Linearized factorization techniques for multidimensional reaction–diffusion equations

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Abstract

An iterative predictor–corrector technique for the elimination of the approximate factorization errors which result from the factorization of linearized θ-methods in multidimensional reaction–diffusion equations is proposed, and its convergence and linear stability are analyzed. Four approximate factorization techniques which do not account for the approximate factorization errors 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 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. © 1999 Elsevier Science Inc. All rights reserved.

1. Introduction

Families of partially linearized, triangular and diagonal θ-methods for the numerical solution of autonomous and nonautonomous, ordinary differential equations and one-dimensional, reaction–diffusion equations, respectively,

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were developed in [1,2]. These methods are implicit, and their accuracy is $O(k)$
where $k$ is the time step. For a system of $N$ ordinary or one-dimensional partial
differential equations, it has been shown [1,2] that there are $N!$ partially line-
arized, triangular $\theta$-methods.

In this paper, factorization techniques are employed to solve numerically the
discretized equations that result from the use of linearized $\theta$-methods in mul-
tidimensional reaction–diffusion equations. 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; unfor-
tunately, their computational solution is very expensive because all the de-
pendent 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 discretization of
multidimensional problems by sequences of one-dimensional ones are opera-
tor-splitting techniques which have received much attention in the recent past
[3–5]. For example, Strang [3] 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 [4] developed linearized block implicit methods for the Navier–
Stokes equations, while Beam and Warming [5] used an implicit factorization
for the compressible Navier–Stokes equations. The formulations of Strang [3]
and Briley and McDonald [4] provide the values of the discretized dependent
variables, whereas Beam and Warming [5] 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 [6] 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. [3–6]
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
[7] who considered methods for reducing them in a three-dimensional, linear,
advection equation. In this paper, an iterative predictor–corrector method is
proposed to eliminate the approximate factorization errors which occur in the
factorization of linearized $\theta$-methods in multidimensional reaction–diffusion
equations. The convergence and the linear or Fourier–von Neumann stability
of the predictor–corrector method is analyzed in Section 3.

In Section 4, four families of approximate factorization techniques which do
not account for the approximate factorization errors are 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 4.2 and 4.3, respectively, where their stability and accuracy is examined. 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 4.4 where its accuracy and linear stability are analyzed. 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 for multidimensional reaction–diffusion equations

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

\[
\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + F(U, t, x, y), \quad (1)
\]

where \( F \) 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 \( y \) (\( 0 \leq x \leq l_y \)) 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 \( \theta \)-methods

\( \theta \)-methods for Eq. (1) can be expressed as

\[
\frac{U_{i,j}^{n+1} - U_{i,j}^n}{k} = \frac{1}{\Delta x^2} [\theta \delta_x^2 U_{i,j}^{n+1} + (1 - \theta) \delta_x^2 U_{i,j}^n] + \frac{1}{\Delta y^2} [\theta \delta_y^2 U_{i,j}^{n+1} + (1 - \theta) \delta_y^2 U_{i,j}^n] + \theta F_{i,j}^n + (1 - \theta) F_{i,j}^n, \quad (2)
\]

where \( k = t^{n+1} - t^n \) is the time step. \( \Delta x = x_{i+1} - x_i \) and \( \Delta y = y_{j+1} - y_j \) denote the constant spatial step sizes in the \( x \)- and \( y \)-directions, respectively, \( U_{i,j}^n = U(t^n, x_i, y_j), F_{i,j}^n = F(U_{i,j}^n, t^n, x_i, y_j) \), \( x_i \) and \( y_j \) denote the location of the \( (i,j) \)th grid point, and
\[ \delta_x^2 U_{i,j}^n = U_{i+1,j}^n - 2U_{i,j}^n + U_{i-1,j}^n, \]  
\[ \delta_y^2 U_{i,j}^n = U_{i,j+1}^n - 2U_{i,j}^n + U_{i,j-1}^n, \]

are central differences operators. The values \( \theta = 0 \) and \( \theta = 1 \) correspond to first-order accurate in time, explicit and implicit, respectively, methods, while \( \theta = 0.5 \) corresponds to a second-order accurate method in time. In this paper, we shall be interested on implicit techniques, and especially on \( 0.5 \leq \theta \leq 1 \).

It must be noted that, 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, \( \theta_x, \theta_y \), and \( \theta_R \) for the diffusion terms in the \( x \)- and \( y \)-directions and the reaction terms, respectively.

Eq. (2) is, in general, nonlinear due to the nonlinearity of \( F \); 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 Section 2.2.

2.2. Fully-linearized, implicit \( \theta \)-methods

If the nonlinear term \( F_{ij}^{n+1} \) is approximated by means of its Taylor polynomial of first degree around \( (U_{i,j}^n, t^n, x_i, y_j) \), Eq. (2) becomes

\[
\frac{U_{i,j}^{n+1} - U_{i,j}^n}{k} = \frac{1}{\Delta x^2} \left[ \theta \delta_x^2 U_{i,j}^{n+1} + (1 - \theta) \delta_x^2 U_{i,j}^n \right] + F_{i,j}^n + \theta T_{i,j}^n k \\
+ \frac{1}{\Delta y^2} \left[ \theta \delta_y^2 U_{i,j}^{n+1} + (1 - \theta) \delta_y^2 U_{i,j}^n \right] + \theta J_{i,j}^n (U_{i,j}^{n+1} - U_{i,j}^n),
\]

where

\[ T_{i,j}^n = \frac{\partial F}{\partial t} (U_{i,j}^n, t^n, x_i, y_j), \]

\[ J_{i,j}^n = \frac{\partial F}{\partial U} (U_{i,j}^n, t^n, x_i, y_j). \]

Eq. (5) coincides with that of Briley and McDonald [4] if \( F \) does not depend on \( t \), and may also be written as

\[
\frac{\Delta U_{i,j}}{k} = \frac{1}{\Delta x^2} \left[ \theta \delta_x^2 \Delta U_{i,j} + \delta_x^2 U_{i,j}^n \right] + F_{i,j}^n \\
+ \theta T_{i,j}^n k + \frac{1}{\Delta y^2} \left[ \theta \delta_y^2 \Delta U_{i,j} + \delta_y^2 U_{i,j}^n \right] + \theta J_{i,j}^n \Delta U_{i,j},
\]

where \( \Delta U_{i,j} = U_{i,j}^{n+1} - U_{i,j}^n \).

Eq. (8) corresponds to a delta formulation and coincides with that of Beam and Warming [5] if \( F \) does not depend on \( t \). Both Eqs. (5) and (8) correspond to large systems of linear algebraic equations and couple all the dependent variables at \((t^{n+1}, x_i, y_j)\). 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

The two-dimensional finite difference operators which appear in Eq. (8) may be written in the following factorization form:

$$\left( I - \frac{k\theta}{\Delta x^2} \delta_x^2 I - k\delta \partial J \right) \left( I - \frac{k\theta}{\Delta y^2} \delta_y^2 I - k\epsilon \partial J \right) \Delta U = k \text{RHS} + E_{AF}, \quad (9)$$

where the subscript $(i,j)$ denoting the grid point has been eliminated for the sake of conciseness, $I$ denotes the unit or identity matrix,

$$\delta + \epsilon = 1, \quad (10)$$

$$\text{RHS} = \frac{1}{\Delta x^2} \delta_x^2 U^n + \frac{1}{\Delta y^2} \delta_y^2 U^n + F^n + \theta T^* k, \quad (11)$$

and $E_{AF}$ denotes the approximate factorization errors, i.e.,

$$E_{AF} = k^2 \theta^2 \left( \frac{1}{\Delta x^2 \Delta y^2} \delta_x^2 \delta_y^2 I + \epsilon \frac{\delta}{\Delta x^2} \delta_y^2 J + \delta \frac{\delta}{\Delta y^2} \delta_x^2 J + \delta \epsilon J^2 \right) \Delta U. \quad (12)$$

Eq. (9) can also be written as

$$L_x(\Delta U^*) = \left( I - \frac{k\theta}{\Delta x^2} \delta_x^2 I - k\delta \partial J \right) \Delta U^* = k \text{RHS} + E_{AF}, \quad (13)$$

$$L_y(\Delta U) = \left( I - \frac{k\theta}{\Delta y^2} \delta_y^2 I - k\epsilon \partial J \right) \Delta U = \Delta U^*, \quad (14)$$

which represent linear systems of one-dimensional equations in the $x$- and $y$-directions, respectively. However, since $E_{AF}$ depends on $\Delta U$ (cf. Eq. (12)), Eqs. (13) and (14) are coupled. In order to solve them 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:

$$L_x(\Delta U^p) = k \text{RHS}, \quad L_y(\Delta U^p) = \Delta U^p, \quad (15)$$

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

\[ L_x(\Delta U^{*k}) = k \ \text{RHS} + E_{AF}^{k-1}, \quad k = 1, 2, \ldots, \] (16a)
\[ L_y(\Delta U^{k}) = \Delta U^{*k}, \quad k = 1, 2, \ldots, \] (16b)

where \( k \) denotes that \( k \)th iteration within the time step and the values corresponding to \( k = 0 \) are those of the predictor step. However, the \( x \)-operator is not solved in this manner because \( E_{AF} \) contains the nine-point finite difference operator \( \delta_x \delta_y^2 \) (cf. Eq. (12)); rather, it is solved in the form provided below.

From Eq. (14), it can be easily shown that

\[ \delta_y^2 \Delta U = \frac{\Delta y^2}{k \theta} [(I - k \epsilon \theta J) \Delta U - \Delta U^*], \] (17)

which substituted into the \( L_x \) operator of the corrector step yields

\[ L_x(\Delta U^{*k}) = k \ \text{RHS} + \frac{k \theta}{\Delta x^2} \delta_y^2 (\Delta U^{k-1} - \Delta U^{*\prime(k-1)}) \]
\[ + k^2 \theta^2 \left( \frac{\delta}{\Delta y^2} \Delta \delta_x^2 I + \delta \epsilon J^2 \right) \Delta U^{k-1}, \] (18)

which only contains the finite difference operators \( \delta_x^2 \) and \( \delta_y^2 \), i.e., it employs five grid points.

The corrector step must be solved as many times as necessary until the following convergence criterion is satisfied

\[ \| \Delta U^{*k} - \Delta U^{*\prime(k-1)} \| \leq \epsilon_c, \] (19)

where \( \epsilon_c \) is a user-specified convergence tolerance.

3.2. Convergence of the predictor-corrector technique

In order to analyze the convergence of the iterative predictor-corrector method presented in the previous subsection, it is convenient to define

\[ \rho^k = \Delta U - \Delta U^k, \quad \delta^k = \Delta U^* - \Delta U^{*k}, \] (20)

so that substraction of Eqs. (16b) and (18), respectively, from Eqs. (14) and (13), respectively, yields

\[ L_y(\rho^k) = \delta^k, \] (21)
\[ L_x(\delta^k) = \frac{k \theta}{\Delta x^2} \delta_y^2 (\rho^{k-1} - \delta^{k-1}) + k^2 \theta^2 \left( \frac{\delta}{\Delta y^2} J \delta_x^2 I + \delta \epsilon J^2 \right) \rho^{k-1}, \] (22)

which can be combined to obtain the following expression:

\[ L_x[L_y(\rho^k)] = k^2 \theta^2 \left( \frac{\delta}{\Delta y^2} J \delta_x^2 I + \delta \epsilon J^2 + \frac{1}{\Delta x^2 \Delta y^2} \delta_x^2 \delta_y^2 I + \frac{\epsilon}{\Delta x^2} J \right) \rho^{k-1}, \] (23)

where \( J \) has been assumed to be constant.
Substitution of
\[ \rho_{ij}^k = \phi^k \exp(I(k_x x_i + k_y y_j)), \] (24)
where \( I^2 = -1 \), and \( k_x \) and \( k_y \) are the wave numbers in the \( x \)- and \( y \)-directions, respectively, in Eq. (23) yields the following equation:
\[ R\phi^k = S\phi^{k-1}, \] (25)
where
\[ R = R_x R_y, \] (26)
\[ R_x = \left(1 + 4 \frac{k\theta}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2}\right) I - k\theta \delta J, \] (27)
\[ R_y = \left(1 + 4 \frac{k\theta}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2}\right) I - k\theta \epsilon J, \] (28)
\[ S = k^2 \theta^2 \left(- \frac{\delta}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2} J + \delta \epsilon J^2 \right. \]
\[ + \frac{16}{\Delta x^2 \Delta y^2} \sin^2 \frac{k_x \Delta x}{2} \sin^2 \frac{k_y \Delta y}{2} I - 4 \frac{\epsilon}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} J \bigg). \] (29)

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

### 3.3. Linear stability of the factorization method

In order to analyze the linear or Fourier-von Neumann stability of the factorization method presented in Section 3.2, it will be assumed that \( T = 0 \) and \( F \) is linear in \( U \) so that \( J \) is a constant matrix. Then, substitution of
\[ U_{ij}^n = \psi^n \exp(I(k_x x_i + k_y y_j)), \] (30)
into Eq. (9) yields
\[ G\psi^n = H\psi^{n-1}, \] (31)
where
\[ G = \left(1 + 4 \frac{k\theta}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} + 4 \frac{k\theta}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2}\right) I - k\theta J, \] (32)
\[ H = \left(1 - 4 \frac{k(1 - \theta)}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} - 4 \frac{k(1 - \theta)}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2}\right) I + k(1 - \theta) J, \] (33)
which is the same expression which could have been obtained from the linear stability analysis of Eq. (5).

A necessary condition for linear stability is that the norm of the amplification matrix, \( G^{-1}H \), be less than unity. The factorization methods presented in this section are here referred to as F-FLM.
4. Approximate factorization of linearized, implicit $\theta$-methods

4.1. Approximately factorized, fully linearized, implicit $\theta$-methods

In Section 3, it was shown that the factorization of fully linearized $\theta$-methods requires an iterative technique due to the approximate factorization errors. Approximate factorization techniques use Eqs. (13) and (14) without the EAF 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 following equations:

$$L_x^F(\Delta U^*) = \left( I - \frac{kR}{\Delta x^2} \frac{\delta^2}{\delta x^2} I - k\delta\theta J \right) \Delta U^* = k \text{ RHS}, \quad (34)$$

$$L_y^F(\Delta U) = \left( I - \frac{kR}{\Delta y^2} \frac{\delta^2}{\delta y^2} I - k\epsilon\theta J \right) \Delta U = \Delta U^*, \quad (35)$$

where

$$L_x^F[L_y^F(\Delta U)] = k \text{ RHS} + E_{AF}, \quad (36)$$

and the approximate factorization errors of approximately factorized, fully linearized $\theta$-methods are $O(k^2)$ (cf. Eq. (12)). These methods are here referred to as AF-FLM and yield systems of block-tridiagonal matrices which may be written at interior points as, for example,

$$A_{i,j}\Delta U_{i-1,j} + B_{i,j}\Delta U_{i,j} + C_{i,j}\Delta U_{i+1,j} = Q_{i,j}, \quad (37)$$

for the $L_x$ operator, where $A$ and $C$ are diagonal matrices whose elements are $-k\theta/\Delta x^2$, whereas $B = 2(k\theta/\Delta x^2)I - k\delta\theta J$ may be a dense matrix. This implies that the solution of Eq. (37) by means of the method of Thomas or block-tridiagonal matrix algorithm requires the inversion of $B$ and this may be very expensive if the number of equations is large or if $J$ is a dense matrix. Such an expense may be reduced substantially if the Jacobian matrix is approximated by means of diagonal or triangular matrices as indicated in Sections 4.2 and 4.3.

The linear stability of approximately factorized, fully linearized, implicit $\theta$-methods is governed by Eq. (31) with

$$G = \left( \frac{1 + 4k\theta}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} I - k\delta\theta J \right) \times \left( \frac{1 + 4k\theta}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2} I - k\epsilon\theta J \right), \quad (38)$$

$$H = G + kJ - \left( 4 \frac{k}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} + 4 \frac{k}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2} \right) I. \quad (39)$$
Eqs. (34) and (35) clearly indicate that, for a second-order accurate discretization of the spatial derivatives, there is a two-parameter family of approximately-factorized, fully-linearized, implicit θ-methods which depend on θ (0 < θ ≤ 1) and δ (0 ≤ δ ≤ 1).

4.2. Approximately factorized, diagonally linearized, implicit θ-methods

The Jacobian matrix, J, may be written as $J = L + D + M$ where D is a diagonal matrix, and L and M are strictly lower and upper, respectively, triangular matrices. If J is approximated by D in Eqs. (34) and (35), the following system results:

$$L_x^D(ΔU^*) = \left( I - \frac{kθ}{Δx^2} \delta_x^2I - kδθD \right) ΔU^* = k \text{ RHS}, \quad (40)$$

$$L_y^D(ΔU) = \left( I - \frac{kθ}{Δy^2} \delta_y^2I - kεθD \right) ΔU = ΔU^*, \quad (41)$$

and the resulting method is here referred to as AF-DLM. The approximation of the Jacobian matrix by a diagonal one results in $O(k)$ approximate factorization errors since

$$L_x^D[L_y^D(ΔU)] = k \text{ RHS} + E^D_{AF}, \quad (42)$$

where

$$E^D_{AF} = kθ(L + M)ΔU + k^2θ^2 \left( \frac{1}{Δx^2Δy^2} \delta_x^2\delta_y^2I + ε \frac{δ_x^2D + δ_y^2D}{Δy^2} + δεD^2 \right) ΔU. \quad (43)$$

The linear stability of approximately factorized, diagonally linearized, implicit θ-methods is governed by Eq. (31) with

$$G = \left( 1 + 4 \frac{kθ}{Δx^2} \sin \frac{k_xΔx}{2} \right) I - kθδD \left( 1 + 4 \frac{kθ}{Δy^2} \sin \frac{k_yΔy}{2} \right) I - kεD$$

$$H = G + kJ - \left( 4 \frac{k}{Δx^2} \sin \frac{k_xΔx}{2} + 4 \frac{k}{Δy^2} \sin \frac{k_yΔy}{2} \right) I. \quad (44)$$

In Eqs. (40) and (41), the dependent variables are uncoupled at each time step and may be easily determined by means of the method of Thomas or tridiagonal matrix algorithm.
4.3. Approximately factorized, triangularly linearized, implicit \( \theta \)-methods

If the Jacobian matrix, \( J \), is approximated by \( N = L + D, B \) in Eq. (37) is a lower triangular matrix which may be easily inverted by forward substitution, and Eqs. (34) and (35) may be written as

\[
L_x^T(\Delta U^*) = \left( I - \frac{k\theta}{\Delta x^2} \delta_x^2 I - k \delta \theta N \right) \Delta U^* = k \text{ RHS},
\]

\[

L_y^T(\Delta U) = \left( I - \frac{k\theta}{\Delta y^2} \delta_y^2 I - k \epsilon \theta N \right) \Delta U = \Delta U^*,
\]

whose approximate factorization errors are \( O(k) \) since

\[
L_x^T[L_y^T(\Delta U)] = k \text{ RHS} + E_{AF}^T,
\]

where

\[
E_{AF}^T = k \theta M \Delta U + k^2 \theta^2 \left( \frac{1}{\Delta x^2 \Delta y^2} \delta_x^2 \delta_y^2 I + \frac{\epsilon}{\Delta x^2} \delta_x^2 N + \frac{\delta}{\Delta y^2} N \delta_y^2 I + \delta \epsilon N^2 \right) \Delta U.
\]

Furthermore, since for a system of \( N \) equations, these can be arranged in \( N! \) manners, there are \( N! \) approximately factorized, triangularly linearized, implicit \( \theta \)-methods which are here referred to as AF-TLM.

The linear stability of approximately factorized, triangularly linearized, implicit \( \theta \)-methods is governed by Eq. (31) with

\[
G = \left( 1 + 4 \frac{k\theta}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} \right) I - k \theta \delta N
\]

\[
\times \left( 1 + 4 \frac{k\theta}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2} \right) I - k \theta \epsilon N,
\]

\[
H = G + kJ - \left( 4 \frac{k}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} + 4 \frac{k}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2} \right) I.
\]

Since \( N \) is a lower triangular matrix, the dependent variables in Eqs. (46) and (47) are sequentially coupled, i.e., the \( k \)th component of \( \Delta U, \Delta U_k \), depends only on \( \Delta U_m, m = 1, 2, \ldots, k - 1 \), and may be easily solved by means of the method of Thomas or tridiagonal matrix algorithm.

4.4. Other approximately factorized, fully linearized, implicit \( \theta \)-methods

It is clear from Section 4.1 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 [3]. Furthermore, the fully linearized methods of Section 4.1 may require the inversion of dense matrices, although their approximate factorization errors are second-order accurate in time, whereas the techniques of Sections 4.2 and 4.3 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, implicit $\theta$-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

$$L_x^N(\Delta U^*) = \left(I - \frac{k\theta}{\Delta x^2} \delta_x^2 I - k\theta(L + \mu D)\right)\Delta U^* = k \text{ RHS},$$  

(52)

$$L_y^N(\Delta U) = \left(I - \frac{k\theta}{\Delta y^2} \delta_y^2 I - k\theta(M + v D)\right)\Delta U = \Delta U^*,$$  

(53)

where $\mu + v = 1$, is here referred to as AF-NFLM and results in a matrix $B$ (cf. Eq. (37)) which is lower and upper, respectively, triangular for the $L_x$ and $L_y$, respectively, operators.

Note that

$$L_x^N[L_y^N(\Delta U)] = k \text{ RHS} + E_{\text{AF}},$$  

(54)

where

$$E_{\text{AF}} = k^2\theta^2 \left(\frac{1}{\Delta x^2 \Delta y^2} \delta_x^2 \delta_y^2 I + \frac{1}{\Delta x^2} \delta_x^2 (M + v D) + \frac{1}{\Delta y^2} (L + \mu D) \delta_y^2 I + \delta(L + \mu D)(M + v D)\right)\Delta U.$$  

(55)

The linear stability of the approximately factorized, linearized, implicit $\theta$-methods presented in this subsection is governed by Eq. (31) with

$$G = \left(1 + 4 \frac{k\theta}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} \right) I - k\theta \delta(L + \mu D)$$  

$$\times \left(1 + 4 \frac{k\theta}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2} \right) I - k\theta \epsilon(M + v D),$$  

(56)

$$H = G + kJ - \left(4 \frac{k}{\Delta x^2} \sin^2 \frac{k_x \Delta x}{2} + 4 \frac{k}{\Delta y^2} \sin^2 \frac{k_y \Delta y}{2} \right) I.$$  

(57)

Since $L + \mu D$ in Eq. (52) and $M + v D$ in Eq. (53) 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.
5. 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

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

subject to

$$\begin{align*}
u(x,y,0) &= 1, & v(x,y,0) &= \exp(-\lambda(x^2 + y^2)), \\
u(x,20,t) &= 1, & v(x,20,t) &= 0, \\
u(20,y,t) &= 1, & v(20,y,t) &= 0, \\
\frac{\partial u}{\partial x}(0,y,t) &= \frac{\partial v}{\partial x}(0,y,t) = \frac{\partial u}{\partial y}(x,0,t) = \frac{\partial v}{\partial y}(x,0,t) = 0,
\end{align*}$$

where $K = 0.5$ and $\lambda = 1$.

Fig. 1. $u$ (top left), $v$ (top right), and errors in $u$ (bottom left) and $v$ (bottom right) at $t = 0$. (The top figures were obtained with AF-FLM, $k = 0.04$, $\theta = 0.5$ and $\delta = 0$. The bottom figures correspond to the difference between the results of AF-FLM and F-FLM, $k = 0.04$, $\theta = 0.5$ and $\delta = 0$.)
Fig. 2. $u$ (top left), $v$ (top right), and errors in $u$ (bottom left) and $v$ (bottom right) at $t = 6$. (The top figures were obtained with AF-FLM, $k = 0.04$, $\theta = 0.5$ and $\delta = 0$. The bottom figures correspond to the difference between the results of AF-FLM and F-FLM, $k = 0.04$, $\theta = 0.5$ and $\delta = 0$.)

Fig. 3. $u$ (top left), $v$ (top right), and errors in $u$ (bottom left) and $v$ (bottom right) at $t = 10$. (The top figures were obtained with AF-FLM, $k = 0.04$, $\theta = 0.5$ and $\delta = 0$. The bottom figures correspond to the difference between the results of AF-FLM and F-FLM, $k = 0.04$, $\theta = 0.5$ and $\delta = 0$.)
Fig. 4. $u$ (top left), $v$ (top right), and errors in $u$ (bottom left) and $v$ (bottom right) at $t = 16$. (The top figures were obtained with AF-FLM, $k = 0.04, \theta = 0.5$ and $\delta = 0$. The bottom figures correspond to the difference between the results of AF-FLM and F-FLM, $k = 0.04, \theta = 0.5$ and $\delta = 0$.)

Fig. 5. $u$ (top left), $v$ (top right), and errors in $u$ (bottom left) and $v$ (bottom right) at $t = 20$. (The top figures were obtained with AF-FLM, $k = 0.04, \theta = 0.5$ and $\delta = 0$. The bottom figures correspond to the difference between the results of AF-FLM and F-FLM, $k = 0.04, \theta = 0.5$ and $\delta = 0$.)
These equations were solved with $k = 0.04$ and $\Delta x = \Delta y = 0.4$, and the convergence of the factorization method presented in Section 3 was established when $\epsilon_c = 10^{-12}$ in Eq. (19) with the $L_2$-norm. For this convergence criterion, F-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. 1–13.

The top graphs in Figs. 1–5 show the spatial distributions of $u$ and $v$ at selected times obtained by means of AF-FLM. Initially, i.e., at $t = 0$, $u = 1$, while $v$ exhibits a spike of unit amplitude at $x = y = 0$ (Fig. 1). 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. 2 which corresponds to $t = 6$.

Fig. 3 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 Figs. 4 and 5.

The bottom graphs in Figs. 1–5 show the difference between the results obtained with F-FLM and AF-FLM, i.e., they show the approximate factorization

![Graphs showing spatial distributions of u and v at selected times](image)

Fig. 6. Errors in $u$ (left) and $v$ (right) at $t = 10$. (The top figures correspond to the difference between the results of AF-FLM with $\delta = 1$ and AF-FLM with $\delta = 0.5, k = 0.04$ and $\theta = 0.5$. The bottom figures correspond to the difference between the results of AF-FLM with $\delta = 0$ and AF-FLM with $\delta = 0.5, k = 0.04$ and $\theta = 0.5$.)
Fig. 7. Errors in u (left) and v (right) at $t = 20$. (The top figures correspond to the difference between the results of AF-FLM with $\delta = 1$ and AF-FLM with $\delta = 0.5, k = 0.04$ and $\theta = 0.5$. The bottom figures correspond to the difference between the results of AF-FLM with $\delta = 0$ and AF-FLM with $\delta = 0.5, k = 0.04$ and $\theta = 0.5$.)

Fig. 8. Errors in u (left) and v (right) at $t = 10$. (The top figures correspond to the difference between the results of AF-NFLM with $\mu = 1$ and AF-FLM with $\delta = 0.5, k = 0.04$ and $\theta = 0.5$. The bottom figures correspond to the difference between the results of AF-NFLM with $\mu = 0$ and AF-FLM with $\delta = 0.5, k = 0.04$ and $\theta = 0.5$.)
errors $E_{AF}$, at selected times. These errors are initially zero as indicated in Fig. 1, and exhibit the same trends as, but have opposite sign to, the spatial distributions of $u$ and $v$. The largest errors in $u$ are 0.002 and occur $x = y = 0$ at $t = 2, 4, 6$ and 8, and at the inflection points of $u$ at $t = 10$. For $t \geq 10$, the largest errors in $u$ are still positive and equal to 0.0015, and occur at the inflection points of $u$.

The errors in $v$ 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, using the results presented in Figs. 1–5, it may be stated that the relative approximate factorization errors in $u$ and $v$ are at most 0.002 and are positive for $u$ and negative for $v$.

The effects of the allocation of the reaction terms in AF-FLM to the one-dimensional operators in the $x$- and $y$- directions are presented in Figs. 6 and 7 at $t = 10$ and 20, respectively. The cases $\delta = 0$ and 1 correspond to the allocation of the reaction or source terms to the $y$- and $x$-operators, respectively, whereas, the case $\delta = 0.5$ allocates the source term in equal proportion to these operators (cf. Eqs. (34) and (35)). The results presented in Figs. 6 and 7 clearly illustrate that the errors corresponding to $\delta = 1$ are of the same magnitude as

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Fig. 9. Errors in $u$ (left) and $v$ (right) at $t = 20$. (The top figures correspond to the difference between the results of AF-NFLM with $\mu = 1$ and AF-FLM with $\delta = 0.5, k = 0.04$ and $\theta = 0.5$. The bottom figures correspond to the difference between the results of AF-NFLM with $\mu = 0$ and AF-NFLM with $\delta = 0.5, k = 0.04$ and $\theta = 0.5$.)
and opposite sign to those corresponding to \( \delta = 0 \); furthermore, these errors are at most 0.001 and 0.0003 in \( u \) and \( v \), respectively, at \( t = 10 \), and 0.001 and 0.0004, respectively, at \( t = 20 \). Moreover, the total approximate factorization errors of AF-FLM with \( \delta = 0 \) and 1 at \( t = 10 \) and 20 may be easily obtained from Figs. 3 and 6 and Figs. 5 and 7, respectively.

The effects of the allocation of the reaction terms in AF-NFLM to the one-dimensional operators in the \( x \)- and \( y \)-directions are presented in Figs. 8 and 9 at \( t = 10 \) and 20, respectively. The cases \( \mu = 0 \) and 1 correspond to the allocation of the reaction or source terms to the \( y \)- and \( x \)-operators, respectively (cf. Eqs. (52) and (53)). These figures indicate that the errors in \( v \) resemble those presented in Figs. 6 and 7, except that the magnitude of the errors in the former is larger than that of the latter; the errors in \( u \) and \( v \) exhibit the same shape for \( \mu = 0 \) and 1; and, the errors in \( u \) show an annular peak before reaching a relative minimum at \( t = 10 \). Moreover, the largest errors in \( u \) and \( v \) at \( x = y = t = 10 \) are about 0.001 and 0.0006, respectively, for \( \mu = 1 \), and 0.002 and 0.001, respectively, for \( \mu = 0 \).

The errors of AF-NFLM are lower for \( \mu = 0.5 \) than, although exhibit similar shapes to, those corresponding to \( \mu = 0 \) and 1 as indicated in the top graphs of Figs. 10 and 11. For example, the largest errors in \( u \) and \( v \) at \( t = 10 \) for \( \mu = 0.5 \)

![Fig. 10. Errors in \( u \) (left) and \( v \) (right) at \( t = 10 \). (The top figures correspond to the difference between the results of AF-NFLM with \( \mu = 0.5 \) and AF-FLM with \( \delta = 0.5, k = 0.04 \) and \( \theta = 0.5 \). The bottom figures correspond to the difference between the results of AF-DLM and AF-FLM with \( \delta = 0.5, k = 0.04 \) and \( \theta = 0.5 \).)
are about 0.001 and 0.0003, respectively, and 0.001 and 0.0004, respectively, at 
$t = 20$.

The bottom graphs of Figs. 10 and 11 illustrate the errors in $u$ and $v$ corresponding to AF-DLM; these errors are larger than those corresponding to AF-NFLM with $\mu = 0.5$. Furthermore, the annular peak observed in these figures before the relative minimum in $u$ is of larger amplitude for AF-DLM than that for AF-NFLM at $t = 10$.

The errors of the approximately factorized, triangularly linearized $\theta$-methods are illustrated in Figs. 12 and 13 when the equations are solved in the sequences $u \rightarrow v$ and $v \rightarrow u$. At $t = 10$, the results presented in Figs. 12 and 13 indicate 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. 6–13 and others not shown here clearly indicate that AF-FLM with $\delta = 0.5$ is more accurate than AF-FLM with $\delta = 0$.
or 1; the accuracy of AF-FLM with $\delta = 0.5$ is comparable to that of AF-NFLM with $\mu = 0.5$ and AF-TLM in the sequence $v \rightarrow u$ with $\delta = 0.5$; AF-NFLM with $\mu = 0.5$ is more accurate than AF-NFLM with $\mu = 1$ which, in turn, is more accurate 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 $\delta = 0$. 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.

6. Conclusions

An iterative, predictor-corrector technique has been developed to eliminate the second-order approximate factorization errors which result from the factorization of 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,
Fig. 13. Errors in u (left) and v (right) at t = 20. (The top figures correspond to the difference between the results of AF-TLM in the sequence u → v and AF-FLM with δ = 0.5, k = 0.04 and θ = 0.5. The bottom figures correspond to the difference between the results of AF-TLM in the sequence v → u and AF-FLM with δ = 0.5, k = 0.04 and θ = 0.5.)

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 wavenumbers in the x- and y-directions.

Four approximately factorized, implicit, noniterative, linearized θ-methods, i.e., techniques which do not account for the approximate factorization errors, have been developed and their linear stability has been analyzed. 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, linearized θ-methods whose
approximate factorization errors are only first-order accurate in time, and, although they are much more efficient than fully linearized 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, linearized θ-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, θ-method which requires the inversion of the full Jacobian matrix and to that of approximately factorized, implicit, triangularly linearized θ-techniques, and higher than that of approximately factorized, implicit, diagonally linearized θ-schemes.

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