite difference formulae, Eqs. (10) and (13) are transformed into systems of linear algebraic equations which have a block tridiagonal structure for the dependent variables at interior points, and these systems may be easily solved by means of the tridiagonal matrix algorithm for each spatial direction. If, however, the spatial derivatives in Eqs. (10) and (13) are discretized by means of three-point, compact difference expressions, i.e.,

\[ \Delta F_{i,j} = \frac{1}{h_x^2 \left( 1 + \frac{\delta_x^2}{12} \right)} \delta_x^2 \Delta U_{i,j}, \quad \Delta G_{i,j} = \frac{1}{h_y^2 \left( 1 + \frac{\delta_y^2}{12} \right)} \delta_y^2 \Delta U_{i,j}, \]

where

\[ \Delta F \equiv \frac{\partial^2 \Delta U}{\partial x^2}, \quad \Delta G \equiv \frac{\partial^2 \Delta U}{\partial y^2}, \]

\((i,j)\) denotes the grid point whose coordinates are \((x_i, y_j)\), \(h_x\) and \(h_y\) denote the constant step sizes in the \( x \)- and \( y \)-coordinates, respectively, and

\[ \delta_x^2 \Delta U_{i,j} = \Delta U_{i+1,j} - 2 \Delta U_{i,j} + \Delta U_{i-1,j}, \]

\[(i,j)\]
\[ \delta_y^2 \Delta U_{i,j} = \Delta U_{i,j+1} - 2 \Delta U_{i,j} + \Delta U_{i,j-1}, \]  \hfill (19)

It can be easily shown that substitution of Eq. (16) into Eq. (13) couples the \(x\)- and \(y\)-directions due to the appearance of second-order derivatives in the \(y\)-direction in the right-hand side of Eq. (13), and this coupling was just what we wanted to avoid when we factorized the two-dimensional operator into a sequence of one-dimensional ones. Therefore, in order to maintain the factorization and avoid coupling between the \(x\)- and \(y\)-directions when three-point, compact differences are employed to discretize the spatial derivatives, it proves convenient to rewrite Eqs. (10) and (13) as

\[ (I - k\theta J) \Delta U_{i,j} - k\theta \Delta G = \Delta U^*, \]  \hfill (20)

\[ (I - k\delta\theta J) \Delta U^* - k\theta \Delta F^* = k(F^* + G^* + S^* + k\theta T^*) + k\theta(\Delta F - \Delta F^*) + k^2 \theta^2 (\delta J \Delta G + \delta \epsilon J^2 \Delta U), \]  \hfill (21)

which are applied at the \((i,j)\) grid point together with Eq. (16), and, for the sake of conciseness, the subindex \((i,j)\) has been eliminated in Eqs. (20) and (21).

This formulation for three-point, compact methods has also a block tridiagonal structure for the \(x\)- and \(y\)-finite difference operators, but the resulting matrices in each coordinate direction are twice as large, for the solution of the equations in the \(x\)- and \(y\)-directions requires the solution of Eq. (16) (first equation) and Eq. (21) and Eq. (16) (second equation) and Eq. (20), respectively.

The predictor–corrector strategy employed to solve Eqs. (20) and (21) is presented in the next section.

### 3.2. Predictor–corrector technique for compact differences

In the predictor step, i.e., \(m = 0\), the following one-dimensional operators are solved

\[ (I - k\delta\theta J) \Delta U^*_{i,m} - k\theta \Delta F^*_{i,m} = k(F^* + G^* + S^* + k\theta T^*), \]  \hfill (22)

\[ \Delta F^*_{i,m} = \frac{1}{h_x^2} \frac{\delta_x^2 \Delta U^*_{i,m}}{1 + \delta_x^2/12}, \]  \hfill (23)

followed by

\[ (I - ke\theta J) \Delta U_{i,m} - k\theta \Delta G_{i,m} = \Delta U^*_{i,m}, \]  \hfill (24)

\[ \Delta G_{i,m} = \frac{1}{h_y^2} \frac{\delta_y^2 \Delta U_{i,m}}{1 + \delta_y^2/12}, \]  \hfill (25)

which represent systems of linear equations in the \(x\)- and \(y\)-directions, respectively.
In the corrector step \((m \geq 0)\), the following coupled systems are solved in an iterative manner

\[
(I - k\delta\theta J)\Delta U^{*(m+1)} - k\theta \Delta F^{*(m+1)} = k(F^n + G^n + S^n + k\theta T^n) + k\theta(\Delta F^m - \Delta F^m) + k^2\theta^2(\delta J\Delta G^m + \delta\epsilon J^2 \Delta U^m),
\]

(26)

\[
\Delta F^{*(m+1)} = \frac{1}{h_x^2} \frac{\delta^2\Delta U^{*(m+1)}}{1 + \delta_x^2 / 12}, \quad \Delta F^m = \frac{1}{h_x^2} \frac{\delta^2\Delta U^m}{1 + \delta_x^2 / 12},
\]

(27)

followed by

\[
(I - ke\theta J)\Delta U^{m+1} - k\theta \Delta G^{m+1} = \Delta U^{*(m+1)},
\]

(28)

\[
\Delta G^{m+1} = \frac{1}{h_x^2} \frac{\delta^2\Delta U^{m+1}}{1 + \delta_x^2 / 12},
\]

(29)

until the following criterion is satisfied

\[
\|\Delta U^{m+1} - \Delta U^m\| \leq \epsilon_c,
\]

(30)

where \(\epsilon_c\) is a user-specified convergence tolerance. A similar criterion applies when the second-order spatial derivatives are discretized by means of three-point, second-order accurate formulae.

### 3.3. Convergence of the predictor–corrector technique for compact differences

In order to analyze the convergence of the iterative predictor–corrector method presented in Section 3.2, it is convenient to define

\[
\rho^m = \Delta U - \Delta U^m, \quad \beta^m = \Delta U - \Delta U^m,
\]

(31)

\[
\mu^m = \Delta F - \Delta F^m, \quad \nu^m = \Delta F - \Delta F^m,
\]

(32)

\[
\pi^m = \Delta G - \Delta G^m,
\]

(33)

so that subtraction of Eqs. (26)–(29), respectively, from Eqs. (21) and (16) (first equation), Eqs. (20) and (16) (second equation), respectively, yields

\[
(I - k\delta\theta J)\beta^{(m+1)} - k\theta\nu^{(m+1)} = k\theta(\mu^m - \nu^m) + k^2\theta^2(\delta J\mu^m + \delta\epsilon J^2 \rho^m),
\]

(34)

\[
\left(1 + \frac{\delta^2}{12}\right)\nu^{(m+1)} = \frac{1}{h_x^2} \frac{\delta^2\beta^{(m+1)}}{1 + \delta_x^2 / 12},
\]

(35)

\[
\left(1 + \frac{\delta^2}{12}\right)\mu^{(m+1)} = \frac{1}{h_x^2} \frac{\delta^2\rho^{(m+1)}}{1 + \delta_x^2 / 12},
\]

(36)
Substitution of
\[ (\rho, \beta, \mu, \nu, \pi)^m_{i,j} = (R, E, M, N, P)^m \exp(I(k_x x_i + k_y y_j)), \]
where \( I^2 = -1 \), and \( k_x \) and \( k_y \) are the wavenumbers in the \( x \)- and \( y \)-directions, respectively, into Eqs. (34)–(38) yields, after lengthy calculations, the following linear system of equations:
\[ AR^{m+1} = BR^m, \]  
where
\[ A = I - (\Delta + \Sigma) + \Delta \Sigma + \alpha_x (I - \Delta) + \alpha_x ((1 + \alpha_y)I - \Sigma), \]
\[ B = \alpha_x (\alpha_y I - \Sigma) + \Delta \Sigma - \alpha_y \Delta, \]
\[ \Delta = k \theta \delta J, \quad \Sigma = k \epsilon \delta J \]
\[ \alpha_x = \frac{12k \theta}{h_x^2} \frac{\sin^2(k_x h_x/2)}{3 - \sin^2(k_x h_x/2)}, \]
\[ \alpha_y = \frac{12k \theta}{h_y^2} \frac{\sin^2(k_y h_y/2)}{3 - \sin^2(k_y h_y/2)}. \]

A necessary condition for the convergence of the iterative predictor–corrector method is that \( \| A^{-1} B \| \) be less than unity.

### 3.4. Linear stability of the factorization method with compact differences

In order to analyze the linear or Fourier–von Neumann stability of the factorization method presented in Section 3.3, it will be assumed that \( T = 0 \) and \( S \) is linear in \( U \) so that \( J \) is a constant matrix. Then, substitution of
\[ (U, F, G)^n_{i,j} = (\alpha, \beta, \gamma)^n \exp(I(k_x x_i + k_y y_j)), \]
into Eqs. (10) and (11) yields
\[ Q \alpha^{n+1} = Z \alpha^n, \]
where
\[ Q = (1 + \alpha_x + \alpha_y) I - k \theta J, \]
\[ Z = (1 - \beta_x - \beta_y) I + k(1 - \theta) J, \]
where
\[
\beta_x = \frac{12k(1 - \theta)}{h_x^2} \frac{\sin^2(k_x h_x/2)}{3 - \sin^2(k_x h_x/2)},
\]
\[
\beta_y = \frac{12k(1 - \theta)}{h_y^2} \frac{\sin^2(k_y h_y/2)}{3 - \sin^2(k_y h_y/2)}.
\]

Eq. (47) is the same expression which could have been obtained from the linear stability analysis of Eq. (3).

A necessary condition for linear stability is that the norm of the amplification matrix, \( \mathbf{Q}^{-1} \mathbf{Z} \), be less than unity. The factorization methods presented in this section are here referred to as \( \mathbf{F-FLM} \) and depend on \( \theta \) and \( \delta \), i.e., on the implicitness of the method and the allocation of the source terms to the one-dimensional operators, respectively, in addition to \( k \), \( h_x \) and \( h_y \).

4. Approximately factorized, fully linearized, implicit, compact \( h \)-methods

In the previous section, it was shown that the factorization of fully linearized, implicit, compact \( h \)-methods requires an iterative technique due to the approximate factorization errors. Approximate factorization techniques use Eqs. (10) and (11) without the \( \mathbf{E}_{AF} \) term and, therefore, uncouple the one-dimensional operators in the \( x \)- and \( y \)-directions. This implies that no iterative technique is required to solve the resulting system of equations which coincides with Eqs. (22)–(25) and is repeated here for the sake of completeness

\[
(I - k\delta \theta \mathbf{J}) \Delta \mathbf{U}^* - k\theta \Delta \mathbf{F}^* = k(\mathbf{F}^n + \mathbf{G}^n + \mathbf{S}^n + k\theta \mathbf{T}^n),
\]

\[
\Delta \mathbf{F}^* = \frac{1}{h_x^2} \frac{\delta_x^2 \Delta \mathbf{U}^*}{1 + \delta_x^2/12},
\]

followed by

\[
(I - k\epsilon \theta \mathbf{J}) \Delta \mathbf{U} - k\theta \Delta \mathbf{G} = \Delta \mathbf{U}^*,
\]

\[
\Delta \mathbf{G} = \frac{1}{h_y^2} \frac{\delta_y^2 \Delta \mathbf{U}}{1 + \delta_y^2/12}.
\]

Eqs. (52) and (53) and (54) and (55) represent systems of linear equations in the \( x \)- and \( y \)-directions, respectively. Furthermore, comparison between Eqs. (10) and (11) and Eqs. (52)–(55) indicates that the approximate factorization errors of approximately factorized, fully linearized \( \theta \)-methods are \( O(k^2) \) (cf. Eq. (9)). These methods are here referred to as \( \mathbf{AF-FLM} \) and yield systems of block-tridiagonal matrices for \( \mathbf{U} \) and \( \mathbf{F} \) in the \( x \)-direction and \( \mathbf{U} \) and \( \mathbf{G} \) in the \( y \)-direction. The blocks in the diagonal are, in general, dense if the matrix is ensembled so
as to determine \((U_1, U_2, \ldots, U_N, F_1, F_2, \ldots, F_N)^T\) where the subscripts denote the
components of the vectors and the superscript \(T\) denotes transpose; however,
the off-diagonal matrices are sparse and contain many zeros. (For \(N = 2\), the
blocks are of \(4 \times 4\) and there are only four elements in each off–diagonal block
matrix which are different from zero.)

The linear stability of Eqs. (52)–(55) may be analyzed in exactly the same
way as that of Section 3.4, i.e., substitution of Eq. (46) into Eqs. (52)–(55)
yields Eq. (47) with

\[
Q = (1 + \alpha_x + \alpha_y)I - k\theta J + k^2\theta^2(\delta \epsilon J^2 - \epsilon \alpha_x J + \alpha_x J + \alpha_y J),
\]

\[
Z = (1 - \beta_x - \beta_y)I + k(1 - \theta)J + k^2\theta^2(\delta \epsilon J^2 - \epsilon \alpha_x J - \alpha_x J + \alpha_x J).
\]

The differences between Eqs. (48) and (56) and Eqs. (49) and (57) are of order \(O(k^2)\) and are a consequence of the approximate factorization errors (cf. Eq. (9)).

5. Approximately factorized, partially linearized, implicit, compact \(\theta\)-methods

In the previous section, it was shown that, in approximately factorized, fully
linearized, compact, implicit, \(\theta\)-methods, all the components of \(\Delta U^*\) are
coupled in Eqs. (52) and (53) because of the Jacobian matrix \(J\). A similar comment
applies to Eqs. (54) and (55). Since \(J = L + D + M\), where \(D\) is a diagonal
matrix, and \(L\) and \(M\) are strictly lower and upper, respectively, triangular matrices,
different approximately factorized, partially linearized, compact, implicit,
\(\theta\)-methods may be obtained from Eqs. (52)–(55) depending on the approxima-
tion used to evaluate the Jacobian matrices as indicated in the next sections.

5.1. Approximately factorized, diagonally linearized, implicit, compact \(\theta\)-methods

If \(J\) is approximated by \(D\), Eqs. (52)–(55) are then approximated by

\[
(I - k\delta \theta D)\Delta U^* - k\theta \Delta F^* = k(F^n + G^n + S^n + k\theta T^n),
\]

\[
\Delta F^* = \frac{1}{h^2_x} \frac{\delta_x^2 \Delta U^*}{1 + \delta_x^2/12},
\]

\[
(I - k\epsilon \theta D)\Delta U - k\theta \Delta G = \Delta U^*,
\]

\[
\Delta G = \frac{1}{h^2_y} \frac{\delta_y^2 \Delta U}{1 + \delta_y^2/12},
\]

and the resulting method is here referred to as \(AF-DLM\) which uncouples the
dependent variables, i.e., the \(i\)th component of \(\Delta U\) is uncoupled from the other
components. The approximation of the Jacobian matrix by a diagonal one results in $O(k)$ approximate factorization errors, i.e., (cf. Eqs. (8)–(11))

$$E^D_{AF} = k\theta (L + M)\Delta U + k^2 \theta^2 \left( \frac{\partial^4}{\partial x^2 \partial y^2} I + \epsilon \frac{\partial^2}{\partial x^2} D + \delta D \frac{\partial^2}{\partial y^2} I + \delta^2 \epsilon D^2 \right) \Delta U,$$

(62)

where the superscript $D$ denotes diagonal.

5.2. Approximately factorized, triangularly linearized, implicit, compact $\theta$-methods

If $J$ is approximated by $N = L + D$, i.e., a lower triangular matrix, Eqs. (52)–(55) are then approximated by

$$(I - k\delta \theta N)\Delta U^* - k\theta \Delta F^* = k(F^n + G^n + S^n + k\theta T^n),$$

(63)

$$\Delta F^* = \frac{1}{h^2} \frac{\delta^2 \Delta U^*}{1 + \delta^2 / 12},$$

(64)

$$(I - k\epsilon \theta N)\Delta U - k\theta \Delta G = \Delta U^*,$$

(65)

$$\Delta G = \frac{1}{h^2} \frac{\delta^2 \Delta U}{1 + \delta^2 / 12},$$

(66)

and the resulting method is here referred to as $AF\text{-}TLM$ which sequentially couples the dependent variables, i.e., the $i$th component of $\Delta U$ is coupled to the $1, 2, \ldots, i - 1$, components of $\Delta U$. The approximation of the Jacobian matrix by a diagonal one results in $O(k)$ approximate factorization errors, i.e., (cf. Eqs. (8)–(11))

$$E^T_{AF} = k\theta M \Delta U + k^2 \theta^2 \left( \frac{\partial^4}{\partial x^2 \partial y^2} I + \epsilon \frac{\partial^2}{\partial x^2} N + \delta N \frac{\partial^2}{\partial y^2} I + \delta^2 N^2 \right) \Delta U,$$

(67)

where the superscript $T$ denotes triangular.

5.3. Other approximately factorized, triangularly linearized, implicit, compact $\theta$-methods

It is clear from Sections 3 and 4 that the approximate factorization of two-dimensional systems of reaction-diffusion equations is not unique; for example, the allocation of the reaction terms to the $x$- and $y$-operators depends on $\delta$. Furthermore, the order of these operators may be inverted, or a symmetric sequence of these operators may be used to determine the numerical solution. Furthermore, the fully-linearized methods of Section 4 may require the inversion of dense matrices, although their approximate factorization errors
are second-order accurate in time, whereas the techniques of Section 5 only require the inversion of diagonal or triangular matrices and have approximate factorization errors which are first-order accurate in time. In this section, a fully linearized, compact, implicit \( h \)-method whose approximate factorization errors are second-order accurate in time and only requires the inversion of triangular matrices is presented. This method can be written as

\[
(I - k\theta(L + \mu D))\Delta U^* - k\theta \Delta F^* = k(F^* + G^* + S^* + k\theta T^*),
\]

where \( L \) and \( M \) are lower and upper triangular matrices, respectively. The approximation of the Jacobian matrix by lower and upper, respectively, triangular matrices in the \( x \)- and \( y \)-directions, results in the following approximate factorization errors, i.e., (cf. Eqs. (8)–(11))

\[
E_{AF} = k^2(\partial^4 x / \partial x^2) I + \partial^2 (M + v D) + (L + \mu D) \partial^2 y / \partial y^2 I
\]

Since \( L + \mu D \) in Eq. (68) and \( M + v D \) in Eq. (70) are lower and upper triangular matrices, respectively, the \( k \)th component of \( \Delta U^* \), \( \Delta U_k^* \), depends only on \( \Delta U_m^*, m = 1, 2, \ldots, k - 1 \), while the \( k \)th component of \( \Delta U \), \( \Delta U_k \), depends only on \( \Delta U_m, m = N, N - 1, \ldots, k - 1 \), and may be easily solved by means of the method of Thomas or tridiagonal matrix algorithm.

**Remark 2.** The linearized, implicit, compact \( \theta \)-methods presented in Sections 3–5 can be used to solve multidimensional reaction-diffusion equations subject to Dirichlet boundary conditions in equally spaced grids. When the boundary conditions are of the Neumann or Robin type, i.e., first-order, spatial derivatives appear at the boundaries, Eqs. (22)–(29) and Eqs. (52)–(55) must be solved together with the following expressions

\[
\Delta f^* = \frac{1}{2h_x} \frac{\mu_x \Delta U^*}{1 + \delta_x^2/6}, \quad \Delta F^* = \frac{1}{2h_x} \frac{\mu_x \Delta f^*}{1 + \delta_x^2/6},
\]

\[
\Delta g = \frac{1}{2h_y} \frac{\mu_x \Delta U}{1 + \delta_y^2/6}, \quad \Delta G = \frac{1}{2h_y} \frac{\mu_x \Delta g}{1 + \delta_y^2/6},
\]
\[ \frac{1}{2h_x} \mu_x \Delta F_x = \frac{1}{h_x^2} \delta_x^2 \Delta F_x, \quad \frac{1}{2h_y} \mu_y \Delta G = \frac{1}{h_y^2} \delta_y^2 \Delta g, \]  
\tag{75}

where

\[ \Delta f \equiv \frac{\partial \Delta U}{\partial x}, \quad \Delta g \equiv \frac{\partial \Delta U}{\partial y}, \]  
\tag{76}

\[ \mu_x f_{i,j} = f_{i+1,j} - f_{i-1,j}, \quad \mu_y g_{i,j} = g_{i,j+1} - g_{i,j-1}. \]  
\tag{77}

Eqs. (73)–(75) represent three-point, fourth-order accurate discretizations of the first- and second-order spatial derivatives. Furthermore, Eqs. (73) and (75) (first equation) and Eqs. (74) and (75) (second equation) are to be solved with Eqs. (52) and (53) and Eqs. (54) and (55), respectively; therefore, the numerical solution of multidimensional reaction-diffusion equations by means of implicit, compact differences requires the inversion of block tridiagonal matrices and the dimensions of these blocks are \( 3N \times 3N \). However, there is no need to solve such a large matrix since the use of Eq. (52) at the \((i - 1, j), (i, j)\) and \((i + 1, j)\)th grid points combined with Eqs. (53), (73) and (75) (first equation) at \((i, j)\) provide seven equations for \( \Delta U_{k,j}^*, \Delta f_{k,j}^* \) and \( \Delta F_{k,j}^* \) with \( k = i - 1, i, i + 1 \), i.e., nine unknowns. Therefore, \( \Delta f_{k,j}^* \) and \( \Delta F_{k,j}^* \) can be written in terms of \( \Delta U_{k,j}^* \) with \( k = i - 1, i, i + 1 \), and one single equation for \( \Delta U_{k,j}^* \) with \( k = i - 1, i, i + 1 \), may be obtained. Such an equation only involves the unknown dependent variables at three consecutive grid points and results in a block tridiagonal matrix.

**Remark 3.** For advection–reaction-diffusion equations, it is also necessary in factorization techniques to solve one-dimensional operators for \( \Delta U^* \), \( \Delta f^* \) and \( \Delta F^* \) in the \( x \)-direction, and \( \Delta U \), \( \Delta g \) and \( \Delta G \) in the \( y \)-direction when compact differences are employed. By way of contrast, it is only necessary to solve one-dimensional operators for \( \Delta U^* \) and \( \Delta U \) when the first- and second-order spatial derivatives are discretized by means of second-order accurate formulae. However, the factorization of advection–reaction-diffusion equations may also be written as a block tridiagonal matrix for the dependent variables of each one-dimensional operator as indicated in Remark 2.

**Remark 4.** For non-equally spaced grids, Eq. (16) (first equation) and Eq. (73) (first equation) are to be replaced by

\[ h_{i+1} \Delta U_{i-1,j}^* + h_i \Delta U_{i+1,j}^* - (h_i + h_{i+1}) \Delta U_{i,j}^* \\
= \frac{1}{2} \left( h_i h_{i+1} (h_i + h_{i+1}) \Delta F_{i,j}^* + \frac{h_i^2 + h_{i+1}^2}{12 h_i + h_{i+1}} \right) \times \left( h_{i+1} \Delta F_{i-1,j}^* + h_i \Delta F_{i+1,j}^* - (h_i + h_{i+1}) \Delta F_{i,j}^* \right), \]  
\tag{78}
\[
\begin{align*}
    h_i^2 \Delta U_{i+1,j} - h_i^2 \Delta U_{i-1,j} & = \left( h_i^2 - h_{i+1}^2 \right) \Delta U_{i,j} + h_i h_{i+1} \left( h_i + h_{i+1} \right) \Delta f_{i,j}^r \\
    & + \frac{1}{3} h_i h_{i+1} \left( h_{i+1} \Delta f_{i+1,j}^r + h_i \Delta f_{i+1,j} - (h_i + h_{i+1}) \Delta f_{i,j}^r \right),
\end{align*}
\]

where \( h_i = x_i - x_{i-1} \), and similar expressions may be obtained for the spatial discretizations of the \( y \)-derivatives. Eqs. (78) and (79) reduce to Eq. (16) (first equation) and Eq. (73) (first equation), respectively, for \( h_i = h_x = \text{const.} \)

**Remark 5.** The delta formulation used in this paper permits to determine a steady state which is independent of the time step employed in the calculations except for \( F-\text{FLM} \) (cf. Eq. (9)). Therefore, the methods presented here may be used to determine the solution of elliptic equations using a time-dependent method.

### 6. Presentation of results

The factorization techniques presented in this paper have been used to obtain the numerical solution of the following two-species, two-dimensional reaction-diffusion system of equations

\[
\begin{align*}
    \frac{\partial u}{\partial t} & = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - u^4 v, \\
    \frac{\partial v}{\partial t} & = \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + u^4 v - Kv,
\end{align*}
\]

subject to

\[
\begin{align*}
    u(x, y, 0) & = 1, \quad v(x, y, 0) = \exp(-\hat{\lambda}(x^2 + y^2)), \\
    u(x, 20, t) & = 1, \quad v(x, 20, t) = 0, \\
    u(20, y, t) & = 1, \quad v(20, y, t) = 0,
\end{align*}
\]

\[
\begin{align*}
    \frac{\partial u}{\partial x}(0, y, t) & = \frac{\partial v}{\partial x}(0, y, t) = \frac{\partial u}{\partial y}(x, 0, t) = \frac{\partial v}{\partial y}(x, 0, t) = 0,
\end{align*}
\]

where \( K = 0.5 \) and \( \hat{\lambda} = 1 \).

These equations were solved with \( k = 0.04 \) and \( \Delta x = \Delta y = 0.2 \), and the convergence of the factorization method presented in Section 3 was established when \( \epsilon_c = 10^{-12} \) in Eq. (30) with the \( L_2 \)-norm for the vector \( \Delta U \). For this convergence criterion, \( F-\text{FLM} \) was observed to converge in two or three iterations; the number of iterations was found to increase as \( \epsilon_c \) was decreased. Some sample results obtained with the factorization methods presented in this paper are
shown in Figs. 1–4 which were obtained with $\theta_x = \theta_y = \theta_R = \delta = 0.5$. In these figures as well as the others presented in this section, only grid points $(i,j)$ where $i$ or $j$ are even are illustrated; this explains why, for example, the $v$ profile shown in Fig. 1 does not look symmetric.

Figs. 1–4 show the spatial distributions of $u$ and $v$ at selected times obtained by means of $\text{AF-FLM}$. Initially, i.e., at $t = 0$, $u = 1$, while $v$ exhibits a spike of unit amplitude at $x = y = 0$ (Fig. 1 (top)). Due to the chemical reactions and diffusion, $u$ decreases and a valley is formed which spreads radially, while $v$ decreases in amplitude and also spreads radially as indicated in Fig. 1 (bottom) which corresponds to $t = 4$.

Fig. 2 also shows the radial spreading of $v$ which also exhibits a valley at $x = y = 0$. The depth of this valley increases as $t$ increases as illustrated in Fig. 3. The solutions at $t = 400$ and $500$ are shown in Fig. 4 which indicate that the problem has reached a steady state characterized by $u \approx 0.8$ in most of the domain and large gradients of $u$ near the boundaries, whereas $v$ has peaks at the corners of the computational domain and somewhat steep gradients at the domain’s boundaries.

The effect of the allocation of the reaction terms on the numerical solution are illustrated in Figs. 5 and 6 for $\text{AF-FLM}$ with $\theta_x = \theta_y = \theta_R = 0.5$. For $\delta = 0$, all the reaction terms are allocated to the $y$-operator (cf. Eqs. (7), (52) and (54)), whereas, for $\delta = 1$, all the reaction terms are allocated to the $x$-operator, and the difference between the solution corresponding to $\delta = 0$ and that for $\delta = 0.5$ and the difference between the solution corresponding to $\delta = 1$ and that for $\delta = 0.5$ are of about the same absolute value but opposite sign. The largest differences between the solution corresponding to $\delta = 0.5$ and that for $\delta = 0$ are (in absolute value) $0.002$ and $0.002$, $0.003$ and $0.002$, $0.004$ and $0.002$, $0.006$ and $0.004$, $0.01$ and $0.004$, $0.01$ and $0.004$, $0.01$ and $0.004$, $0.015$ and $0.004$, $0.015$ and $0.004$, $0.015$ and $0.005$ for $u$ and $v$, respectively, at $t = 2, 4, 6, 8, 10, 12, 14, 16, 18$ and $20$, respectively. The largest differences between the solution corresponding to $\delta = 0.5$ and that for $\delta = 1$ are (in absolute value) $0.002$ and $0.002$, $0.003$ and $0.002$, $0.004$ and $0.004$, $0.006$ and $0.004$, $0.01$ and $0.004$, $0.01$ and $0.004$, $0.01$ and $0.004$, $0.015$ and $0.004$, $0.015$ and $0.004$, $0.015$ and $0.005$, $0.015$ and $0.005$ for $u$ and $v$, respectively, at $t = 2, 4, 6, 8, 10, 12, 14, 16, 18$ and $20$, respectively.

Figs. 7–10 show the effect of both the first- and second-order accurate treatment of the reaction terms and the allocation of these terms to the one-dimensional operators in $\text{AF-FLM}$ measured with respect to $\theta_R = \delta = 0.5$. For example, the top graphs in Figs. 7–10 show the difference between the solution obtained with $\theta_R = 1$ and $\delta = 0.5$ and that with $\theta_R = \delta = 0.5$, i.e., between first-and second-order accurate discretizations of the reaction terms with equal allocation to the one-dimensional operators. The bottom graphs in Figs. 7 and 8 exhibit the difference between the solution obtained with $\theta_R = 1$ and $\delta = 0$ and that with $\theta_R = \delta = 0.5$, whereas the bottom graphs in Figs. 9 and 10 show...
the difference between the solution obtained with $\theta_R = 1$ and $\delta = 1$ and that with $\theta_R = \delta = 0.5$. The differences in $u$ and $v$ between the solutions obtained with $\theta_R = 1$ and $\delta = 0.5$ and those with $\theta_R = \delta = 0.5$ are (in absolute value), respectively, 0.002 and 0.002, 0.003 and 0.002, 0.006 and 0.004, 0.004, 0.01 and 0.004, 0.01 and 0.004, 0.015 and 0.005, 0.015 and 0.01, 0.02 and 0.01, and 0.02 and 0.005, respectively, at $t = 2, 4, 6, 8, 10, 12, 14, 16, 18$ and 20, respectively.

The differences in $u$ and $v$ between the solutions obtained with $\theta_R = 1$ and $\delta = 0$ and those with $\theta_R = \delta = 0.5$ are (in absolute value), respectively, 0.002 and 0.002, 0.002 and 0.002, 0.003 and 0.002, 0.004 and 0.004, 0.004, 0.01 and 0.004, 0.01 and 0.004, 0.01 and 0.004, 0.01 and 0.004, and 0.01 and 0.004, respectively, at $t = 2, 4, 6, 8, 10, 12, 14, 16, 18$ and 20, respectively.

The differences in $u$ and $v$ between the solutions obtained with $\theta_R = 1$ and $\delta = 1$ and those with $\theta_R = \delta = 0.5$ are (in absolute value), respectively, 0.005 and 0.01, 0.01 and 0.01, 0.015 and 0.01, 0.02 and 0.01, 0.03 and 0.02, 0.03 and 0.02, 0.04 and 0.02, 0.04 and 0.02, 0.06 and 0.02, and 0.06 and 0.02, respectively, at $t = 2, 4, 6, 8, 10, 12, 14, 16, 18$ and 20, respectively.

The top graphs in Figs. 11 and 12 show the differences in the solutions for $u$ and $v$ obtained with AF-FML and $\theta_x = \theta_y = \theta_R = \delta = 0.5$ and $\theta_z = 1$, and those obtained with AF-FML and $\theta_z = \theta_x = \theta_y = \theta_R = \delta = 0.5$, i.e., the difference between $O(k)$ and $O(k^2)$ discretizations of the diffusion term in the $y$-direction, whereas
Fig. 2. $u$ (left) and $v$ (right) (top: $t = 8$; bottom: $t = 12$; $\mathbb{AP}-\text{FLM}; \theta_s = \theta_y = \theta_R = \delta = 0.5$).

Fig. 3. $u$ (left) and $v$ (right) (top: $t = 16$; bottom: $t = 20$; $\mathbb{AP}-\text{FLM}; \theta_s = \theta_y = \theta_R = \delta = 0.5$).
the bottom graphs of these figures illustrate the differences in $u$ and $v$ between the solutions obtained with $\theta_y = \theta_R = \delta = 0.5$ and $\theta_x = 1$, and those with $\theta_x = \theta_y = \theta_R = \delta = 0.5$, i.e., the difference between $O(k)$ and $O(k^2)$ discretizations of the diffusion term in the $x$-direction.

The differences in $u$ and $v$ between the solutions obtained with $\text{AF-FML}$ and $\theta_x = \theta_R = \delta = 0.5$ and $\theta_y = 1$ and those obtained with $\text{AF-FML}$ and $\theta_x = \theta_y = \theta_R = \delta = 0.5$ are (in absolute value), respectively, 0.001 and 0.001, 0.0005 and 0.0004, 0.0004 and 0.0002, 0.001 and 0.0004, 0.001 and 0.0004, 0.001 and 0.0004, 0.002 and 0.0004, 0.002 and 0.0004, 0.001 and 0.0004, and 0.001 and 0.0002, respectively, at $t = 2, 4, 6, 8, 10, 12, 14, 16, 18$ and $20$, respectively.

The differences in $u$ and $v$ between the solutions obtained with $\text{F-FLM}$ and $\theta_x = \theta_R = \delta = 0.5$ and $\theta_y = 1$ and those obtained with $\text{AF-FML}$ and $\theta_x = \theta_y = \theta_R = \delta = 0.5$ are, respectively, 0.001 and 0.001, 0.0005 and 0.0004, 0.0004 and 0.0002, 0.001 and 0.0004, 0.001 and 0.0004, 0.001 and 0.0004, 0.002 and 0.0004, 0.002 and 0.0004, 0.001 and 0.0004, and 0.001 and 0.0002, respectively, at $t = 2, 4, 6, 8, 10, 12, 14, 16, 18$ and $20$, respectively.

Although not shown here, the differences between the results obtained with $\text{F-FLM}$ and $\text{AF-FLM}$, i.e., the approximate factorization errors $E_{\text{AF}}$, for $\theta_x = \theta_y = \theta_R = \delta = 0.5$ are initially zero, and exhibit the same trends as, but have opposite sign to, the spatial distributions of $u$ and $v$. The largest
Fig. 5. Errors in $u$ (left) and $v$ (right) at $t = 8$ (the errors are the difference between the results obtained with $\delta = 0$ and $\delta = 0.5$ (top) and between those with $\delta = 1$ and $\delta = 0.5$ (bottom); AF-FLM; $\theta_s = \theta_r = \theta_R = 0.5$).

Fig. 6. Errors in $u$ (left) and $v$ (right) at $t = 16$ (the errors are the difference between the results obtained with $\delta = 0$ and $\delta = 0.5$ (top) and between those with $\delta = 1$ and $\delta = 0.5$ (bottom); AF-FLM; $\theta_s = \theta_r = \theta_R = 0.5$).
Fig. 7. Errors in $u$ (left) and $v$ (right) at $t = 8$ (the errors are the difference between the results obtained with $\theta_R = 1$ and $\delta = 0.5$ and those with $\theta_R = 0.5$ and $\delta = 0.5$ (top) and between those with $\theta_R = 1$ and $\delta = 0$ and those with $\theta_R = 0.5$ and $\delta = 0.5$ (bottom); AF-FLM; $\theta_i = \theta_j = 0.5$).

Fig. 8. Errors in $u$ (left) and $v$ (right) at $t = 16$ (the errors are the difference between the results obtained with $\theta_R = 1$ and $\delta = 0.5$ and those with $\theta_R = 0.5$ and $\delta = 0.5$ (top) and between those with $\theta_R = 1$ and $\delta = 0$ and those with $\theta_R = 0.5$ and $\delta = 0.5$ (bottom); AF-FLM; $\theta_i = \theta_j = 0.5$).
The differences in \( u \) between the two solutions are 0.002 and occur at \( x = y = 0 \) at \( t = 2, 4, 6 \) and 8, and at the inflection points of \( u \) at \( t = 10 \). For \( t \geq 10 \), the largest differences in \( u \) are still positive and equal to 0.0015, and occur at the inflection points of \( u \).

The differences in \( v \) between the results obtained with F-FLM and AF-FLM are negative and occur at \( x = y = 0 \) for \( t \leq 20 \); their largest absolute value is 0.002 and occurs at \( t = 0 \), and decreases as \( t \) increases, so that their magnitude is about 0.0005 at \( t = 20 \). Furthermore, the relative approximate factorization errors in \( u \) and \( v \) are at most 0.002 and are positive for \( u \) and negative for \( v \).

It has also been found that the absolute values of the differences between the results obtained with AF-NFLM and F-FLM are larger than those between AF-FLM and F-FLM, the differences in \( u \) and \( v \) between the results obtained with AF-NFLM and F-FLM exhibit the same shape for \( \mu = 0 \) and 1 and their largest values at \( x = y = t = 10 \) are about 0.001 and 0.0006, respectively, for \( \mu = 1 \), and 0.002 and 0.001, respectively, for \( \mu = 0 \), and the differences in \( u \) show an annular peak before reaching a relative minimum at \( t = 10 \).

The differences between the results obtained with AF-NFLM and F-FLM are smaller for \( \mu = 0.5 \) than, although exhibit similar shapes to, those corresponding to \( \mu = 0 \) and 1. For example, the largest differences in \( u \) and \( v \) at \( t = 10 \) for
The differences in $u$ and $v$ between the results obtained with $\text{AF-DLM}$ and $\text{F-FLM}$ are larger than those between $\text{AF-NFLM}$ with $\mu = 0.5$ and $\text{AF-DLM}$, and the annular peak which these differences show before the relative minimum in $u$ is of larger amplitude for $\text{AF-DLM}$ than that for $\text{AF-NFLM}$ at $t = 10$.

The errors of the approximately factorized, triangularly linearized $\theta$-methods with respect to $\text{F-FLM}$ were evaluated when the equations were solved in the sequences $u \rightarrow v$ and $v \rightarrow u$. At $t = 10$, it was found that the largest errors in $u$ and $v$ are about $0.0005$ and $0.0006$, respectively, for the sequence $u \rightarrow v$, and $0.001$ and $0.0003$, respectively, for the sequence $v \rightarrow u$. Furthermore, at the same time, the sequence $u \rightarrow v$ shows an annular peak of positive errors in $u$. At $t = 20$, the largest errors in $u$ and $v$ are about $0.001$ and $0.0005$, respectively, for the sequence $u \rightarrow v$, and $0.001$ and $0.0004$, respectively, for the sequence $v \rightarrow u$.

The results presented in Figs. 1–12 and others not shown here clearly indicate that $\text{AF-FLM}$ with $\delta = 0.5$ is more accurate than $\text{AF-FLM}$ with $\delta = 0$ or $1$; the accuracy of $\text{AF-FLM}$ with $\delta = 0.5$ is comparable to that of $\text{AF-NFLM}$ with $\mu = 0.5$ and $\text{AF-TLM}$ in the sequence $v \rightarrow u$ with $\delta = 0.5$; $\text{AF-NFLM}$ with $\mu = 0.5$ is more accurate than $\text{AF-NFLM}$ with $\mu = 1$ which, in turn, is more accurate.

Fig. 10. Errors in $u$ (left) and $v$ (right) at $t = 16$ (the errors are the difference between the results obtained with $\theta_R = 1$ and $\delta = 0.5$ and those with $\theta_R = 0.5$ and $\delta = 0.5$ (top) and between those with $\theta_R = 1$ and $\delta = 1$ and those with $\theta_R = 0.5$ and $\delta = 0.5$ (bottom): $\text{AF-FLM}; \theta_i = \theta_j = 0.5$).
Fig. 11. Errors in $u$ (left) and $v$ (right) at $t = 8$ (the errors are the difference between the results obtained with $\theta_i = \delta_R = \delta = 0.5$ and $\theta_i = 1$ and those with $\theta_i = \delta_i = \delta = 0.5$ (top) and between those with $\theta_i = \delta_R = \delta = 0.5$ and $\theta_i = 1$ and those with $\theta_i = \delta_i = \delta = 0.5$ (bottom); \(\mathcal{AP}\)-FLM).

Fig. 12. Errors in $u$ (left) and $v$ (right) at $t = 16$ (the errors are the difference between the results obtained with $\theta_i = \delta_R = \delta = 0.5$ and $\theta_i = 1$ and those with $\theta_i = \delta_i = \delta = 0.5$ (top) and between those with $\theta_i = \delta_R = \delta = 0.5$ and $\theta_i = 1$ and those with $\theta_i = \delta_i = \delta = 0.5$ (bottom); \(\mathcal{AP}\)-FLMd).
than AF-NFLM with $\mu = 0$; the accuracy of AF-NFLM with $\mu = 1$ is comparable to that of AF-TLM in the sequence $u \rightarrow v$ with $\delta = 0.5$; and, the accuracy of AF-NFLM with $\mu = 0$ is comparable to that of AF-DLM with $\delta = 0.0$. Therefore, the accuracy of approximately factorized, implicit, linearized $\theta$-methods depends on the allocation of the source terms to the one-dimensional operators, and degrades as the Jacobian matrix is approximated by triangular or diagonal ones.

7. Conclusions

An iterative, predictor–corrector technique has been developed to eliminate the second-order approximate factorization errors which result from the factorization of implicit, compact, linearized $\theta$-methods in multidimensional reaction-diffusion equations. It is shown that this iterative technique converges in two or three iterations at a rate which depends on the spatial and temporal step sizes, Jacobian matrix of the reaction terms, implicitness of the discretization and allocation of the reaction or source terms to the one-dimensional operators which result from the factorization. The linear or Fourier–von Neumann stability of the predictor–corrector method is also shown to depend on the above and on the wave numbers in the $x$- and $y$-directions. Moreover, the predictor–corrector method employs only compact, three-point finite discretizations for each spatial coordinate which result in fourth-order spatial accuracy.

Four approximately factorized, implicit, non-iterative, compact, linearized $\theta$-methods, i.e., techniques which do not account for the approximate factorization errors, have been developed. The first method is second-order accurate in time and accounts for the full Jacobian matrix of the reaction terms. As a consequence, the use of the tridiagonal matrix algorithm for the inversion of the block-tridiagonal matrices which result from the one-dimensional operators coming from the approximate factorization may be computationally very demanding for systems of highly coupled, nonlinear reaction-diffusion equations because this Jacobian matrix may be dense. Such a computational cost may be substantially reduced by approximating the Jacobian matrix by diagonal or triangular ones which require the easy inversion of either diagonal or triangular matrices, respectively. Unfortunately, diagonal and triangular approximations to the Jacobian matrix result in approximately factorized, implicit, compact, linearized $\theta$-methods whose approximate factorization errors are only first-order accurate in time, and, although they are much more efficient than fully linearized, implicit, compact techniques which employ the full Jacobian matrix, they may require smaller time steps because they uncouple or sequentially couple, respectively, the dependent variables at each time step.

Finally, an approximately factorized, implicit, compact, linearized $\theta$-method whose approximate factorization errors are second-order accurate in time and requires the inversion of lower and upper triangular matrices has been
developed. The accuracy of this scheme is highest when the reaction terms are allocated in the same proportion to each one-dimensional operator, is comparable to that of the fully linearized, implicit, $\theta$-method which requires the inversion of the full Jacobian matrix and to that of approximately factorized, implicit, trianglerly linearized $\theta$-techniques, and higher than that of approximately factorized, compact, implicit, diagonally linearized $\theta$-schemes.

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