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PDE-W-methods for parabolic problems with mixed derivatives

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Abstract The present work considers the numerical solution of differential equations that are obtained by space discretization (method of lines) of parabolic evolution equations. Main emphasis is put on the presence of mixed derivatives in the elliptic operator. An extension of the alternating-direction-implicit (ADI) approach to this situation is presented. Our stability analysis is based on a scalar test equation that is relevant to the considered class of problems. The novel treatment of mixed derivatives is implemented in 3rd order W-methods. Numerical experiments and comparisons with standard methods show the efficiency of the new approach. An extension of our treatment of mixed derivatives to 3D and higher dimensional problems is outlined at the end of the article.

1 Introduction

This work is concerned with time integrators applied to the space discretization (method of lines) of parabolic partial differential equations with mixed derivatives. We focus on W-methods, which avoid the solution of nonlinear equations and only require an approximate solution of linear systems with matrix $I - \theta\tau W$, where I is the identity, θ is a real parameter, τ the time step size, and W is an approximation to the Jacobian matrix of the ordinary differential equation.

To reduce the work in the solution of the arising linear systems the alternating-direction-implicit (ADI) method has been proposed by Peaceman, Rachford, and Douglas (see [14] and [2]). One only needs to solve a sequence of

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tridiagonal linear systems (one for each space variable). An ADI method for parabolic problems with mixed derivatives has been proposed in [1].

There are a few well-established time integrators for the numerical solution of parabolic problems with mixed derivatives based on ADI techniques. An extension of the Douglas scheme, including stabilizing correction stages, is given in [9]. It is called Hundsdorfer–Verwer (HV) scheme in [11]. With the aim of getting more freedom in the scheme of [1] and thus improving its stability, in't Hout & Welfert [11] propose a modified Craig–Sneyd (MCS) scheme. Convergence has been considered in [9,10] for the HV scheme and in [12] for the MSC scheme. These methods have been developed mainly in view of applications in financial mathematics.

The methods HV and MCS are second order in space and second order in time. Much effort has been made to extend the ADI approach to higher order (in space). Based on the time integrator HV, space discretizations of order 4 (either using five nodes or as a compact scheme) are given in [3] with an application to financial option pricing in [4]. Based on either the MCS or the HV scheme, compact schemes of order 4 (in space) are derived in [7,8]. All these extensions are fourth order in space and second order in time.

The present work is mainly concerned with improving the accuracy of the time integration by targeting an order in time that is higher than two. This can be achieved by considering W-methods ([17], see also [6, Section IV.7]) of classical order at least three. Extending the ADI approach to the solution of the linear system with matrix $I - \theta\tau W$ (where mixed derivatives are present in the elliptic operator) an efficient implementation is possible. In contrast to a von Neumann stability analysis, which requires periodic boundary conditions, our stability analysis is based on a test problem with Dirichlet boundary conditions.

1.1 Class of evolution equations

On a rectangular domain $(x,y) \in [a,b] \times [c,d]$ and for $t \geq 0$ we consider the partial differential equation

$$\partial_t u = A\,\partial^2_{xx} u + B\,\partial^2_{yy} u + 2\,C\,\partial^2_{xy} u + g\big(t, x, y, u, \partial_x u, \partial_y u\big) \qquad (1.1)$$

with suitable boundary conditions and an initial condition at $t = 0$. The coefficients A, B, C may depend on space and time. We assume that pointwise

$$A > 0, \quad B > 0, \quad AB > C^2, \qquad (1.2)$$

so that the leading part represents an elliptic operator. The stability analysis of Section 3 below is carried out for the case of constant coefficients A, B, C, and for vanishing function g.

We apply a space discretization (method of lines or MOL) using finite differences. Let $a = x_0 < x_1 < \cdots < x_{n_x+1} = b$ and $c = y_0 < y_1 < \cdots < y_{n_y+1} = d$ be subdivisions inducing a grid on the rectangular domain $[a,b] \times$

$[c, d]$, and denote by $U_{ij}(t)$ an approximation to the solution $u(t, x_i, y_j)$ of (1.1) at the grid points. Using differentiation matrices D_{xx} and D_{yy} for the second partial derivatives, and D_x, D_y for the first partial derivatives, we obtain an ordinary differential equation

$$\begin{aligned}\dot{U} &= A(I \otimes D_{xx})U + B(D_{yy} \otimes I)U + 2\,C(D_y \otimes D_x)U \\ &\quad + \big(g\big(t, x_i, y_j, U_{ij}, ((I \otimes D_x)U)_{ij}, ((D_y \otimes I)U)_{ij}\big)\big)_{i,j=1,1}^{n_x,n_y} + b(t)\end{aligned} \tag{1.3}$$

for the vector $U(t) = \big(U_{ij}(t)\big)_{i,j=1,1}^{n_x,n_y}$ (in the case of Dirichlet boundary conditions). The vector $b(t)$ contains terms arising from non-homogeneous boundary conditions. For the differential equation (1.3) we use the compact notation

$$\dot{U} = F(t, U). \tag{1.4}$$

Since the differentiation matrices contain divisions by the small quantities $\Delta x_i = x_{i+1} - x_i$ and $\Delta y_j = y_{j+1} - y_j$, the differential equation (1.4) is stiff and suitable time integrators (implicit or linearly implicit) are recommended.

For the study of convergence of the MOL approach, connecting the errors of the space discretization with those of the time integrator, we refer to the standard literature on the numerical treatment of partial differential equations, e.g., the monograph by Hundsdorfer & Verwer [10].

1.2 W-methods

In principle, all time integrators for stiff differential equations are suitable for the numerical solution of (1.4). We focus our interest to W-methods, because they do not require the solution of nonlinear systems, and they permit the use of non-exact approximations for the Jacobian of the vector field. Augmenting (1.4) with $\dot{t} = 1$ we get formally the autonomous differential equation

$$\dot{y} = f(y), \qquad f(y) = \begin{pmatrix} 1 \\ F(t, U) \end{pmatrix} \quad \text{for} \quad y = \begin{pmatrix} t \\ U \end{pmatrix}. \tag{1.5}$$

For its numerical integration we consider s-stage W-methods (originally proposed in [17], see also [6, Section IV.7]). Denoting by τ the time step size, and by y_n, y_{n+1} the numerical approximations to $y(t)$ at t_n and $t_{n+1} = t_n + \tau$, it is defined by

$$\begin{aligned}(I - \theta\tau\widehat{W}_n)k_i &= \tau f\Big(y_n + \sum_{j=1}^{i-1} a_{ij}k_j\Big) + \sum_{j=1}^{i-1} \ell_{ij}k_j, \quad i = 1, 2, \ldots, s, \\ y_{n+1} &= y_n + \sum_{i=1}^{s} b_i k_i.\end{aligned} \tag{1.6}$$

The coefficients of the method are collected in $A = (a_{ij})_{j<i}$, $L = (\ell_{ij})_{j<i}$ and $b = (b_i)_i$, so that the W-method is characterized by (A, L, b, θ).

The matrix $\widehat{W}_n$ is arbitrary, in principle, but it is expected to be a rough approximation to $f'(y_n)$. The construction of methods of order 3 and higher simplifies considerably under the assumption

$$\big(f'(y_n)\widehat{W}_n - \widehat{W}_n f'(y_n)\big)\,\dot{y}(t_n) = \mathcal{O}(\tau), \tag{1.7}$$

which is satisfied if $\widehat{W}_n = f'(y_n) + \mathcal{O}(\tau)$.

In view of an application to discretized parabolic differential equations, W-methods of order 3 and higher have been constructed in [5, 16, 13, 15].

1.3 Splitting of the Jacobian

To get reasonably high accuracy, fine grids have to be considered, so that the dimension of the semi-discretized differential equation (1.3) is very high. Therefore, the solution of the linear system with matrix $I - \theta\tau\widehat{W}_n$ is often the most costly part in the implementation of method (1.6).

We consider the situation, where a splitting of the vector field and of its Jacobian exists,

$$f(y) = \sum_{j=0}^{d} f_j(y), \qquad f'(y) = \sum_{j=0}^{d} f_j'(y), \tag{1.8}$$

such that the solution of the linear systems with matrices $I - \theta\tau f_j'(y_n)$ can be done much more efficiently than with the matrix $I - \theta\tau f'(y_n)$. In this situation it is advantageous to approximate[1]

$$I - \theta\tau f'(y_n) \approx \prod_{j=0}^{d}\Big(I - \theta\tau f_j'(y_n)\Big). \tag{1.9}$$

This is the essence of the alternating-direction-implicit (ADI) approach [14, 2], where each $f_j(y)$ contains the terms in (1.3) that correspond to partial derivatives with respect to only one space variable. The splitting could also be into a stiff and a non-stiff part. In this situation the Jacobian of the non-stiff part is often replaced by the zero matrix.

In the context of W-methods this approach is studied in [18] (see also [10, Section IV.5]). The resulting methods are called AMF-W-methods (approximate matrix factorization W-methods). Such an AMF-W-method is called exact [15], if the matrix $I - \theta\tau\widehat{W}_n$ is equal to the right-hand side of (1.9). This implies that $\widehat{W}_n - f'(y_n) = \mathcal{O}(\tau)$. It is called inexact, if one of the factors in (1.9) is replaced by the identity matrix, so that $\widehat{W}_n - f'(y_n) = \mathcal{O}(\tau)$ is no longer fulfilled.

[1] The notation $\prod_{j=0}^{d} A_j$ is understood to be a multiplication from right to left, i.e., $\prod_{j=0}^{d} A_j = A_d \dots A_1 A_0$.

1.4 Outline of the rest of the paper

Section 2 explains how the presence of mixed derivatives in the elliptic operator can be efficiently combined with the ADI approach for W-methods. The main idea is presented for the autonomous differential equation (1.5). Mixed derivatives are included in an explicit manner combined with a suitable damping. An algorithmic description is given for the general non-autonomous problem (1.4). The resulting W-methods are called PDE-W-methods.

Stability of these schemes is studied in Section 3. We introduce a new scalar test equation, which takes into account the presence of mixed derivatives in the differential equation.

Numerical experiments are presented in Section 4. We observe the numerically achieved stiff order, and we propose a transformation of non-homogeneous Dirichlet boundary conditions to homogeneous ones. This considerably improves the accuracy of the results. We also compare our implementation of W-methods with the classical methods MCS (modified Craig–Sneyd) and HV (Hundsdorfer–Verwer), see [11].

In a final section we show how our techniques can be applied to 3D (or higher dimensional) problems. Numerical experiments give the same good behaviour as for 2D problems.

2 PDE-W-methods

PDE-W-methods are W-methods, where the arising linear system is solved in a way that is adapted to the treatment of parabolic partial differential equations. We start by explaining the ideas for the autonomous equation (1.5), and then we present the algorithmic form for (1.4).

2.1 Solving the linear system by splitting

Motivated by the alternating-direction-implicit approach (ADI) of [14,2] and by the AMF (approximate matrix factorization) implementation of W-methods (see [15]), we assume that the Jacobian $f'(y_n)$ can be split as

$$f'(y_n) = f_0'(y_n) + f_1'(y_n) + f_2'(y_n). \tag{2.1}$$

Here, $f_1'(y_n)$ and $f_2'(y_n)$ correspond to the discretization of the partial derivatives with respect to the first and second space variables, whereas $f_0'(y_n)$ corresponds to those of the mixed derivative (and further terms that may arise). The idea of the AMF approach is to approximate the inverse of the left-hand matrix in (1.6) by

$$\Big(I - \theta\tau f'(y_n)\Big)^{-1} \approx \prod_{j=0}^{2}\Big(I - \theta\tau f_j'(y_n)\Big)^{-1}. \tag{2.2}$$

Since the discretization of the partial derivatives in $f_1'(y_n)$ and $f_2'(y_n)$ are banded matrices (tridiagonal for the standard second order discretization), the solution of linear systems of the form

$$\big(I - \theta\tau f_j'(y_n)\big)k = v, \qquad j = 1, 2$$

can be done very efficiently. This is less evident for $j = 0$ since the discretization of the mixed derivatives in $f_0'(y_n)$ is not a banded matrix (with small band-width). Moreover, $f_0'(y_n)$ has large positive and negative eigenvalues, so that an application of $\big(I - \theta\tau f_0'(y_n)\big)^{-1}$ would imply a step size restriction as for explicit time integrators. This is what we want to avoid. The idea is to approximate

$$\Big(I - \theta\tau f_0'(y_n)\Big)^{-1} \approx \; I + \theta\tau f_0'(y_n) \prod_{j=1}^{2} \big(I - \theta\tau f_j'(y_n)\big)^{-1}. \tag{2.3}$$

This means that we use $\big(I - \theta\tau f_0'(y_n)\big)^{-1} \approx I + \theta\tau f_0'(y_n)$, but before applying the operator $f_0'(y_n)$ we damp the large eigenvalues by applying successively $\big(I - \theta\tau f_1'(y_n)\big)^{-1}$ and $\big(I - \theta\tau f_2'(y_n)\big)^{-1}$. Such a procedure is only justified in the situation, where the eigenvalues of $f_0'(y_n)$ are related to those of $f_1'(y_n)$ and $f_2'(y_n)$.

2.2 W-methods for non-autonomous differential equations

Splitting the vector y_n into (t_n, U_n), the vector k_i into (M_i, K_i), and denoting the non-zero parts of $\widehat{W}_n$ by w_n and W_n, the ith stage of the W-method (1.6) becomes

$$\begin{aligned} &\left(\begin{pmatrix} 1 & 0 \\ 0 & I \end{pmatrix} - \theta\tau \begin{pmatrix} 0 & 0 \\ w_n & W_n \end{pmatrix}\right)\begin{pmatrix} M_i \\ K_i \end{pmatrix} \\ &\quad = \tau \begin{pmatrix} 1 \\ F\big(t_n + \sum_{j=1}^{i-1} a_{ij} M_j, U_n + \sum_{j=1}^{i-1} a_{ij} K_j\big) \end{pmatrix} + \sum_{j=1}^{i-1} \ell_{ij} \begin{pmatrix} M_j \\ K_j \end{pmatrix}, \end{aligned} \tag{2.4}$$

where w_n and W_n are arbitrary, but ideally they should be approximations to $\partial_t F(t_n, U_n)$ and $\partial_U F(t_n, U_n)$, respectively. The upper equation of this relation gives $M_i = \rho_i \tau$, where ρ_i is defined recursively by $\rho_i = 1 + \sum_{j=1}^{i-1} \ell_{ij} \rho_j$. The first argument of F thus becomes $t_n + c_i \tau$ with $c_i = \sum_{j=1}^{i-1} a_{ij} \rho_j$.

With the splitting

$$F(t, U) = F_0(t, U) + F_1(t, U) + F_2(t, U), \tag{2.5}$$

induced by (2.1), we let $a_{n,j} \approx \partial_t F_j(t_n, U_n)$ and $A_{n,j} \approx \partial_U F_j(t_n, U_n)$. The matrix to the left of (2.4) is then defined via the approach of Section 2.1 by

$$\left(\begin{pmatrix} 1 & 0 \\ 0 & I \end{pmatrix} - \theta\tau \begin{pmatrix} 0 & 0 \\ w_n & W_n \end{pmatrix}\right)^{-1} = \prod_{j=0}^{2} \left(\begin{pmatrix} 1 & 0 \\ 0 & I \end{pmatrix} - \theta\tau \begin{pmatrix} 0 & 0 \\ w_{n,j} & W_{n,j} \end{pmatrix}\right)^{-1}$$

where $w_{n,j} = a_{n,j}$ and $W_{n,j} = A_{n,j}$ for $j = 1, 2$, and

$$\begin{aligned}&\left(\begin{pmatrix}1 & 0\\ 0 & I\end{pmatrix} - \theta\tau \begin{pmatrix}0 & 0\\ w_{n,0} & W_{n,0}\end{pmatrix}\right)^{-1}\\ = &\begin{pmatrix}1 & 0\\ 0 & I\end{pmatrix} + \theta\tau \begin{pmatrix}0 & 0\\ a_{n,0} & A_{n,0}\end{pmatrix} \prod_{j=1}^{2}\left(\begin{pmatrix}1 & 0\\ 0 & I\end{pmatrix} - \theta\tau \begin{pmatrix}0 & 0\\ a_{n,j} & A_{n,j}\end{pmatrix}\right)^{-1}.\end{aligned}$$

An algorithmic presentation of the resulting method is given in the following subsection.

2.3 Implementation of PDE-W-methods

We consider the differential equation (1.4) together with the splitting (2.1). With $a_{n,j} = \partial_t F_j(t_n, U_n)$ and $A_{n,j} = \partial_U F_j(t_n, U_n)$, for $j = 0, 1, 2$ (or approximations if the derivatives are not available analytically), the algorithm for the computation of the internal stages (2.4) of the W-method becomes

$$\begin{aligned}K_i^{(-3)} &= \tau F(t_n + c_i\tau, U_n + \textstyle\sum_{j=1}^{i-1} a_{ij}K_j) + \sum_{j=1}^{i-1} \ell_{ij}K_j\\ (I - \theta\tau A_{n,1})K_i^{(-2)} &= K_i^{(-3)} + \theta\rho_i\tau^2 a_{n,1}\\ (I - \theta\tau A_{n,2})K_i^{(-1)} &= K_i^{(-2)} + \theta\rho_i\tau^2 a_{n,2}\\ K_i^{(0)} &= K_i^{(-3)} + \theta\tau A_{n,0}K_i^{(-1)} + \theta\rho_i\tau^2 a_{n,0}\\ (I - \theta\tau A_{n,1})K_i^{(1)} &= K_i^{(0)} + \theta\rho_i\tau^2 a_{n,1}\\ (I - \theta\tau A_{n,2})K_i^{(2)} &= K_i^{(1)} + \theta\rho_i\tau^2 a_{n,2}\\ K_i &= K_i^{(2)}\end{aligned} \tag{2.6}$$

for $i = 1, \ldots, s$. The numerical solution after one step is then given by

$$U_{n+1} = U_n + \sum_{i=1}^{s} b_i K_i.$$

Note that the above algorithm requires only the numerical solution of linear systems with banded (typically tridiagonal) matrices. Since this implementation is adjusted for the solution of evolution equations with dominant elliptic operator, we call the algorithm PDE-W-method.

2.4 Order

For a differential equation (1.5) the W-method becomes a *Rosenbrock method* if $\widehat{W}_n = f'(y_n)$. Conditions on the coefficients $\theta, a_{ij}, \ell_{ij}, b_j$ that guarantee classical order p are well understood. If $\widehat{W}_n$ is not close to $f'(y_n)$ for $\tau \to 0$, then many more order conditions have to be satisfied (see for example [6, Section IV.7]). An intermediate situation is obtained under the assumption

$$\widehat{W}_n - f'(y_n) = \mathcal{O}(\tau), \qquad \tau \to 0. \tag{2.7}$$

Theorem 2.1 *If the relation (2.1) is satisfied up to an error of size $\mathcal{O}(\tau)$, then the PDE-W-method is equivalent to a W-method (1.6) satisfying the relation (2.7).*

Proof The product of the factorization (2.2) can be considered as exact for a modified vector w_n and a modified matrix W_n which are $\mathcal{O}(\tau)$ close to the original ones. □

This result implies that every W-method, which has order p under the assumption (2.7), yields a PDE-W-method of the same order.

3 Stability

For W-methods the study of stability is a nontrivial task. The difficulty is mainly due to the lack of commutativity of the matrices $\widehat{W}_n$ and $f'(y_n)$. Here, we propose a scalar test equation that is relevant for a large class of partial differential equations for which the dominant part is an elliptic operator with constant coefficients.

3.1 Motivation of a test equation

On a rectangular 2-dimensional domain let us consider the PDE

$$\partial_t u = A\,\partial^2_{xx} u + B\,\partial^2_{yy} u + 2\,C\,\partial^2_{xy} u \tag{3.1}$$

with homogeneous Dirichlet boundary conditions. We assume that the coefficients A, B, C are constant and satisfy (1.2), so that the differential operator on the right-hand side is elliptic. A standard second order space discretization of (3.1) yields the ordinary differential equation

$$\dot{U} = A(I \otimes D_{xx})U + B(D_{yy} \otimes I)U + 2\,C(D_y \otimes D_x)U, \tag{3.2}$$

where D_{xx} and D_{yy} are tridiagonal Toeplitz matrices (with possibly different dimension) having entries $(1, -2, 1)/\Delta x^2$ and $(1, -2, 1)/\Delta y^2$, and D_x, D_y are tridiagonal Toeplitz matrices with entries $(-1, 0, 1)/(2\Delta x)$ and $(-1, 0, 1)/(2\Delta y)$, respectively. Unfortunately, the matrices D_{xx} and D_x do not commute[2], so that they cannot be diagonalized simultaneously, however the full Jacobian matrix of the linear system (3.2) is a symmetric matrix. Moreover, the stability of the system (3.2) is guaranteed by the following result.

[2] For the case of periodic boundary conditions these matrices commute and a von Neumann stability analysis is possible; see [11].

Theorem 3.1 *Under the assumption (1.2), the system (3.2) is asymptotically stable.*

Proof The idea is to approximate the matrices D_{xx} and D_{yy} by the squares D_x^2 and D_y^2, and to study the defect. A direct computation yields the relation

$$D_{xx} = D_x^2 - \frac{\Delta x^2}{4} D_{xx}^2 - \frac{1}{2\Delta x^2} \mathrm{Diag}\,(1, 0, \dots, 0, 1),$$

which implies that the logarithmic norm of the defect $D_{xx} - D_x^2$ is negative. For the study of asymptotic stability of (3.2) we can therefore replace D_{xx} and D_{yy} by D_x^2 and D_y^2, respectively. All matrices of the resulting system can be diagonalized simultaneously. Let v be an eigenvector of D_x for the eigenvalue $\mathrm{i}\tilde{\lambda}$, and w an eigenvector of D_y for the eigenvalue $\mathrm{i}\tilde{\mu}$, then $v \otimes w$ is an eigenvector of the matrices $D_x^2 \otimes I$, $I \otimes D_y^2$ and $D_x \otimes D_y$. Written in the basis of eigenvectors, which is orthonormal, the system (3.2) is decoupled into scalar equations of the form

$$\dot{\nu} = -A\tilde{\lambda}^2 \nu - B\tilde{\mu}^2 \nu - 2C\tilde{\lambda}\tilde{\mu}\nu.$$

Assumption (1.2) guarantees the asymptotic stability of this scalar differential equation which, in turn, implies asymptotic stability of (3.2). □

Motivated by the proof of the previous theorem, we consider the scalar test equation

$$\dot{\nu} = -\lambda^2 \nu - \mu^2 \nu - 2c\lambda\mu\nu. \tag{3.3}$$

where we put $\lambda = \tilde{\lambda}\sqrt{A}$, $\mu = \tilde{\mu}\sqrt{B}$ and $c = C/\sqrt{AB}$. Here, $\lambda \in \mathbb{R}$, $\mu \in \mathbb{R}$, and $|c| < 1$ by assumption (1.2).

3.2 PDE-stability

Applying a PDE-W-method (1.6) with step size τ to the test equation (3.3) and considering in (2.6) the natural splitting for the Jacobian corresponding to the mixed derivative, and to the derivatives with respect to x and y, respectively,

$$A_{n,0} = -2c\lambda\mu, \quad A_{n,1} = -\lambda^2, \quad A_{n,2} = -\mu^2, \tag{3.4}$$

we get the recursion $U_{n+1} = R(z_0, z_1, z_2)U_n$, where $R(z_0, z_1, z_2)$ is a rational function of the real variables,

$$z_1 = -\tau\lambda^2, \quad z_2 = -\tau\mu^2, \quad z_0 = -2\tau c\lambda\mu. \tag{3.5}$$

It is given by

$$R(z_0, z_1, z_2) = 1 + zb^T(\Pi\, I_s - L - zA)^{-1}\mathbf{1}, \tag{3.6}$$

where $z = z_0 + z_1 + z_2$ and

$$\Pi^{-1} = (1 - \theta z_2)^{-1}(1 - \theta z_1)^{-1}\Big(1 + \theta z_0 (1 - \theta z_2)^{-1}(1 - \theta z_1)^{-1}\Big), \tag{3.7}$$

and it is called the *stability function* of the method.

It should be noticed that the exact solution of the test equation (3.3) is stable for all $\lambda \in \mathbb{R}$ and $\mu \in \mathbb{R}$, provided that $|c| < 1$, because

$$z = z_0 + z_1 + z_2 \leq 0, \quad z_1 \leq 0, \quad z_2 \leq 0. \tag{3.8}$$

This motivates the following definition.

Definition 3.1 A numerical time integrator which, when applied to the test equation (3.3), yields the recursion $U_{n+1} = R(z_0, z_1, z_2)U_n$ with z_0, z_1, z_2 given by (3.5), is called PDE-stable if

$$|R(z_0, z_1, z_2)| \leq 1 \quad \text{for all} \quad \lambda \in \mathbb{R},\ \mu \in \mathbb{R},\ |c| < 1.$$

Numerical experiments with various W-methods confirm that PDE-stable methods yield stable numerical solutions also for the system (3.2). It is, of course, an interesting question to study whether PDE-stability implies stability for the system (3.2) in any dimension.

3.3 PDE-stability of 1-stage PDE-W-methods

The most simple W-method is given by, (see e.g. [10, p. 398])

$$\big(I - \theta\tau\widehat{W}_n\big)(y_{n+1} - y_n) = \tau f(y_n). \tag{3.9}$$

It is of classical order 1, and for $\theta = 1/2$ it is of order 2 if (2.7) is satisfied. The stability function is

$$R(z_0, z_1, z_2) = 1 + \Pi^{-1} z \tag{3.10}$$

with $z = z_0 + z_1 + z_2$ and Π^{-1} from (3.7).

The stability function (3.10) is identical to that of the modified Craig–Sneyd scheme for the special case $\mu = 0$, $\sigma = \theta$ of the 3-parameter family of methods in [11, Formula (1.11)]. For the important case $\theta = 1/2$, unconditional stability of (3.10) is shown in the article [11]. The following theorem proves unconditional stability for all $\theta \geq 1/2$. The proof is based on the inequality (3.11) which will be an essential ingredient for the stability investigation of W-methods with more than one stage.

Theorem 3.2 *Assume that z_0, z_1, z_2 are given by (3.5). Then, the stability function $R(z_0, z_1, z_2)$ of (3.10) satisfies*

$$|R(z_0, z_1, z_2)| \leq 1 \quad \textit{for all} \quad \lambda \in \mathbb{R},\ \mu \in \mathbb{R},\ |c| < 1,\ \tau > 0,$$

if and only if $\theta \geq 1/2$.

Proof It follows from $|c| < 1$ and (3.5) that

$$|z_0| \leq 2\tau|\lambda||\mu| \leq \tau(\lambda^2 + \mu^2) = |z_1| + |z_2|,$$

so that $z_0 \geq z_1 + z_2$ and $z = z_0 + z_1 + z_2 \leq 0$. We thus have

$$1 + \frac{\theta z_0}{(1-\theta z_1)(1-\theta z_2)} \geq 1 + \frac{\theta(z_1 + z_2)}{(1-\theta z_1)(1-\theta z_2)} = \frac{1+\theta^2 z_1 z_2}{(1-\theta z_1)(1-\theta z_2)} > 0,$$

so that $\Pi > 0$. Together with an application of Lemma 3.1 below (by putting $a_i := -\theta z_i$, $i = 0, 1, 2$ and observing $1 + a_0 + a_1 + a_2 = 1 - \theta z \geq 1$) this implies

$$0 < \frac{1}{\Pi} \leq \frac{1}{1-\theta z}. \tag{3.11}$$

Consequently, from (3.8) we have that $R(z_0, z_1, z_2) = 1 + z/\Pi \leq 1$ and also

$$-1 \leq \frac{1 + (1-\theta)z}{1-\theta z} = 1 + \frac{z}{1-\theta z} \leq R(z_0, z_1, z_2).$$

The inequality to the left follows from $\theta \geq 1/2$. □

Lemma 3.1 *Assume that* $a_0 \in \mathbb{R}$, $a_1 \geq 0$, $a_2 \geq 0$ *satisfy* $1 + a_0 + a_1 + a_2 > 0$. *Then we have*

$$\frac{1}{(1+a_1)(1+a_2)}\left(1 - \frac{a_0}{(1+a_1)(1+a_2)}\right) \leq \frac{1}{1 + a_0 + a_1 + a_2}.$$

Proof A straight-forward computation gives

$$\begin{aligned} &\frac{1}{(1+a_1)(1+a_2)} - \frac{a_0}{(1+a_1)^2(1+a_2)^2} - \frac{1}{1+a_0+a_1+a_2} \\ &= -\frac{(a_0 - \frac{a_1 a_2}{2})^2 + a_1 a_2 + a_1^2 a_2 + a_1 a_2^2 + \frac{3}{4} a_1^2 a_2^2}{(1+a_1)^2(1+a_2)^2(1+a_0+a_1+a_2)} \leq 0 \end{aligned}$$

which proves the statement of the lemma. □

3.4 PDE-stability of 2-stage PDE-W-methods

There is a two-parameter family of 2-stage W-methods of order ≥ 2, see [10, p. 400]. It is straightforward to check that the stability function only depends on the stability parameter θ and that it is given by

$$R(z_0, z_1, z_2) = 1 + \frac{2z}{\Pi} + \frac{z(z-2)}{2\Pi^2} \tag{3.12}$$

with z and Π as in Section 3.2.

Theorem 3.3 *Assume that z_0, z_1, z_2 are given by (3.5). Then, the stability function $R(z_0, z_1, z_2)$ of (3.12) satisfies*

$$|R(z_0, z_1, z_2)| \leq 1 \quad \textit{for all} \quad \lambda \in \mathbb{R},\ \mu \in \mathbb{R},\ |c| < 1,\ \tau > 0,$$

if and only if $\theta \geq 1/4$.

Proof By putting $\mu = 0$ and considering the limit $|\lambda| \to \infty$, we find that $\theta \geq 1/4$ is a necessary condition for stability.

It follows from $z = z_0 + z_1 + z_2 \leq 0$ (see the proof of Theorem 3.2) that

$$R(z_0, z_1, z_2) + 1 = 2 + \frac{2z}{\varPi} + \frac{z(z-2)}{2\varPi^2} = 2\Big(1 + \frac{z}{2\varPi}\Big)^2 - \frac{z}{\varPi^2} \geq 0,$$

so that $R(z_0, z_1, z_2) \geq -1$. From the inequalities (3.11) we get

$$R(z_0, z_1, z_2) = 1 + \frac{z}{\varPi}\Big(2 + \frac{z-2}{2\varPi}\Big) \leq 1 + \frac{z}{\varPi}\Big(2 + \frac{z-2}{2(1-\theta z)}\Big) \leq 1,$$

because the expression in the bracket is positive for $z \leq 0$ and $\theta \geq 1/4$. This proves the statement of the theorem. □

3.5 PDE-stability of 3-stage PDE-W-methods

The family of 3-stage W-methods of order ≥ 3, under the special assumption (1.7), were studied in [15, Theorem 1]. All these methods have the same stability function (depending only on θ), which is given by

$$R(z_0, z_1, z_2) = 1 + \frac{3z}{\varPi} + \frac{3z(z-2)}{2\varPi^2} + \frac{z(z^2 - 6z + 6)}{6\varPi^3} \tag{3.13}$$

with z and $\varPi$ as in Section 3.2. We also recall that there do not exist 3-stage W-methods that are of order 3 without any restriction on W [17].

Theorem 3.4 *Assume that z_0, z_1, z_2 are given by (3.5). Then, the stability function $R(z_0, z_1, z_2)$ of (3.13) satisfies*

$$|R(z_0, z_1, z_2)| \leq 1 \quad \textit{for all} \quad \lambda \in \mathbb{R},\ \mu \in \mathbb{R},\ |c| < 1,\ \tau > 0,$$

if and only if $\theta \geq 1/3$.

Proof a) Assume first that $|\mu| \to \infty$. In this case $z \to -\infty$, but $z/\varPi$ converges to a limit which we denote by $-\alpha$. We have

$$\lim_{|\mu| \to \infty} R(z_0, z_1, z_2) = 1 - 3\alpha + \frac{3}{2}\alpha^2 - \frac{1}{6}\alpha^3, \qquad \alpha = \frac{1}{\theta(1 + \tau\theta\lambda^2)}.$$

The value $\alpha^* = 3$ is maximal such that the modulus of this limit is bounded by 1 for all $\alpha \in [0, \alpha^*]$. This proves the necessity of $\theta \geq 1/3$.

b) By abuse of notation we write $R(z, \Pi) = R(z_0, z_1, z_2)$, and we let

$$R(z,\Pi) - 1 = \frac{z}{6\Pi^3} f(z,\Pi), \quad f(z,\Pi) = 18\Pi^2 + 9\Pi(z-2) + 6 - 6z + z^2,$$

so that also

$$f(z,\Pi) = 18\Big(\Pi + \frac{1}{4}(z-2)\Big)^2 + \frac{1}{8}\Big(12 - 12z - z^2\Big).$$

From (3.11) we have that $\Pi + \frac{1}{4}(z-2) \geq (1-\theta z) + \frac{1}{4}(z-2) = \frac{1}{4}(2 + (1-4\theta)z) \geq 0$ for all $z \leq 0$ and $\theta \geq \frac{1}{3}$. Since $f(z, 1-\theta z)$ is a monotonically increasing function of $\theta \geq 1/3$ we have $f(z,\Pi) \geq f(z, 1+z/3)$ for all $z \leq 0$. It can be checked that the polynomial $f(z, 1+z/3)$ is non-negative for $z \leq 0$. Consequently, we have $f(z,\Pi) \geq 0$ and therefore also $R(z,\Pi) - 1 \leq 0$.

For the proof of $R(z_0, z_1, z_2) \geq -1$ we write

$$R(z,\Pi) + 1 = \frac{1}{6\Pi^3} g(z,\Pi)$$

with

$$\begin{aligned} g(z,\Pi) &= 12\Pi^3 + 18z\Pi^2 + \Pi(9z^2 - 18z) + z(6 - 6z + z^2) \\ &= 12\Big(\Pi + \frac{1}{2}z\Big)^3 - 18z\Pi + z\Big(6 - 6z - \frac{1}{2}z^2\Big). \end{aligned}$$

For $z \leq 0$ this function is monotonically increasing with Π. From (3.11) and $\theta \geq 1/3$ we have $\Pi \geq 1 - \theta z \geq 1 - z/3$, so that $g(z,\Pi) \geq g(z, 1-z/3)$. A straight-forward computation shows that the polynomial $g(z, 1-z/3)$ is non-negative. This completes the proof of the theorem. □

4 Numerical experiments

We consider advection-diffusion-reaction partial differential equations, where mixed derivatives of the solution are present. Our aim is to demonstrate numerically that a stiff order larger than 2 can be achieved by the proposed time integrator.

4.1 Advection-diffusion equation with constant coefficients

We first consider a linear advection-diffusion equation with constant coefficients,

$$\partial_t u = A\,\partial^2_{xx} u + B\,\partial^2_{yy} u + 2C\,\partial^2_{xy} u + D\partial_x u + E\partial_y u + g(t,x,y) \tag{4.1}$$

on the square $(x, y) \in [0, 1] \times [0, 1]$, where $g(t, x, y)$ is selected in such a way that

$$u(t,x,y) = u_e(t,x,y) := x(1-x)y(1-y)\mathrm{e}^t + \kappa\Big(\big(x+\tfrac{1}{3}\big)^2 + \big(y+\tfrac{1}{4}\big)^2\Big)\,\mathrm{e}^t$$

is the exact solution of (4.1). We impose the initial condition $u(0,x,y) = u_e(0,x,y)$ and Dirichlet boundary conditions. If $\kappa = 0$ we have homogeneous boundary conditions, but when $\kappa = 1$ we get non-homogeneous time-dependent Dirichlet conditions. To obtain an elliptic operator we always assume (1.2).

We apply the MOL approach, where D_x, D_y, D_{xx}, D_{yy} are the differentiation matrices corresponding to the first and second order central differences in each spatial direction (as in Section 3.1). The resulting semi-discretized system is

$$\begin{aligned}\dot U &= A(I\otimes D_{xx})U + B(D_{yy}\otimes I)U + 2\,C(D_y\otimes D_x)U\\ &\quad + D(I\otimes D_x)U + E(D_y\otimes I)U + (g(t,x_i,y_j))_{i,j=1,1}^{N,M} + b(t)\end{aligned} \tag{4.2}$$

where $b(t)$ stores the terms due to non-homogeneous boundary conditions. As in (1.4) we write this differential equation as $\dot U = F(t,U)$, and we consider the splitting

$$F(t,U) = F_0(t,U) + F_1(t,U) + F_2(t,U),$$

where $F_1(t,U)$ and $F_2(t,U)$ correspond to the terms originating from discretizations with respect to x and y, respectively, and $F_0(t,U)$ collects the rest including mixed derivatives.

We have deliberately chosen a problem, where the exact solution is a polynomial of degree 2 in x and also in y. In this situation the space discretization is without error, and it is easier to study the error due to the time discretization.

4.2 Time integrators

There exist time integrators (e.g., MCS and HV below) of orders up to 2 that allow for a treatment of mixed derivatives in the elliptic operator. In addition to them we consider two PDE-W-methods.

MCS is a modification of the Craig–Sneyd [1] scheme that is considered in [11, Formula (1.3)]. Parameters are $\sigma = \theta = 1/3$ and $\mu = 1/2 - \theta$.

$$\begin{aligned} Y_0 &= U_n + \tau F(t_n,U_n)\\ Y_j &= Y_{j-1} + \theta\tau\big(F_j(t_{n+1},Y_j) - F_j(t_n,U_n)\big), \quad j=1,2\\ \widehat Y_0 &= Y_0 + \sigma\tau\big(F_0(t_{n+1},Y_2) - F_0(t_n,U_n)\big)\\ \widetilde Y_0 &= \widehat Y_0 + \mu\tau\big(F(t_{n+1},Y_2) - F(t_n,U_n)\big)\\ \widetilde Y_j &= \widetilde Y_{j-1} + \theta\tau\big(F_j(t_{n+1},\widetilde Y_j) - F_j(t_n,U_n)\big), \quad j=1,2\\ U_{n+1} &= \widetilde Y_2.\end{aligned} \tag{4.3}$$

HV is an extension of the Douglas scheme [2] and termed *Hundsdorfer–Verwer* scheme in [11, Formula (1.4)]. Parameters are $\mu = 1/2$ and $\theta = 1/3$.

$$\begin{aligned}
Y_0 &= U_n + \tau F(t_n, U_n) \\
Y_j &= Y_{j-1} + \theta\tau\big(F_j(t_{n+1}, Y_j) - F_j(t_n, U_n)\big), \quad j = 1, 2 \\
\widetilde{Y}_0 &= Y_0 + \mu\tau\big(F(t_{n+1}, Y_2) - F(t_n, U_n)\big) \\
\widetilde{Y}_j &= \widetilde{Y}_{j-1} + \theta\tau\big(F_j(t_{n+1}, \widetilde{Y}_j) - F_j(t_{n+1}, Y_2)\big), \quad j = 1, 2 \\
U_{n+1} &= \widetilde{Y}_2.
\end{aligned} \tag{4.4}$$

WPDE2 is the 2-stage PDE-W-method of Section 2.3 with coefficients taken from the book by Hundsdorfer & Verwer [10, p. 155]

$$A = \begin{pmatrix} 0 & 0 \\ 2/3 & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 \\ -4/3 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 5/4 \\ 3/4 \end{pmatrix}.$$

The stability parameter is $\theta = (3 + \sqrt{3})/6$. This method has only 2 stages, but it is of order 3 if (2.7) is fulfilled.

WPDE3 is the 3-stage PDE-W-method with coefficients of the W3a method [15]. The coefficients of $A = (a_{ij})$, $L = (\ell_{ij})$, and $b = (b_i)$ are given by

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ \frac{4-\sqrt{3}}{4} & \frac{1}{4} & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 & 0 \\ -3 + \sqrt{3} & 0 & 0 \\ -\frac{3}{2} & -\frac{3+\sqrt{3}}{4} & 0 \end{pmatrix} \quad b = \begin{pmatrix} \frac{10-\sqrt{3}}{6} \\ \frac{4+\sqrt{3}}{6} \\ \frac{2}{3} \end{pmatrix}$$

and the stability parameter is chosen as $\theta = 0.435866\ldots$. The method is of classical order 3 under the assumption (1.7).

4.3 Homogeneous Dirichlet boundary conditions

We apply the four time integrators of Section 4.2 to the space-discretized differential equation (4.2). We fix the coefficients as $A = B = 1$, $C = 0.5$, $D = 0.8$, $E = -0.7$, and we assume homogeneous Dirichlet boundary conditions ($\kappa = 0$). The integration interval is $0 \le t \le 1$.

For our first numerical experiment we put $\Delta x_i = 1/(n_x + 1)$ and $\Delta y_i = 1/(n_y+1)$ with $n_x = n_y = 64$, so that the dimension of the ordinary differential equation is $n_x n_y = 4096$. We apply the four time integrators with constant time step $\tau = 2^{-r}$, for $r = 2, 3, \ldots, 16$ with the methods MCS and HV, and for $r = 2, 3, \ldots, 14$ with the two W-methods. In Figure 4.1 we plot the ℓ_2-error for all methods. The left picture shows the error as a function of the cpu-time, and the right picture as a function of the number of calls to a subroutine that solves a tridiagonal linear system. It is equal to four times the number of time steps for the methods MCS and HV, eight times the number of time steps for the 2-stage method WPDE2, and twelve times the number of time steps for the 3-stage method WPDE3. Both pictures are qualitatively identical, which

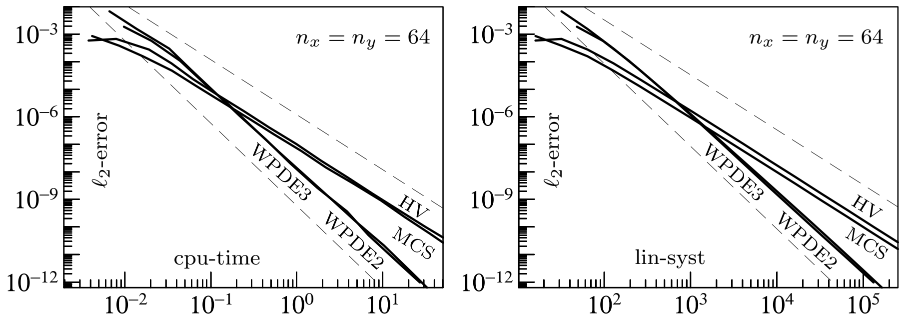

Fig. 4.1 Comparison of four time-integrators applied to the equation (4.2) with parameters $A = B = 1$, $C = 0.5$, $D = 0.8$, $E = -0.7$, and $\kappa = 0$.

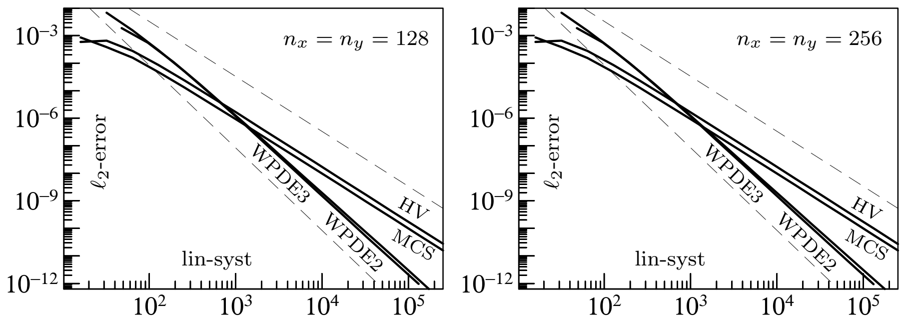

Fig. 4.2 Comparison of four time-integrators with data as in Figure 4.1, but for finer space discretizations, $n_x = n_y = 128$ (left) and $n_x = n_y = 256$ (right).

shows that the number of calls to the linear system solver is a reliable measure for the work.

In the figures we have included thin broken lines of slopes 2 (upper) and 3 (lower). They permit us to guess the numerical convergence order. One sees that the methods MCS and HV show a stiff convergence order that is close to 2. The PDE-W-methods, WPDE2 and WPDE3, show a nearly identical ℓ_2-error. Their convergence order is close to 3.

In our second experiment we study the performance of the methods for finer space discretizations. We repeat the previous experiment, but we choose $n_x = n_y = 128$ and also $n_x = n_y = 256$. The result is shown in Figure 4.2. This time we plot the ℓ_2-errors only as a function of the number of calls to a linear system solver. The pictures for all different choices of the spatial discretization parameter are nearly identical. The only difference is in the cpu-time. Since the cpu-time is dominated by the time for solving the arising linear systems, and these systems are all tridiagonal, the cpu-time depends linearly on the dimension of the ordinary differential equation.

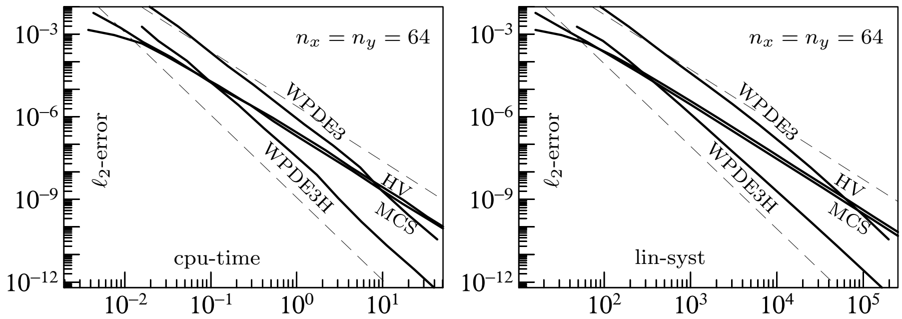

Fig. 4.3 Comparison of time-integrators applied to the equation (4.2) with parameters as in Figure 4.1, but with time-dependent non-homogeneous boundary conditions ($\kappa = 1$).

4.4 Non-homogeneous Dirichlet boundary conditions

It turns out that the PDE-W-methods lose accuracy when they are applied to problems with time-dependent, non-homogeneous Dirichlet boundary conditions (see the method WPDE3 in Figure 4.3). To avoid this drawback, we apply the usual trick and transform the problem to an equivalent one having homogeneous Dirichlet boundary conditions.

WPDE3H is identical to **WPDE3**, but applied to an equivalent problem with homogeneous Dirichlet boundary conditions.

Let us explain the transformation to homogeneous boundary conditions. We use the four cardinal directions to denote the boundary functions: we denote by $u_S(t,x)$ and $u_N(t,x)$ (south and nord) the functions on the bottom and upper sides of the square, and by $u_W(t,y)$ and $u_E(t,y)$ (west and east) those on the left and right sides. The expressions on the four corners are denoted by $u_{SW}(t)$, $u_{SE}(t)$, $u_{NE}(t)$, and $u_{NW}(t)$. We let

$$\widetilde{u}(t,x,y) = xyu_{NE}(t) + x(1-y)u_{SE}(t) + (1-x)yu_{NW}(t) + (1-x)(1-y)u_{SW}(t)$$

be the bilinear interpolation at the four corners, and we define

$$\widehat{u}(t,x,y) = (1-x)u_W(t,y) + xu_E(t,y) + (1-y)u_S(t,x) + yu_N(t,x) - \widetilde{u}(t,x,y).$$

The change of variables $w(t,x,y) = u(t,x,y) - \widehat{u}(t,x,y)$ then transforms the equation (4.1) into a similar one, where only the function $g(t,x,y)$ is changed. To perform this transformation we assume that the first and second derivatives of the boundary functions are analytically available. Discretizing the resulting PDE as above, we get an ordinary differential equation, similar to (4.2), for the transformed variables $W_{ij}(t) = U_{ij}(t) - \widehat{u}(t,x_i,y_j)$. Applying a PDE-W-method to this differential equation yields approximations to $W_{ij}(t_n)$, which in turn gives the desired approximations to $U_{ij}(t_n)$.

Figure 4.3 shows the numerical results for the problem of Section 4.1 with parameter $\kappa = 1$. We compare the PDE-W-method with the methods MCS

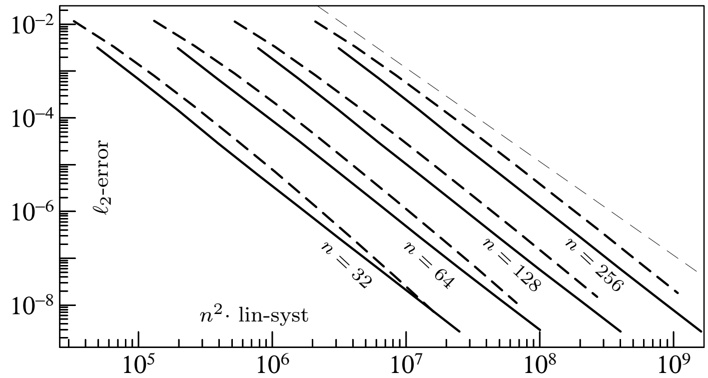

Fig. 4.4 Error at the endpoint of integration of the methods WPDE3 (solid lines) and WPDE2 (broken lines). The thin broken line indicates a slope 2.

and HV, which do not require the transformation to homogeneous boundary conditions. The pictures as a function of the cpu-time (left) and as a function of the required calls to a linear system solver (right) show that the overhead for the above transformation is nearly negligible. Evidently, the good behaviour of Section 4.3 is recovered with the implementation of WPDE3H.

4.5 Diffusion with nonlinear reaction

We consider a diffusion-reaction equation on the square $(x, y) \in [0, 1] \times [0, 1]$,

$$\partial_t u = A\,\partial^2_{xx} u + B\,\partial^2_{yy} u + 2\,C(x, y)\,\partial^2_{xy} u + u^2(1 - u) + \mathrm{e}^t, \tag{4.5}$$

where $A = B = 1$, and $C(x, y) = 0.5\big(1+(x-0.5)(y-0.5)\big)$ is a space-dependent diffusion coefficient. The reaction term is the same as in the experiment of [9], and the term e^t is included to avoid the stationary solution $u = 0$. We assume homogeneous Dirichlet boundary conditions and the initial function $u_0(x, y) = 4x(1 - x)y(1 - y)$ for $t = 0$, which is consistent with the boundary conditions.

We consider the space discretization as in Section 4.3 with $n_x = n_y = n$, and we apply the methods WPDE2 and WPDE3 of Section 4.2 with the splitting as in Section 4.1, where the reaction term is included in $F_0(t, U)$.[3] Figure 4.4 shows the ℓ_2-error (i.e., the difference between the numerical solution and the exact solution of the space-discretized ordinary differential equation) as a function of n^2 times the number of calls to the linear systems solver (which is approximately proportional to the cpu-time of the integration). The reference solution of the ordinary differential equation is obtained numerically by an integration with very small time steps. Both integrators are applied with constant time steps $\tau = 2^{-r}$, $r = 2, \ldots, 11$. We observe from Figure 4.4 that the convergence order is uniform from very large to very small time step sizes,

[3] For a stiff reaction it is recommended to use an additional term in the splitting.

and it is slightly larger than 2. This convergence order is specific for the example (an order close to 3 has been observed in the previous experiments for a linear problem). A study of the convergence order is an interesting question, but it goes beyond the scope of the present article.

5 Extension to higher dimensions

PDE-W-methods, as introduced in Section 2, can be extended with some care to any number m of spatial variables to cope with the time integration of parabolic problems

$$\partial_t u = \sum_{i,j=1}^{m} \alpha_{ij}\, \partial^2_{x_i x_j} u + g(t, x_1, \ldots, x_m, u, \partial_{x_1} u, \ldots, \partial_{x_m} u), \tag{5.1}$$

where $\mathcal{A} = (\alpha_{ij})_{i,j=1}^m$ is symmetric positive definite, so that the second order differential operator on the right-hand side is elliptic. In the present work we restrict our considerations to a rectangular domain $[0,1] \times \ldots \times [0,1]$ and to Dirichlet boundary conditions.

5.1 Space discretization

Standard central second order discretization for the first and second order partial derivatives leads to the ODE system

$$\dot{U} = \mathcal{M}U + G(t, U) + b(t). \tag{5.2}$$

Here, $U(t) \in \mathbb{R}^{n_{x_1} \cdot \ldots \cdot n_{x_m}}$, $\mathcal{M}$ is a symmetric matrix given by

$$\begin{aligned} \mathcal{M} := &\sum_{i=1}^{m} \alpha_{ii} (I \otimes \ldots \otimes D_{x_i x_i} \otimes \ldots \otimes I) \\ &+ 2 \sum_{1 \le i < j \le m} \alpha_{ij} (I \otimes \ldots \otimes D_{x_j} \otimes \ldots \otimes D_{x_i} \otimes \ldots \otimes I), \end{aligned} \tag{5.3}$$

where $D_{x_i x_i}$ and D_{x_i} are in the $(m-i+1)$th position of the tensor product, and D_{x_j} is in the $(m-j+1)$th position. The function $G(t, U)$ corresponds to the spatial discretization of $g(t, x_1, \ldots, x_m, u, \partial_{x_1} u, \ldots, \partial_{x_m} u)$, and the vector $b(t)$ contains the terms arising from Dirichlet boundary conditions. The differentiation matrices $D_{x_i x_i}$ and D_{x_i} are assumed to be tridiagonal with entries $(1, -2, 1)/\Delta x_i^2$ and $(-1, 0, 1)/\Delta x_i$, respectively, and $\Delta x_i = 1/(n_{x_i} + 1)$.

Neglecting the expression $g(\ldots)$ in (5.1) we are concerned with a purely parabolic differential equation. Assuming homogeneous Dirichlet boundary conditions its dicretization is

$$\dot{U} = \mathcal{M}U \tag{5.4}$$

with $\mathcal{M}$ given by (5.3). The stability of (5.4) can be studied as in Theorem 3.1.

Theorem 5.1 *If the coefficient matrix $\mathcal{A} = (\alpha_{ij})_{i,j=1}^m$ in (5.1) is positive definite, then the system (5.4) is asymptotically stable.*

Proof The matrix $\mathcal{M}$ can be decomposed as $\mathcal{M} = \mathcal{M}_0 + \sum_{i=1}^m \mathcal{M}_i$ with

$$\mathcal{M}_i = \alpha_{ii}(I \otimes \ldots \otimes \left(D_{x_i x_i} - D_{x_i}^2\right) \otimes \ldots \otimes I), \qquad i = 1, \ldots, m,$$
$$\mathcal{M}_0 = \sum_{i,j=1}^m \alpha_{ij}(I \otimes \ldots \otimes D_{x_j} \otimes \ldots \otimes D_{x_i} \otimes \ldots \otimes I).$$

As in the proof of Theorem 3.1, the logarithmic norm of the defect $D_{x_i x_i} - D_{x_i}^2$ is negative for $i = 1, \ldots, m$. If we let v_i be an eigenvector of D_{x_i} with eigenvalue $\mathrm{i}\lambda_i$, then $v_m \otimes \ldots \otimes v_1$ is an eigenvector of $\mathcal{M}_0$ corresponding to the eigenvalue

$$\sum_{i,j=1}^m \alpha_{ij}(-\lambda_i \lambda_j) = -(\lambda_m, \ldots, \lambda_1)\mathcal{A}(\lambda_m, \ldots, \lambda_1)^{\mathsf{T}} < 0.$$

This proves the asymptotic stability of the system (5.4). □

5.2 Numerical algorithm

As in Section 2 we write the differential equation (5.2) as $\dot{U} = F(t, U)$ with $F(t, U) = \mathcal{M}U + G(t, U) + b(t)$. We split vector field $F(t, U)$ as

$$F(t, U) = F_0(t, U) + F_1(t, U) + \ldots + F_m(t, U), \tag{5.5}$$

where $F_j(t, U)$ (for $j = 1, \ldots, m$) correspond to the discretization of the partial derivatives with respect to each space variable, whereas $F_0(t, U)$ corresponds to what remains including the mixed derivatives. We let $a_{n,j} = \partial_t F_j(t_n, U_n)$ and $A_{n,j} = \partial_U F_j(t_n, U_n)$. The PDE-W-methods of Section (2.3) allow for a straight-forward extension to the $m-$dimensional PDE problem (5.1) as follows:

$$\begin{aligned}
K_i^{-(m+1)} &= \tau F(t_n + c_i\tau, U_n + \textstyle\sum_{j=1}^{i-1} a_{ij} K_j) + \sum_{j=1}^{i-1} \ell_{ij} K_j \\
(I - \theta\tau A_{n,l}) K_i^{l-(m+1)} &= K_i^{l-(m+2)} + \theta\rho_i\tau^2 a_{n,l}, \qquad l = 1, \ldots, m, \\
K_i^{(0)} &= K_i^{-(m+1)} + \theta\tau A_{n,0} K_i^{(-1)} + \theta\rho_i\tau^2 a_{n,0} \\
(I - \theta\tau A_{n,l}) K_i^{(l)} &= K_i^{(l-1)} + \theta\rho_i\tau^2 a_{n,l}, \qquad l = 1, \ldots, m, \\
K_i &= K_i^{(m)}
\end{aligned} \tag{5.6}$$

for $i = 1, \ldots, s$, and with advancing solution after one step given by

$$U_{n+1} = U_n + \sum_{i=1}^s b_i K_i.$$

5.3 Stability of PDE-W-methods

The stability analysis of Section 5.1 suggests to consider the scalar equation $\dot{u} = -\sum_{i,j=1}^{m} \alpha_{ij}\lambda_i\lambda_j\, u$ for the study of the stability of PDE-W-methods. Substituting $\sqrt{a_{ii}}\lambda_i \to \lambda_i$ this equation becomes

$$\dot{\nu} = -\sum_{i=1}^{m} \lambda_i^2 \nu - 2 \sum_{1\le i<j\le m} c_{i,j}\lambda_i\lambda_j\nu, \tag{5.7}$$

with $c_{i,j} = \alpha_{ij}/\sqrt{\alpha_{ii}\cdot\alpha_{jj}}$ for $1 \le i,j \le m$. Note that with $\mathcal{A} = (\alpha_{ij})_{i,j=1}^{m}$ also the matrix $\mathcal{C} = (c_{i,j})_{i,j=1}^{m}$ is positive definite.

Applying a PDE-W-method to (5.7) with $A_{n,i} = -\lambda_i^2$ for $i = 1,\dots,m$, and $A_{n,0} = -2\sum_{i<j} c_{i,j}\lambda_i\lambda_j$ yields a recursion $U_{n+1} = R(z_0, z_1, \dots, z_m)U_n$, where $R(z_0, z_1, \dots, z_m)$ is a rational function of the real variables

$$z_i = -\tau\lambda_i^2, \quad i = 1,\dots,m, \qquad z_0 = -2\tau \sum_{1\le i<j\le m} c_{i,j}\lambda_i\lambda_j. \tag{5.8}$$

It is given by (3.6), where $z = z_0 + z_1 + \ldots + z_m$, and

$$\Pi := \prod_{j=1}^{m}(1-\theta z_j)\Big(1+\theta z_0\prod_{j=1}^{m}(1-\theta z_j)^{-1}\Big)^{-1}. \tag{5.9}$$

According to Definition 3.1 we have PDE-stability if

$$|R(z_0, z_1, \dots, z_m)| \le 1$$

for all $\lambda_i \in \mathbb{R}$ and for all symmetric matrices $(c_{i,j})_{i,j=1}^{m}$ (with $c_{i,i} = 1$ for all i) that are positive definite. An essential ingredient of such a stability analysis is upper and lower bounds for the AMF factor.

Theorem 5.2 *Let $\lambda_i \in \mathbb{R}$ and assume that $\mathcal{C} = (c_{i,j})_{i,j=1}^{m}$ (with $c_{i,i} = 1$) is positive definite. With z_i of (5.8) and $z = z_0 + z_1 + \ldots + z_m$ the AMF factor Π (with $\theta \ge 0$) given by (5.9) satisfies*

$$\frac{1}{\Pi} \le \frac{1}{1-\theta z}. \tag{5.10}$$

Proof This inequality follows from Lemma 5.1 below by putting $a_i = -\theta z_i$ for $0 \le i \le m$. □

Lemma 5.1 *Assume that $a_0 \in \mathbb{R}$, $a_i \ge 0$, $1 \le i \le m$ $(m \ge 1)$, satisfy $1 + a_0 + \sum_{i=1}^{m} a_i > 0$. Then*

$$\frac{1}{\prod_{i=1}^{m}(1+a_i)}\left(1-\frac{a_0}{\prod_{i=1}^{m}(1+a_i)}\right) \le \frac{1}{1+a_0+\sum_{i=1}^{m} a_i}.$$

Proof Let $P_m := \prod_{i=1}^m (1+a_i) \geq 1$ and $S_m := \sum_{i=1}^m a_i \geq 0$. A direct computation shows that

$$\frac{1}{P_m}\left(1-\frac{a_0}{P_m}\right)-\frac{1}{1+a_0+S_m}$$
$$=\frac{-\left(a_0+\frac{1}{2}(1+S_m-P_m)\right)^2+\frac{1}{4}(1+S_m+P_m)^2-P_m^2}{P_m^2(1+a_0+S_m)}.$$

To prove the non-positivity of this expression, we notice that

$$\frac{1}{4}(1+S_m+P_m)^2-P_m^2=\frac{1}{4}\Big(1+S_m+3P_m\Big)\Big(1+S_m-P_m\Big).$$

The first factor is positive, and the second one is ≤ 0, because

$$P_m=(1+a_1)\cdot\ldots\cdot(1+a_m)=1+a_1+\ldots+a_m+a_1a_2+\ldots\geq 1+S_m.$$

This proves the inequality of the lemma. □

The stability analysis of PDE-W-methods (Section 3) also needs the positivity of Π, which we formulate as an assumption.

Assumption P *The matrix $\mathcal{C}=(c_{i,j})_{i,j=1}^m$ (with $c_{i,i}=1$) satisfies*

$$\prod_{j=1}^m(1+\lambda_j^2)-\sum_{i\neq j}c_{i,j}\lambda_i\lambda_j>0 \qquad \textit{for all } \lambda_i\in\mathbb{R}. \tag{5.11}$$

With the substitution $\lambda_i \to \sqrt{\theta\tau}\lambda_i$, this inequality becomes equivalent to the positivity of the factor Π of (5.9). It would be desirable to have a result that states the validity of Assumption P for all positive definite matrices $\mathcal{C}$. This is true in dimension $m=3$ (Theorem 5.3), but it is not true in general for $m\geq 4$ (Remark 5.1 below).

Theorem 5.3 *Let $\mathcal{C}=(c_{i,j})_{i,j=1}^3$ be positive definite, with $c_{i,i}=1$ for all i. Then, (5.11) holds.*

Proof Since $|c_{i,j}|<\sqrt{c_{i,i}\cdot c_{j,j}}=1$ $(1\leq i,j\leq 3)$, it holds for all $\lambda_j\in\mathbb{R}$ that

$$\prod_{j=1}^3(1+\lambda_j^2)-\sum_{i\neq j}c_{i,j}\lambda_i\lambda_j \geq 1+\sum_{j=1}^3\lambda_j^2+\sum_{i<j}\lambda_i^2\lambda_j^2-\sum_{i\neq j}|\lambda_i||\lambda_j|$$
$$\geq -2+\sum_{j=1}^3\lambda_j^2+\sum_{i<j}(|\lambda_i||\lambda_j|-1)^2.$$

Now, consider $f(x,y,z)=-2+(x^2+y^2+z^2)+(xy-1)^2+(xz-1)^2+(yz-1)^2$ for $x,y,z\geq 0$. It is not difficult to check that the critical points of $f(x,y,z)$ fulfil $x=y=z$. In fact, the minimum value of f is $f(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}})=\frac{1}{4}>0$. This completes the proof. □

Remark 5.1 The previous result for dimension $m=3$ does not extend to higher dimension. Here, we state a sufficient condition and a necessary one.

Sufficient condition. If the matrix $\mathcal{C}$ is such that $2I-\mathcal{C}$ is positive semi-definite, then Assumption P is fulfilled. Expanding the product in (5.11) and neglecting some positive terms shows that Assumption P holds, if

$$\lambda_1^2 + \ldots + \lambda_m^2 - \sum_{i\neq j} c_{i,j}\lambda_i\lambda_j \geq 0. \tag{5.12}$$

Because of $c_{i,i} = 1$ this is equivalent to $2I - \mathcal{C} \geq 0$.

Necessary condition. Assumption P does not hold for general positive definite matrices $\mathcal{C} = (c_{i,j})_{i,j=1}^m$, with $c_{i,i} = 1$ $(1 \leq i \leq m)$ whenever $m \geq 4$. To see this, it is enough to take in (5.11) $\lambda_j = \lambda \geq 0$ $(1 \leq j \leq m)$ and consider

$$f(\lambda) = (1+\lambda^2)^m - \mathcal{K}\lambda^2, \qquad \mathcal{K} = \sum_{i\neq j} c_{i,j}.$$

If $\mathcal{K} \geq m$, the function $f(\lambda)$ attains its minimum at $\lambda^* \geq 0$, where

$$(\lambda^*)^2 = -1 + \Big(\frac{\mathcal{K}}{m}\Big)^{1/(m-1)}.$$

For this value, one has $f(\lambda^*) > 0$ if and only if

$$\mathcal{K} = \sum_{i\neq j} c_{i,j} < m\Big(\frac{m}{m-1}\Big)^{m-1}.$$

This is a necessary condition for Assumption P.

We are now in the position to formulate PDE-stability of W-methods also in dimension $m \geq 3$ under Assumption P.

Theorem 5.4 *Consider parabolic problems (5.1) in any number m of spatial dimensions (mixed derivatives are allowed), i.e. having a positive definite matrix $\mathcal{A}$. Under Assumption P, the PDE-W-methods of 1, 2, and 3 stages with stability functions given by (3.10), (3.12) and (3.13) are PDE-stable for $\theta \geq 1/2$, $\theta \geq 1/4$ and $\theta \geq 1/3$, respectively.*

Proof By taking into account the Assumption P and the bound (5.10), the proof follows the same steps as the proofs of Theorem 3.2 for $s = 1$ stage, of Theorem 3.3 for the case of $s = 2$ stages and of Theorem 3.4 for $s = 3$. □

5.4 Numerical experiment

Extending the example of Section 4.1 we consider the partial differential equation

$$\partial_t u = \sum_{i,j=1}^{3} \alpha_{i,j}\, \partial^2_{x_i x_j} u + \sum_{i=1}^{3} \alpha_i\, \partial_{x_i} u + g(t,x,y,z)$$

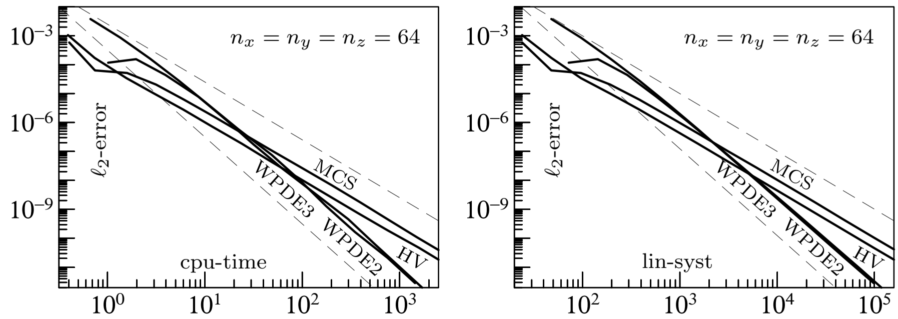

Fig. 5.1 Comparison of four time-integrators applied to the problem of Section 5.4 with coefficients of (5.13).

on the cube $(x, y, z) \in [0, 1] \times [0, 1] \times [0, 1]$, where $g(t, x, y, z)$ is chosen such that

$$u(t, x, y, z) = x(1 - x)y(1 - y)z(1 - z)\mathrm{e}^t$$

is the solution of the differential equation. We arbitrarily fix the coefficients as

$$\begin{gathered} \alpha_{1,1} = \alpha_{2,2} = \alpha_{3,3} = 1, \quad \alpha_{1,2} = 0.5, \quad \alpha_{1,3} = 0.25, \quad \alpha_{2,3} = -0.5, \\ \alpha_1 = 0.8, \quad \alpha_2 = -0.7, \quad \alpha_3 = 0.6 \end{gathered} \tag{5.13}$$

guaranteeing that the second order operator is elliptic. We assume homogeneous Dirichlet boundary conditions.

To this problem we apply PDE-W-methods with the implementation of Section 5.2. For a comparison with standard methods we also apply the MCS method (with parameters as in Section 4.2) and the HV method (again with $\mu = 1/2$ and $\theta = 1/3$). We discretize the cube in such a way that we have in every direction 64 grid points in the interior of $[0, 1]$. Figure 5.1 shows the ℓ_2-error as a function of the cpu-time (left picture) and as a function of the number of calls to the subroutine that solves a linear tridiagonal system (right picture), which equals six times the number of steps for the MCS and HV methods and for each stage of the PDE-W-methods. The results are very similar to those of Figure 4.1.

6 Conclusions

This article considers parabolic partial differential equations, where mixed derivatives are present in the elliptic operator of the problem. Dirichlet boundary conditions are considered and the MOL (method of lines) approach is used for the space discretization. The resulting ordinary differential equation is numerically integrated with methods that allow for an efficient application of the AMF (approximate matrix factorization) technique to solve the arising linear systems. An important class of such integrators are W-methods, which are linearly implicit time integrators that only require an approximation to the Jacobian of the vector field.

In the present work a new treatment of discretized mixed derivatives in the AMF technique is proposed. These mixed derivatives are treated in an explicit manner, however, due to the application of suitable damping matrices time step size restrictions are avoided. For a stability analysis a new scalar test equation is considered. PDE-stability (i.e., unconditional stability with respect to the test equation) is studied for s-stage W-methods with $s \leq 3$. Numerical experiments indicate that the proposed test equation is relevant for the system obtained by the MOL approach.

An interesting question for further research is to study whether PDE-stability of a PDE-W-method is sufficient for the stability of the method, when it is applied to the MOL discretization in any dimension.

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