Linearization Methods for Reaction-Diffusion Equations: 1-D Problems

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ABSTRACT

Three types of linearized finite difference methods are presented. The first type is based on a \( \theta \)-formulation which provides discrete solutions in both space and time. It is shown that this type is a linearly-implicit Rosenbrock's or a \( W \)-method depending on whether the full or an appropriate Jacobian is employed. The second one requires the solution of two-point, linear, ordinary differential equations and provides either piecewise continuous or piecewise differentiable solutions in space and discrete in time. The third type is based on the discretization of the spatial coordinate and provides a system of linear, ordinary differential equations in time which can be integrated analytically. Therefore, the third type of linearized finite difference methods provides continuous solutions in time and discrete in space, and may be transformed into one of the first type by discretizing the time variable. © Elsevier Science Inc., 1997

1. INTRODUCTION

The numerical solution of nonlinear, ordinary differential equations by means of implicit methods requires the solution of nonlinear algebraic equations. This may be a serious drawback since it adds to the problem of stability that of convergence of the iterative process. In 1962–1963, Rosenbrock [1] developed a large class of methods which try to avoid nonlinear systems and replace them by a sequence of linear ones. These methods are
frequently referred to as linearly-implicit Runge-Kutta techniques, although they are also called semi-implicit, generalized, modified, adaptive or additive Runge-Kutta methods [2]. A derivation of Rosenbrock's methods starting from a diagonally-implicit Runge-Kutta technique, together with an analysis of their stability, is given in Hairer and Wanner [2].

Linearly-implicit techniques employ the full Jacobian and, since this matrix has to be evaluated at each time step, they are computationally costly. For this reason, Steihaug and Wolfbrandt [3] developed a family of linearly-implicit techniques which use an approximate Jacobian and which assure classical order. The resulting methods are referred to as W-techniques.

Recently, Ramos and García-López [4] developed a family of linearly-implicit θ-methods for nonautonomous, nonlinear, ordinary differential equations which are based on the linearization of the nonlinear terms with respect to the previous time step. They also introduced fully-, triangularly- and diagonally-linearized θ-methods which employ the full, the lower triangular part or the diagonal of the Jacobian matrix. As a consequence, the fully-linearized methods require the inversion of the full Jacobian at each time step, while no such inversion is needed for triangularly- and diagonally-linearized θ-techniques. In fact, the dependent variables at each time step are uncoupled and may be calculated explicitly in diagonally-linearized θ-techniques. On the other hand, the dependent variables are sequentially coupled in triangularly-linearized θ-techniques, and may be determined explicitly in a sequential manner.

Rosenbrock's, W- and linearized θ-methods may also be used to solve nonlinear, partial differential equations which can be transformed into ordinary differential ones by discretizing the spatial coordinates while keeping the time variable continuous. The resulting technique is referred to as a method of lines [5].

Block-tridiagonal, linearized-implicit methods based on the linearization of θ-techniques have also been developed for nonlinear, partial differential equations both in standard [6, 7] and delta [8, 9] formulations. In both formulations, the time variable is discretized by means of a θ-method; the resulting equations are then time-linearized; and, finally, the spatial coordinates are discretized. In the standard formulation, the dependent variables are determined at each time step, whereas, in the delta formulation, one determines the difference between the values of the dependent variables at two subsequent time steps. Both formulations provide discrete solutions in both space and time; therefore, interpolation of the discrete values is required to obtain approximate continuous solutions.

The objective of this paper is three-fold. First, implicit, linearized θ-methods for one-dimensional, reaction-diffusion equations are presented in
Section 2 where it is proved that these methods are either Rosenbrock's [1, 2] or \( \mathcal{W} \)-techniques [2, 3] depending on whether the full or an approximate Jacobian is employed to determine the discrete values of the dependent variables at each time step. The approximate Jacobian employed in \( \mathcal{W} \)-techniques is either the lower triangular part or the diagonal part of the full Jacobian. The methods presented in Section 2 provide discrete solutions in both space and time and result in block-tridiagonal matrices at each time level.

Second, linear implicit methods based on the discretization of the time variable are presented in Section 3. These methods result in systems of linear, non-constant coefficients, ordinary differential equations for the values of the dependent variables at each time step, and the solutions of the piecewise spatial linearization of these equations provide either piecewise continuous or piecewise differentiable solutions in space depending on the interval where the spatial linearization is performed. Moreover, the values of the nodal amplitudes are the solutions of linear systems of algebraic equations governed by tridiagonal matrices. Therefore, these linearized methods of lines provide continuous solutions in space which are discrete in time. Furthermore, depending on the linearization, these methods of lines use either the full or an approximate Jacobian.

Finally, linearized methods of lines in time are developed by first discretizing the spatial coordinate while keeping continuous the time variable, and the resulting ordinary differential equations are linearized with respect to the previous time level in order to obtain linear, ordinary differential equations which have analytical solutions in time. Therefore, the linearized methods presented in Section 4 provide continuous solutions in time which are discrete in space. Furthermore, if the time variable in methods of lines in time is discretized, these methods result in the linearized \( \theta \)-techniques presented in Section 2.

2. LINEARIZED \( \theta \)-METHODS

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

\[
 u_t = u_{xx} + f(u), \quad t \geq 0, \quad 0 \leq x \leq L, \tag{1}
\]

where the subscripts denote partial differentiation, \( u \in \mathbb{R}^N \), and \( f(u) \in \mathbb{R}^N \) is a nonlinear function of \( u \).
Due to the nonlinearity, (1) cannot be integrated analytically and numerical methods must be used to obtain approximate solutions. If a $\theta$-method is employed to discretize the time derivative, (1) may be written as

\[
\Delta = k\theta \Delta_{xx} + ku^n_{xx} + k\theta f(u^{n+1}) + k(1 - \theta) f(u^n),
\]

(2)

where $k$ is the time step, $u^n = u(t^n, x)$, $\Delta = u^{n+1} - u^n$, and $0 < \theta \leq 1$. The values $\theta = 1$ and $\frac{1}{2}$ correspond to the implicit and Crank-Nicolson methods, respectively, which are $O(k)$ and $O(k^2)$ accurate in time, respectively.

Equation (2) corresponds to a method of lines in space because the time has been discretized while the $x$-coordinate has been kept continuous, and is a nonlinear, ordinary differential equation which cannot, in general, be integrated analytically. However, if the nonlinear terms are linearized with respect to $u^n$, (2) is transformed into the following linear equation

\[
\Delta = k\theta \Delta_{xx} + ku^n_{xx} + kf(u^n) + k\theta J(u^n) \Delta,
\]

(3)

where $J(u^n) = \frac{\partial f}{\partial u}(u^n)$ is a Jacobian matrix which is a function of $x$ for $t^n < t < t^{n+1}$; therefore, (3) is a linear, ordinary differential equation with variable coefficients whose solution may not, in general, be obtained in a simple manner. However, if the spatial-derivatives are discretized, (3) can be transformed into a system of linear algebraic equations which can be readily solved. For example, if a second-order accurate discretization of the spatial derivatives is used in an equally-spaced grid, (3) can be written as

\[
-\frac{\theta}{h^2} \Delta_{i-1} + \left(\frac{1}{k} + \frac{2\theta}{h^2} - \theta J^n_i\right) \Delta_i - \frac{\theta}{h^2} \Delta_{i+1} = \frac{1}{h^2} \delta^2 u^n_i + f(u^n_i),
\]

(4)

where, for example, $u^n_i = u(t^n, x_i)$, $h$ is the constant step size, and

\[
\delta^2 u_i = u_{i+1} - 2u_i + u_{i-1}.
\]

(5)

Equation (4) corresponds to a block-tridiagonal matrix where each block is an $N \times N$ square matrix. In this equation, all the dependent variables are coupled through the Jacobian matrix $J$, and is here referred to as a fully-linearized method because the full Jacobian matrix is used. However, if this matrix is approximated by its lower triangular part, i.e., $L_{ij} = J_{ij}$ for $i \geq j$ or by its diagonal, i.e., $D_{kk} = J_{kk}$, then the dependent variables are
coupled in a sequential manner or uncoupled, respectively, and the resulting methods are referred to as triangularly- and diagonally-linearized techniques, respectively. In the case that \( J \) is approximated by \( D \), (4) reduces to \( N \) tridiagonal matrices for each component of \( u \) which can be easily and speedily solved by means of the method of Thomas or the tridiagonal matrix algorithm. This diagonal approximation to \( J \) uncouples the dependent variables at each time step. On the other hand, when \( J \) is approximated by its lower triangular part, the dependent variables are coupled in a sequential manner, and the method of Thomas can also be used to solve for each component of \( u \).

**Remark 1.** If the spatial derivatives in (2) are discretized by means of, for example, a fourth-order accurate, compact finite difference expression [10, 11], i.e.,

\[
    u_{xx}(t, x_i) \approx \frac{\delta^2 u_i}{h^2 \left(1 + \frac{\delta^2}{12}\right)}, \tag{6}
\]

the \( \theta \)-method for (2) can be expressed as

\[
    \left( \frac{1}{12} - \frac{k\theta}{h^2} \right) \Delta_{i-1} + \left( \frac{10}{12} + \frac{2k\theta}{h^2} \right) \Delta_i + \left( \frac{1}{12} - \frac{k\theta}{h^2} \right) \Delta_{i+1} = \frac{k}{h^2} \delta^2 u_i^n + \frac{k\theta}{12} \left( f(u_{i-1}^{n+1}) + 10f(u_i^{n+1}) + f(u_{i+1}^{n+1}) \right) + \frac{k(1 - \theta)}{12} \left( f(u_{i-1}^n) + 10f(u_i^n) + f(u_{i+1}^n) \right), \tag{7}
\]

while the linearized \( \theta \)-method corresponding to (7) is

\[
    \left( \frac{1}{12} - \frac{k\theta}{12} J_{i-1}^n - \frac{k\theta}{h^2} \right) \Delta_{i-1} + \left( \frac{10}{12} - \frac{10}{12} k\theta J_i^n + \frac{2\theta}{h^2} \right) \Delta_i + \left( \frac{1}{12} - \frac{k\theta}{12} J_{i+1}^n - \frac{k\theta}{h^2} \right) \Delta_{i+1} = \frac{k}{h^2} \delta^2 u_i^n + \frac{k}{12} \left( f(u_{i-1}^n) + 10f(u_i^n) + f(u_{i+1}^n) \right), \tag{8}
\]
which also corresponds to a block tridiagonal matrix since it only involves three grid points.

**Remark 2.** The linearized \( \theta \)-methods presented in this section provide a discrete approximation in both space and time to the solution of (1); therefore, in order to obtain approximate continuous solutions, interpolation in space and time has to be used.

**Remark 3.** Although only equally-spaced grids have been employed, second-order accurate discretizations of the spatial derivatives in unequally-spaced grids which involve only three grid points may be easily obtained. Furthermore, if \( f = f(t, x, u) \), then the term \( k^2 \theta f_i(t^n, x, u^n) \) must be added to the right-hand sides of (2) and (3), while \( k \theta f_i(t^n, x, u^n) \) must be added to the right-hand side of (4).

**Remark 4.** The linearized \( \theta \)-methods presented in this section can also be used with fractional steps or operator-splitting schemes [12–14] where the reaction-diffusion operator is replaced by a sequence of reaction and diffusion ones. As an illustration, let us assume that (1) is replaced by

\[
\begin{align*}
u_t &= u_{xx} = L_D(u), \\
u_t &= f(u) = L_R(u),
\end{align*}
\]

(9)

and

\[
u^{n+1} = L_R^M \left[ L_D^K \left[ L_R^M (u^n) \right] \right],
\]

(10)

where the subscripts \( D \) and \( R \) denote diffusion and reaction, respectively, and \( M \) and \( K \) denote the number of times that the reaction and diffusion, respectively, operators are solved; for example, \( K = 1 \) indicates that the diffusion operator is only solved once, while \( M \) is the natural number closest to one half of the ratio between the characteristic diffusion and reaction times.

Both the reaction and the diffusion operators can be discretized as in (4) where \( J = 0 \) and \( f(u) = 0 \) for the diffusion operator, whereas the reaction one can be expressed as

\[
\left( \frac{1}{k} - \theta J_i^n \right) \Delta_i = f(u_i^n).
\]

(11)
The Jacobian matrix $J$ may be, in general, dense and the determination of $\Delta_i$ may be costly. However, if $J$ is approximated by a diagonal or a lower triangular matrix, there is no need to invert the matrix on the left side of (11), because $\Delta_i$ may be calculated explicitly or in a sequential manner as a function of $\Delta_i$ for $i = 1, 2, \ldots, i - 1$, by forward substitution.

The fully-linearized $\theta$-methods presented in this section and, in particular, (11) are linearly implicit techniques which are, in fact, Rosenbrock's methods as shown in the next theorem.

**Theorem 1.** Fully-linearized $\theta$-methods are Rosenbrock's techniques.

**Proof.** Consider the following nonlinear, nonautonomous, ordinary differential equation

$$u_t = f(t, u), \quad (12)$$

whose discretization by means of a linearly implicit, $s$-stages, one-step method may be written as

$$u^{n+1} = u^n + k \sum_{i=1}^{s} b_i U_{ni}^n, \quad (13)$$

where

$$U_{ni} = u^n + k \sum_{j=1}^{i-1} \alpha_{ij} U_{nj}^n, \quad (14)$$

$$U_{ni}^n = f(t^n + \alpha_i k, U_{ni}) - k J^n \sum_{j=1}^{i} \gamma_{ij} U_{nj}^n - k \gamma_i g^n, \quad (15)$$

$$\alpha_i = \sum_{j=1}^{i-1} \alpha_{ij}, \quad \gamma_i = \sum_{j=1}^{i} \gamma_{ij}. \quad (16)$$

Rosenbrock's methods correspond to

$$J^n = -f_u(t^n, u^n), \quad g^n = -f_i(t^n, u^n), \quad (17)$$
for which, (15) becomes

\[
(I + kJ^n \gamma_{ii}) U_n^r = G_n^r,
\]

where

\[
G_n^r = f(t^n + \alpha_i k, U_{ni}) - hJ^n \sum_{j=1}^{i-1} \gamma_{ij} U_{nj}^r - h\gamma_i g^n,
\]

only depends on the previous steps and \( I \) is the \( N \times N \) unit matrix.

Equations (13) and (18) imply that

\[
\sum_{i=1}^{s} b_i (I + kJ^n \gamma_{ii})^{-1} G_n^r.
\]

A fully-linearized \( \theta \)-method applied to (12) yields

\[
u^{n+1} = u^n + k(I + k\theta J^n)^{-1}(f(t^n, u^n) - \theta kg^n).
\]

Equation (21) coincides with (20) if \( s = 1, \gamma_{ii} = \theta, \alpha_i = 0, \alpha_{ij} = 0, \) and \( \gamma_{ij} = 0 \) for \( j = 1, 2, \ldots, i - 1 \). Therefore, linearized \( \theta \)-methods are Rosenbrock’s techniques [1, 2, 15].

**THEOREM 2.** *Diagonally- and triangularly-linearized \( \theta \)-methods are W-techniques.*

**PROOF.** \( W \)-methods are linearly implicit techniques in which \( J^n \) is approximated by a simpler matrix. Therefore, \( W \)-methods may be easily obtained from Rosenbrock’s techniques by approximating \( J \) in (20) by a simpler matrix [2, 3, 15].

The diagonally- and triangularly-linearized \( \theta \)-techniques presented in this paper when applied to (12) can be written as

\[
u^{n+1} = u^n + k(I + k\theta Q^n)^{-1}(f(t^n, u^n) - \theta kg^n),
\]

where \( Q = D = diag(J), \ Q = L = trian(J) \) and \( diag \) and \( trian \) indicate the diagonal and lower triangular, respectively, parts of the Jacobian.
matrix. Therefore, these matrices are approximations to $J^n$, and (22) correspond to a $W$-method since this equation corresponds to the approximation of $J$ by simpler matrices in (21) which is a Rosenbrock’s method.

The following two corollaries are consequences of Theorems 1 and 2, and the stability and error analysis derived by Lubich and Ostermann [15].

**Corollary 1.** The stability of one-stage Rosenbrock’s methods implies the stability of fully-linearized $\theta$-techniques.

**Corollary 2.** The stability of one-stage $W$-methods implies the stability of diagonally- and triangularly-linearized $\theta$-techniques.

3. LINEARIZED METHODS OF LINES IN SPACE

The methods of lines in space developed in this section are all based on (3) and allow to obtain approximate solutions which are either piecewise continuous or piecewise differentiable in space as shown in the next subsections.

3.1. Piecewise Continuous Solutions

Equation (3) cannot be, in general, solved analytically because the Jacobian matrix which appears in that equation is a function of $x$; however, if this equation is employed in the interval $[x_{i-1}, x_{i+1}]$ and linearized about $x_i$, one obtains a system of linear, constant-coefficients, ordinary differential equations which may be solved analytically. For the sake of conciseness, here we assume that $N = 1$, and write the linearization of (3) about $x_i$ as

$$\Delta_{xx} + \lambda_i^2 \Delta = G(x_i),$$

where

$$\lambda_i^2 = J_i^n - \frac{1}{k\theta},$$

$$G(x) = -\frac{1}{\theta}(u_{xx}^n + f(u^n)).$$

(23)

(24)

(25)
In the local coordinate \( z = x - x_i \) with \( x \in [x_i, x_{i+1}] \), the solution of (23) is, for \( \lambda^2 > 0 \),

\[
\Delta = A_i \sin(\lambda_i z) + B_i \cos(\lambda_i z) + \frac{G_i}{\lambda_i^2},
\]

(26)

where \( A_i \) and \( B_i \) are integration constants which can be determined from the conditions

\[
\Delta(z = -h_{i-1}) = \Delta_{i-1}, \quad \Delta(z = h_i) = \Delta_{i+1},
\]

(27)

which together with the condition

\[
\Delta(z = 0) = \Delta_i,
\]

(28)

yield

\[
A_i = \frac{1}{\sin \lambda_i(h_i + h_{i-1})} \left( \Delta_{i+1} \cos \lambda_i h_{i-1} - \Delta_{i-1} \cos \lambda_i h_i - \frac{G_i}{\lambda_i^2} (\cos \lambda_i h_{i-1} - \cos \lambda_i h_i) \right),
\]

(29)

\[
B_i = \Delta_i - \frac{G_i}{\lambda_i^2},
\]

(30)

\[
-\Delta_{i-1} \sin \lambda_i h_i + \Delta_i \sin \lambda_i(h_i + h_{i-1}) - \Delta_{i+1} \sin \lambda_i h_{i-1}
\]

\[
= \frac{G_i}{\lambda_i^2} (\sin \lambda_i(h_i + h_{i-1}) - \sin \lambda_i h_i - \sin \lambda_i h_{i-1}),
\]

(31)

\( h_i = x_{i+1} - x_i \) and \( G_i = G(x_i) \).

Equation (31) is a linear finite difference formula which provides the values of \( \Delta_i \). These values can then be substituted into (26) to obtain \( \Delta = u^{n+1} - u^n \) in each interval \([ x_{i-1}, x_{i+1} ]\). Therefore, the piecewise continuous methods presented here provide a tridiagonal matrix for the determination of \( \Delta_i \), and an approximate continuous solution for \( 0 \leq x \leq L \). Furthermore, within each interval \([ x_{i-1}, x_{i+1} ]\), the method provides analytical solutions which are not differentiable at \( x_{i-1} \) and \( x_{i+1} \). Differentiable
solutions based on piecewise linearization are obtained in the next subsections.

The cases \( \lambda_i^2 \leq 0 \) can be analyzed analogously.

### 3.2. Piecewise Differentiable Solutions: Left Expansions

If (3) is linearized with respect to the left end point of the interval \( I_i = [x_i, x_{i+1}] \) with \( 0 \leq x_i \leq L \) for \( N = 1 \), the solution of the resulting linearized equation can be written as (26) where

\[ \Delta(z = h_i) = \Delta_{i+1}, \quad \Delta(z = 0) = \Delta_i, \]  

which yield

\[ A = \frac{1}{\sin \lambda_i h_i} \left( \Delta_{i+1} - \Delta_i \cos \lambda_i h_i + \frac{G_i}{\lambda_i^2} (\cos \lambda_i h_i - 1) \right), \]  

\[ B = \Delta_i - \frac{G_i}{\lambda_i^2}. \]  

Continuity of the first-order derivative of \( \Delta \) with respect to \( x \) for the solutions in \( I_i \) and \( I_{i-1} \) at \( x_i \) implies that

\[ \frac{\lambda_{i-1}}{\sin \lambda_{i-1} h_{i-1}} \Delta_{i-1} - \left( \frac{\lambda_{i-1}}{\tan \lambda_{i-1} h_{i-1}} + \frac{\lambda_i}{\tan \lambda_i h_i} \right) \Delta_i + \frac{\lambda_i}{\sin \lambda_i h_i} \Delta_{i+1} \]

\[ = \frac{G_{i-1}}{\lambda_{i-1} \sin \lambda_{i-1} h_{i-1}} (1 - \cos \lambda_{i-1} h_{i-1}) + \frac{G_i}{\lambda_i \sin \lambda_i h_i} (1 - \cos \lambda_i h_i), \]  

which, for \( |\lambda_i h_i| \ll 1 \), reduces to

\[ \frac{\Delta_{i-1}}{h_{i-1}} - \left( \frac{1}{h_{i-1}} + \frac{1}{h_i} \right) \Delta_i + \frac{1}{h_i} \Delta_{i+1} = \frac{G_{i-1} h_{i-1} + G_i h_i}{2}. \]  

Equation (35) is a linear finite difference formula which provides the values of \( \Delta_i \). These values can then be substituted into (26) to obtain \( \Delta = u^{n+1} - u^n \) in each interval \([ x_i, x_{i+1} ]\). Therefore, the piecewise differentiable methods presented here provide a tridiagonal matrix for the determi-
nation of $\Delta$, and an approximate piecewise differentiable solution for $0 \leq x \leq L$. Furthermore, within each interval $[x_i, x_{i+1}]$, the method provides analytical solutions which are not $C^2$ at $x_i$.

The cases $\lambda^2 \leq 0$ can be analyzed analogously.

3.3. Piecewise Differentiable Solutions: Right Expansions

If (3) is linearized with respect to the right end point of the interval $I_i = [x_i, x_{i+1}]$ with $0 \leq x_i \leq L$, it becomes

$$
\Delta_{xx} + \lambda^2_{i+1} \Delta = G(x_{i+1}),
$$

whose solution can be written as

$$
\Delta = A_i \sin(\lambda_{i+1} z) + B_i \cos(\lambda_{i+1} z) + \frac{G_{i+1}}{\lambda^2_{i+1}},
$$

where

$$
\Delta(z = h_i) = \Delta_{i+1}, \quad \Delta(z = 0) = \Delta_i,
$$

which yield

$$
A_i = \frac{1}{\sin \lambda_{i+1} h_i} \left( \Delta_{i+1} - \Delta_i \cos \lambda_{i+1} h_i + \frac{G_{i+1}}{\lambda^2_{i+1}} (\cos \lambda_{i+1} h_i - 1) \right),
$$

$$
B_i = \Delta_i - \frac{G_{i+1}}{\lambda^2_{i+1}}.
$$

Continuity of the first-order derivative of $\Delta$ with respect to $x$ for the solutions in $I_i$ and $I_{i-1}$ at $x_i$ implies that

$$
\frac{\lambda_i}{\sin \lambda_i h_{i-1}} \Delta_{i-1} - \left( \frac{\lambda_i}{\tan \lambda_i h_{i-1}} + \frac{\lambda_{i+1}}{\tan \lambda_{i+1} h_i} \right) \Delta_i + \frac{\lambda_{i+1}}{\sin \lambda_{i+1} h_i} \Delta_{i+1}
$$

$$
= \frac{G_i}{\lambda_i \sin \lambda_i h_{i-1}} (1 - \cos \lambda_i h_{i-1}) + \frac{G_{i+1}}{\lambda_{i+1} \sin \lambda_{i+1} h_i} (1 - \cos \lambda_{i+1} h_i),
$$

(42)
which, for $|\lambda_i h_i| \ll 1$, reduces to

$$
\frac{\Delta_{i-1}}{h_{i-1}} - \left( \frac{1}{h_{i-1}} + \frac{1}{h_i} \right) \Delta_i + \frac{1}{h_i} \Delta_{i+1} = \frac{G_i h_{i-1} + G_{i+1} h_i}{2}.
$$

Equation (43) is a linear finite difference formula which provides the values of $\Delta_i$. These values can then be substituted into (38) to obtain $\Delta = u^{n+1} - u^n$ in each interval $[x_i, x_{i+1}]$. Therefore, the piecewise differentiable methods presented here provide a tridiagonal matrix for the determination of $\Delta_i$, and an approximate piecewise differentiable solution for $0 \leq x \leq L$. Furthermore, within each interval $[x_i, x_{i+1}]$, the method provides analytical solutions which are not $C^2$ at $x_i$.

The cases $\lambda_i^2 < 0$ can be analyzed analogously.

### 3.4. Piecewise Differentiable Solutions: Composite Expansions

Approximate, piecewise differentiable solutions can also be obtained by combining those corresponding to the left and right expansions. These solutions require, however, the solution of two tridiagonal systems of difference equations, i.e., (35) and (42), and are more costly than those associated with the left and right expansions.

**Remark 5.** Approximate analytical solutions can also be obtained if $J$ in (3) is linearized while $f(u^n)$ is not. In this case the solution to the partial linearization of (3) may be determined by means of the method of variation of parameters and involves a nonhomogeneous term which is an integral of $f(u^n)$ that, in general, may not be integrated analytically.

**Remark 6.** The methods of lines presented in this section provide piecewise continuous or piecewise differentiable solutions in space at each time level. Continuous solutions in time may be obtained by interpolating the solutions in space at different times.

**Remark 7.** When $N > 1$, $\lambda_i^2$ in (23) is an $N \times N$ matrix and $\Delta$ and $G(x_i)$ are $N \times 1$ column vectors which will be referred to as $\Lambda_i$, $\Delta$ and $G(x_i)$, respectively, where

$$
\Lambda_i = J_i^n - \frac{1}{k \theta} I,
$$

and $I$ is the $N \times N$ identity matrix.
In this case, (23) may be written as the following system of $2N$, first-order, ordinary differential equations

$$\frac{dQ}{dx} = B + F,$$

where $F = (0, G)^T$, $Q = (\Delta, P)^T$, the superscript denotes transpose, and

$$B = \begin{bmatrix} 0 & I \\ -\Lambda & 0 \end{bmatrix}.$$

Equation (45) can be integrated analytically in each interval $I_i$ subject to appropriate continuity conditions at the ends of the interval. Since analytical solutions to equations similar to (45) are presented in the next section, they will be omitted here. Approximate solutions to (45) can be obtained if $J$ is approximated by a diagonal or lower triangular matrix because these approximations imply that $\Lambda_i$ is diagonal or lower triangular, respectively. If $\Lambda_i$ is approximated by a diagonal matrix, the components of $\Delta$ are uncoupled in each interval and can be solved independently of each other as indicated in the previous subsections; however, if $\Lambda_i$ is approximated by a lower triangular matrix, the components of $\Delta$ are coupled sequentially in each interval and the $i$-th component depends on the solutions of the $j = 1, 2, \ldots, i - 1$ components; therefore, it can be solved as indicated in the previous subsections with a nonhomogeneous term which depends on the solutions of the $j = 1, 2, \ldots, i - 1$ components.

REMARK 8. The methods of lines presented in this section may also be used when (1) is solved by means of operator-splitting techniques. In this case, however, the diffusion operator is a linear one and its solution may be determined analytically; therefore, there is no need to obtain approximate solutions by splitting the $0 \leq x \leq L$ interval into subintervals. The reaction operator may be solved, after the time variable is discretized, by means of iterative techniques or the fully-, diagonally- and triangularly-linearized $\theta$-methods presented in Section 2.

4. LINEARIZED METHODS OF LINES IN TIME

If the space coordinate in (1) is discretized by means of, for example, a second-order accurate formula in an equally-spaced grid, the following
system of nonlinearly coupled differential equations is obtained

\[
\frac{dU}{dt} + AU = F, \quad (46)
\]

where \( U = (u_2, u_3, \ldots, u_{NP-1})^T \), \( u_i = u(t, x_i) \), the superscript \( T \) denotes transpose, \( NP \) is the number of grid points, and \( A \) is a tridiagonal matrix which comes from the discretization of the spatial derivatives in (1). In (46), it has been assumed that Dirichlet boundary conditions are imposed at \( x = 0 \) and \( x = L \), so that \( u_1 \) and \( u_{NP} \) do not appear in \( U \).

Equation (46) is, in general, nonlinear; therefore, if the time variable is discretized, a system of nonlinear algebraic equations has to be solved iteratively. Alternatively, the linearized \( \theta \)-methods presented in Section 2 may be used to find the solution of the resulting linear system of algebraic equations. In this section, we propose a different method to solve (46) in an analytical, albeit approximate, manner.

If (46) is linearized in the interval \( t^n \leq t \leq t^{n+1} \) with respect to \( t^n \), the resulting linear ordinary differential equation may be written as

\[
\frac{d\Delta}{dt} + B\Delta = G, \quad (47)
\]

\[
\Delta = U - U^n, \quad (48)
\]

\[
B = A - J(U^n), \quad J = \frac{\partial F}{\partial U}, \quad (49)
\]

\[
G = F(U^n) - AU^n. \quad (50)
\]

Equation (47) can be integrated analytically to yield

\[
\Delta = \exp(-Bt) \int_{t^n}^{t} \exp(Bs)G \, ds. \quad (51)
\]

An approximate solution to (51) may be obtained by employing the Taylor series expansion of the matrix exponential, and integrating the resulting series. Therefore, this method provides piecewise analytical solutions in time which are continuous at \( t^n \). However, for Dirichlet boundary conditions at \( x = 0 \) and \( x = L \) and \( NP \) grid points, the dimensions of the matrix \( A \) are \( (N \times (NP - 2)) \times (N \times (NP - 2)) \) which may be very large. Furthermore, although the linearized method of lines presented here yields
approximate continuous solutions in time, it only provides discrete solutions in space. Continuous solutions in space may be found by means of interpolation.

**Remark 9.** If compact operators are employed to discretize the spatial variables, the left side of (46) is premultiplied by a matrix, and the method presented in this section can also be used to obtain the analytical solution of the resulting system of linear, first-order, ordinary differential equations.

**Remark 10.** Approximate solutions to (46) may also be obtained if $B$ is approximated by either a diagonal or lower triangular matrix. In the first case, the components of $\Delta$ are uncoupled and may be solved independently of each other, whereas in the second case, they are coupled sequentially. These approximations may, however, result in inaccurate solutions, because they may not approximate the diffusion terms faithfully.

**Remark 11.** Instead of using the $\Delta$-formulation, one may employ all the methods presented in this paper to determine $u$ by writing the appropriate algebraic or differential equations for the dependent variables rather than $\Delta$.

5. **APPLICATIONS**

Some of the linearized methods developed in this paper have been applied to the following system of one-dimensional, reaction-diffusion equations [16]

\begin{align*}
  u_t &= u_{xx} - uv, & v_t &= v_{xx} + uv - k_1v, \quad (52)
\end{align*}

in $0 \leq x \leq L = 200$, subject to

\begin{align*}
  u(200, t) &= 1, & v(200, t) &= 0, \quad (53)
  \frac{\partial u}{\partial x}(0, t) &= 0, & v(20, t) &= 0, \quad (53)
  \frac{\partial v}{\partial x}(0, t) &= 0, & v(x, 0) &= \exp(-x^2), \quad (54)
\end{align*}

where $k_1 = 0.5$.

The numerical results obtained with the method presented in Section 4 with compact operators for the diffusion terms and an explicit, fourth-order
accurate Runge-Kutta technique for the integration in time are shown in Figure 1 which corresponds to $h = 0.04$ and $k = 0.05$. This figure shows that $u$ is characterized by a front which propagates in time at a constant speed. Ahead of this front, $u = 1$, while behind it $u = 0$. On the other hand, $v$ is a propagating pulse whose initial value rapidly decreases initially and stabilizes later due to diffusion and reaction.

Figures 2–4 illustrate the errors in both $u$ and $v$ as functions of $x$ and $t$ of the partially linearized techniques presented in Section 2 when the spatial derivatives are discretized by means of compact operators. These errors as well as those of Figures 5 and 6 have been obtained by subtracting the numerical solutions from those of a fully-linearized method which employs compact operators in space. Furthermore, $\theta = 0.5$ in Figures 2–6.

Figure 2 indicates that a diagonal approximation to the Jacobian matrix yields errors in $u$ and $v$ whose maximum values are about 0.01 and 0.005, respectively. Furthermore the errors in $v$ have a similar behavior to the $u$ solution. Both the errors in $u$ and $v$ are located at the fronts of these two variables and increase almost linearly in time. Figure 3 corresponds to a lower triangular matrix approximation to the Jacobian matrix and exhibits similar trends to those of Figure 2, but the largest errors in $u$ and $v$ are about 0.004 and 0.001, respectively, i.e., these errors are smaller than those that result when the Jacobian matrix is approximated by a diagonal one.

Figure 4 corresponds to an upper triangular matrix approximation to the Jacobian matrix and exhibits different trends from those illustrated in Figure 2. The largest errors in $u$ and $v$ are about 0.004 and 0.004, respectively, thus indicating that the approximation to the Jacobian matrix plays an important role on the errors.

Figure 5 corresponds to a standard, second-order discretization of the spatial derivatives and full linearization, and shows that the errors of this discretization are larger than those of compact techniques which employ diagonal or triangular approximations to the Jacobian matrix. Figure 5 also shows that the errors increase almost linearly in time and are largest at the fronts.

Figure 6 shows the errors of the method employed in obtaining Figure 1 which is fourth-order accurate in both space and time. Figure 6 clearly indicates that the errors of fully-linearized $\theta$-techniques which employ compact operators in space are about 0.002 and 0.0005 in $u$ and $v$, respectively, with respect to the solution obtained by means of fourth-order accurate techniques in both space and time.

The CPU times on an HP9000/735 workstation required by the fully-, diagonally-, lower triangularly- and upper triangularly-linearized $\theta$-methods which employ compact operators in space were 63.2, 6.3, 10.1 and 5.8 seconds, respectively, whereas those of the fully-linearized $\theta$-method which
Fig. 1. $u$ (top) and $v$ (bottom) as functions of $x$ and $t$ obtained with a fourth-order accurate method in both space and time.
Fig. 2. Errors in $u$ (top) and $v$ (bottom) as functions of $x$ and $t$ obtained with a $\theta$-linearized method which employs compact differences in space and a diagonal approximation to the Jacobian matrix. These errors are measured with respect to a $\theta$-linearized method which employs compact differences in space and the full Jacobian matrix.
Fig. 3. Errors in $u$ (top) and $v$ (bottom) as functions of $x$ and $t$ obtained with a $\theta$-linearized method which employs compact differences in space and a lower triangular approximation to the Jacobian matrix. These errors are measured with respect to a $\theta$-linearized method which employs compact differences in space and the full Jacobian matrix.
Fig. 4. Errors in $u$ (top) and $v$ (bottom) as functions of $x$ and $t$ obtained with a $\theta$-linearized method which employs compact differences in space and an upper triangular approximation to the Jacobian matrix. These errors are measured with respect to a $\theta$-linearized method which employs compact differences in space and the full Jacobian matrix.
FIG. 6. Errors in $u$ (top) and $v$ (bottom) as functions of $x$ and $t$ obtained with a fourth-order accurate method in both space and time. These errors are measured with respect to a $\theta$-linearized method which employs compact differences in space and the full Jacobian matrix.
employs a second-order accurate discretization of the spatial derivatives and that of the $O(k^4, h^4)$ technique were 30.6 and 29.3 seconds, respectively. These CPU times and Figures 1–6 clearly indicate that diagonally-linearized $\theta$-methods are much faster although incur larger errors than other techniques; however, by appropriately reducing the time step, diagonally-linearized $\theta$-methods can yield as accurate results, while requiring less computer time, than more exact methods.

6. CONCLUSIONS

Three different types of linearly implicit methods for one-dimensional, reaction-diffusion equations have been presented. The first two types are based on $\theta$-techniques, while the third one is based on the discretization of the spatial coordinate and the time linearization of the resulting nonlinear system of ordinary differential equations. Such a linearization yields a system of first-order, linear, ordinary differential equations which have analytical solutions. However, if the time variable in the linear system of ordinary differential equations is discretized, then a linearized method of the first type is obtained.

The first type of time linearization involves the discretization of the time coordinate, the linearization of the resulting system of two-point, ordinary differential equations, and the discretization of the spatial coordinate in the latter. As a consequence, a block-tridiagonal matrix for the discrete values of the dependent variables at each time step is obtained. In general, the Jacobian matrix resulting from the linearization is dense and the linearized $\theta$-method is a linear implicit technique. However, if the Jacobian matrix is approximated by either its diagonal or lower triangular parts, then $W$-techniques are obtained. These techniques allow to determine the nodal values explicitly in a direct or sequential manner depending on whether the Jacobian is approximated by its diagonal or lower triangular part, respectively.

The second type of time linearization also employs a $\theta$-formulation and time linearization but the spatial coordinate is kept continuous so that a system of two-point, boundary-value problems for ordinary differential equations results. These equations may be solved in intervals containing three or two grid points. In the first, a spatial linearization is performed with respect to the middle point of the interval and the resulting linear, ordinary differential equations are solved in such an interval subject to continuity conditions at the three points of the interval. Such continuity requirements result in a tridiagonal system of equations for the nodal values, and piecewise continuous solutions in the whole interval. If intervals with
only two grid points are employed, the condition of continuity of the solution and of its first-order derivative at both points also results in a tridiagonal system of equations for the nodal values, and piecewise differentiable solutions in the whole interval. In either case, the solutions in each interval are analytical except at the end points of each interval.

The three types of time linearization methods developed in the paper provide discrete solutions in both space and time, continuous solutions in space and discrete in time, and continuous solutions in time and discrete in space, respectively. Furthermore, the three types of time linearization methods use the available powerful tools for linear operators. For example, the second type of time linearization uses linearization in time and piecewise linearization in space and provides exponential solutions in each interval.

An application to a one-dimensional system of nonlinear reaction-diffusion equations indicates that the accuracy of the linearized techniques presented in this paper increases as the order of the spatial discretization is increased and as the time and spatial step sizes are decreased. The accuracy of linearized \( \theta \)-methods which employ diagonal or triangular approximations to the Jacobian matrix and which provide the discrete solutions in an explicit or sequential, respectively, manner is lower than, while their numerical efficiency is higher than those of fully-linearized techniques.

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