

AMF-TYPE W-METHODS FOR PARABOLIC PROBLEMS WITH MIXED DERIVATIVES

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Dedicated to the memory of Willem Hundsdorfer.

Abstract. The time integration of differential equations obtained by the space discretization via Finite Differences of evolution parabolic PDEs with mixed derivatives in the elliptic operator is considered (MOL approach). W-methods (Rosenbrock-type methods) are combined with the Approximate Matrix Factorization technique (AMF), which is applied in alternating direction implicit (ADI) sense. A new AMF approach, based on an iterative refinement of the linear system, allows to improve stability properties of the integrator. The focus of the paper is a stability analysis, which is based on a scalar test equation that is relevant for the class of problems when periodic or homogeneous Dirichlet boundary conditions are considered. Unconditional stability, independent of the number of space dimensions m , is proved for a variety of AMF-type W-methods. Numerical experiments with linear parabolic problems in dimension $m = 3$ and $m = 4$, as well as with the Heston problem from financial option pricing are presented.

Key words. Parabolic PDEs, mixed derivatives, time integration, W-methods, Approximate Matrix Factorization, Alternating Direction Implicit schemes, unconditional stability, Heston model.

AMS subject classifications. 65M12, 65M20.

1. Introduction. The time integration of parabolic partial differential equations with mixed derivatives discretized in space by means of the method of lines (MOL) is considered. Well-known time integrators of order less or equal than two of Alternating Direction Implicit type (ADI) for parabolic problems with mixed derivatives are the Craig–Sneyd (CS) [3], Hundsdorfer–Verwer (HV) [19, 20, 22] and the modified Craig–Sneyd (MCS) [22, 23] schemes. The analysis of unconditional stability on linear diffusion problems with constant coefficients for these schemes in the case of periodic boundary conditions and some general finite difference discretizations for the mixed derivatives was carried out in [22]. The HV scheme has been recently considered together with space discretizations of order 4 in [5] and applied to stochastic volatility models in financial option pricing in [6]. Compact schemes of order 4 in space together with both the MCS and the HV schemes have also been treated recently in [16, 17].

In the present paper, our focus is on W-methods ([33], see also [15, Section IV.7]), 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. This paper is a continuation of [8], where the authors introduced the class of PDE-W-methods aimed at increasing the temporal order of convergence in time by considering W-methods of classical order at least three. However, it turns out that these latter methods are only unconditionally stable whenever the spatial dimension is at most three. Here we propose a new class of methods, combining the Approximate Matrix Factorization (AMF) [34, 20] for the matrix $I - \theta\tau W$ with a refinement to the solution of the linear systems [9, Section 3], which can be unconditionally stable regardless of the spatial dimension.

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1.1. Class of evolution equations. On a rectangular domain $\Omega = (0, 1)^m \subset \mathbb{R}^m$ and for $t > 0$ we consider parabolic partial differential equations with mixed derivatives,

$$(1.1) \quad \begin{aligned} \partial_t u &= g(t, \vec{x}, u) + \sum_{j=1}^m \eta_j(t, \vec{x}) \partial_{x_j} u + \sum_{i,j=1}^m \alpha_{i,j}(t, \vec{x}) \partial_{x_i x_j}^2 u \\ \vec{x} &= (x_1, \dots, x_m)^\top \in \Omega, \quad t \in [0, T] \\ u(t, \vec{x}) &= \beta(t, \vec{x}), \quad (t, \vec{x}) \in [0, T] \times \partial\Omega, \\ u(0, \vec{x}) &= a(\vec{x}), \quad \vec{x} \in \Omega, \end{aligned}$$

where $\partial\Omega$ denotes the boundary of Ω ($\bar{\Omega} = \Omega \cup \partial\Omega$), $g(t, \vec{x}, u)$ stands for the reaction terms, $\eta_j(t, \vec{x})$ corresponds to advection terms on each space variable and the diffusion terms are those corresponding to the coefficient matrix $(\alpha_{i,j}(t, \vec{x}))_{i,j=1}^m$, which will be assumed to be symmetric and positive definite for every $(t, \vec{x}) \in [0, T] \times \bar{\Omega}$. In the present work we confine the space variables to the m -dimensional unit square but it straightforwardly extends to any m -dimensional box. The PDE problem is provided with initial conditions and with Dirichlet boundary conditions. PDE problems of the form (1.1) in several spatial variables arise, e.g., when pricing several interest rate derivatives with SABR/LIBOR market models (see, e.g., [27, p. 1620]).

1.2. Space discretization and dimensional splitting of the ODEs. With a space discretization (e.g., by means of Finite Differences or Finite Volumes) we get a large system of ODEs

$$(1.2) \quad \dot{U} = F(t, U), \quad U(0) = U_0, \quad t \in [0, T],$$

where $U(t)$ is a real vector approximating the solution values at grid points, and $F(t, U)$ collects the terms of the spatial discretization, reaction terms, and the contribution of inhomogeneous boundary conditions. The function $F(t, U)$ can be naturally split as (inspired by the alternating direction implicit (ADI) approach [30, 4])

$$(1.3) \quad F(t, U) = \sum_{j=0}^m F_j(t, U),$$

where $F_j(t, U)$ contains, for $j = 1, \dots, m$, the terms corresponding to space derivatives with respect to x_j (including boundary conditions), and $F_0(t, U)$ collects the terms corresponding to mixed derivatives, their respective boundary conditions, and eventually also non-stiff reaction terms.

The present work considers time integrators that can be applied to general problems of the form (1.1), but our emphasis is on a stability analysis that gives insight into the linear diffusion problem

$$(1.4) \quad \partial_t u = \sum_{i,j=1}^m \alpha_{i,j} \partial_{x_i x_j}^2 u$$

with constant coefficients $\alpha_{i,j}$ and homogeneous Dirichlet boundary conditions. We assume that the matrix $\mathbb{A} = (\alpha_{i,j})_{i,j=1}^m$ is symmetric and positive definite¹, so that the right-hand side represents an elliptic operator.

Assuming two space dimensions (i.e., $m = 2$), $\Omega = (0, 1) \times (0, 1)$ and equidistant grids $0 < x_1^1 < x_1^2 < \dots < x_1^{n_1} < 1$ and $0 < x_2^1 < x_2^2 < \dots < x_2^{n_2} < 1$ with spacings $\Delta x_1 = 1/(n_1 + 1)$ and $\Delta x_2 = 1/(n_2 + 1)$, respectively, the standard 2nd order central discretization of (1.4) yields

$$\begin{aligned} \dot{U}_{k,l} &= \alpha_{1,1} \frac{1}{\Delta x_1^2} (U_{k+1,l} - 2U_{k,l} + U_{k-1,l}) + \alpha_{2,2} \frac{1}{\Delta x_2^2} (U_{k,l+1} - 2U_{k,l} + U_{k,l-1}) \\ &+ 2\alpha_{1,2} \frac{1}{4\Delta x_1 \Delta x_2} (U_{k+1,l+1} - U_{k-1,l+1} - U_{k+1,l-1} + U_{k-1,l-1}), \end{aligned}$$

¹In the sequel we shall write $\mathbb{A} > 0$ whenever \mathbb{A} is a positive definite matrix.

where $U_{k,l} \approx u(x_1^k, x_2^l)$ for $1 \leq k \leq n_1$ and $1 \leq l \leq n_2$. Collecting these values in a vector $U = (U_{1,1}, U_{2,1}, \dots, U_{n_1,1}, U_{1,2}, \dots, U_{n_1,2}, \dots, U_{1,n_2}, \dots, U_{n_1,n_2})^\top$, and using tensor product notation, the ordinary differential equation becomes

$$\dot{U} = \alpha_{1,1}(I_{n_2} \otimes D_{x_1 x_1})U + \alpha_{2,2}(D_{x_2 x_2} \otimes I_{n_1})U + 2\alpha_{1,2}(D_{x_2} \otimes D_{x_1})U.$$

Here, I_p denotes the identity matrix of dimension p and $D_{x_i x_i}$ and D_{x_i} are tridiagonal differentiation matrices with entries $(1, -2, 1)/\Delta x_i^2$ and $(-1, 0, 1)/(2\Delta x_i)$, respectively.

For general space dimension m the central discretization yields $\dot{U} = \mathcal{M}U$, where

$$(1.5) \quad \begin{aligned} \mathcal{M} &= \sum_{i=1}^m \alpha_{i,i} (I_{n_m} \otimes \dots \otimes D_{x_i x_i} \otimes \dots \otimes I_{n_1}) \\ &+ 2 \sum_{1 \leq i < j \leq m} \alpha_{i,j} (I_{n_m} \otimes \dots \otimes D_{x_j} \otimes \dots \otimes D_{x_i} \otimes \dots \otimes I_{n_1}). \end{aligned}$$

The differentiation matrices $D_{x_i x_i}$ and D_{x_i} are placed in the $(m - i + 1)$ th position of the tensor product.

1.3. Outline of the paper. The main goal of this paper is the introduction of a new class of AMF-type W-methods for the time integration of (1.2)-(1.3), and a stability analysis for linear parabolic problems with mixed derivatives and constant coefficients. We consider three different approaches for dealing with the time integration, and we pay special attention to the unconditional stability of the proposed schemes. All methods are based on the Approximate Matrix Factorization (AMF), see e.g. [34, 20], or some variants of it applied to a given W-method. The choice of any of the AMF-variants applied on the same underlying W-method supplies different methods, which are determined by the choice of the preconditioner $(I - \theta\tau W)$ in the formulation (2.3). The methods slightly differ in computational costs, stability properties and consistency order (in ODE sense) among other features. In any case, the computational costs are quite reasonable, since very few evaluations of the function $F(t, U)$ are used and the solution of a few linear systems with small bandwidth per integration step are required.

The rest of the paper is organized as follows. In section 2, three different approaches for combining W-methods with a splitting of AMF-type are presented. The corresponding unconditional stability analysis relevant in the context of linear diffusion problems with constant coefficients (1.4) is performed in Section 3. For a practical implementation, the application of AMF-type W-methods to non-autonomous problems is discussed in Section 4. The numerical experiments of Section 5 give a comparison with low order methods of the literature and illustrate the theoretical results of Section 3 on a linear model in three and four spatial dimensions. A comparison of the proposed AMF-type W-methods with the classical Hundsdorfer–Verwer ADI scheme on the 2D Heston model from financial option pricing is also presented. Some conclusions are drawn in Section 6. Finally, Section 7 contains an Appendix with some technical results that are needed in the analysis of Section 3 and in the Subsection 5.4.

2. Time integration – W-methods. Our stability analysis is related to the equation (1.4), which leads to an autonomous differential equation. Therefore, we present the time integrators for the autonomous system

$$(2.1) \quad \dot{y} = f(y), \quad y(0) = y_0, \quad t \in [0, T],$$

where the vector field has a splitting

$$(2.2) \quad f(y) = \sum_{j=0}^m f_j(y).$$

By considering time t as an independent variable, the system (1.2) with the splitting (1.3) can be written in the form (2.1) with (2.2), where $y = (t, U)^\top$, $f_0(y) = (1, F_0(t, U))^\top$ and $f_j(y) = (0, F_j(t, U))^\top$, $1 \leq j \leq m$. This will be discussed in more detail in Section 4.

2.1. W-methods for autonomous differential equations. Concerning the time integration we focus our interest on W-methods, originally proposed in [33], see also [15, Section IV.7]. They do not require the solution of nonlinear systems and they permit the use of non-exact approximations (i.e., approximations W violating (2.4)) for the Jacobian of the vector field. Consider the problem (2.1), and let y_n be a numerical approximation to $y(t)$ at t_n . Then, with a step size $\tau > 0$, the numerical approximation y_{n+1} at $t_{n+1} = t_n + \tau$ is defined by

$$(2.3) \quad \begin{aligned} (I - \theta\tau W)\tilde{K}_i &= \tau f\left(y_n + \sum_{j=1}^{i-1} a_{i,j}\tilde{K}_j\right) + \sum_{j=1}^{i-1} \ell_{i,j}\tilde{K}_j, \quad i = 1, 2, \dots, s, \\ y_{n+1} &= y_n + \sum_{i=1}^s b_i\tilde{K}_i. \end{aligned}$$

The matrix W is arbitrary, but it is expected to be a rough approximation to $f'(y_n)$. For $W = f'(y_n)$ we obtain the underlying Rosenbrock method. It is characterized by $(\mathcal{A}, L, b, \theta)$, where $\mathcal{A} = (a_{i,j})_{j < i}$, $L = (\ell_{i,j})_{j < i}$ and $b = (b_i)$.

Many W-methods of low order can be found in the literature. To get methods of order 3 and higher it is convenient to assume

$$(2.4) \quad W - f'(y_n) = \mathcal{O}(\tau), \quad \tau \rightarrow 0,$$

see [7, 32, 26, 10]. Under the slightly less restrictive condition

$$(2.5) \quad [W, f'(y_n)] = Wf'(y_n) - f'(y_n)W = \mathcal{O}(\tau), \quad \tau \rightarrow 0,$$

some families of third order methods are presented in [11]. The construction of efficient W-methods of order ≥ 3 in the general setting $W - f'(y_n) = \mathcal{O}(1)$ is a challenging issue due to the high number of order conditions to be satisfied, see e.g. [15, 24]. Some W-methods of order four and six stages have been constructed in [31].

2.2. AMF-type W-methods. In the splitting (2.2), we assume that $f_j(y)$ (for $j = 1, \dots, m$) contains the terms corresponding to the spatial derivative with respect to x_j , and $f_0(y)$ collects discretizations of mixed derivatives (and eventually also non-stiff reaction terms). In the following we denote

$$(2.6) \quad A = f'(y_n), \quad A_j = f'_j(y_n), \quad j = 0, 1, \dots, m,$$

so that $A = A_0 + A_1 + \dots + A_m$. The idea of Approximate Matrix Factorization (AMF) is to write the matrix of the linear system in (2.3) as a product of matrices, for which the linear systems can be solved efficiently. In our situation A_j are tri-diagonal for $j = 1, \dots, m$, but this is not the case for A_0 . For an approximation of the inverse of $(I - \theta\tau f'(y_n))$ we consider the following cases

(A) The direct AMF approach uses

$$(I - \theta\tau W)^{-1} = \prod_{j=m}^1 (I - \theta\tau A_j)^{-1}.$$

This approach has been studied in [20, Section IV.5] for problems without mixed derivatives. Note that in the presence of mixed derivatives condition (2.4) is violated.

(B) With the aim of verifying (2.4) the following modification of approach (A), leading to the so-called PDE-W-methods, is proposed in [8]:

$$(I - \theta\tau W)^{-1} = \prod_{j=m}^1 (I - \theta\tau A_j)^{-1} (I + \theta\tau A_0 \prod_{j=m}^1 (I - \theta\tau A_j)^{-1}).$$

Instead of completely neglecting mixed derivatives, they are treated explicitly combined with a damping of large eigenvalues.

- (C) For solving the arising linear system in Rosenbrock methods the authors of [9] suggest the use of a fixed number of preconditioned iterations with the approach (A) as preconditioner, where θ is replaced by a new parameter ν . In our situation this leads to the approximation

$$(I - \theta\tau W)^{-1} = \prod_{j=m}^1 (I - \nu\tau A_j)^{-1} (2I - (I - \theta\tau A) \prod_{j=m}^1 (I - \nu\tau A_j)^{-1}).$$

Similar as in the approach (B) mixed derivatives (which are present in A) are treated explicitly, but a suitable choice of the new parameter ν allows us to improve the stability properties of the method. Note that this approximation also verifies the condition (2.4). We call the resulting method AMFR-W-method, where “R” stands for refinement.

Remark 2.1. Since the approach (C) is new in the context of W-methods applied to parabolic problems with mixed derivatives, let us explain it in some more detail. The idea is to solve the linear system $(I - \theta\tau A)x = \tilde{d}$ iteratively by using the preconditioner $\prod_{j=m}^1 (I - \nu\tau A_j)$. This gives the iteration

$$\prod_{j=m}^1 (I - \nu\tau A_j)(x^{(p)} - x^{(p-1)}) = \tilde{d} - (I - \theta\tau A)x^{(p-1)},$$

whose convergence is analyzed in [9]. In the context of low order Rosenbrock methods it was observed that two iterations are sufficient to give an efficient algorithm. Starting the iteration with $x^{(0)} = 0$ yields $x^{(2)} = (I - \theta\tau W)^{-1}\tilde{d}$ with the matrix $(I - \theta\tau W)^{-1}$ given by approach (C).

3. Stability. The space discretization of (1.4) leads to the linear ordinary differential equation with natural splitting

$$\dot{U} = \mathcal{M}U, \quad U(0) = U_0, \quad \mathcal{M} = \sum_{j=0}^m \mathcal{M}_j,$$

where \mathcal{M} is given by (1.5). The difficulty of studying the stability of time integrators lies in the fact that the differentiation matrices D_x and D_{xx} do not commute. Here, we consider a scalar test equation that is relevant for problems with periodic boundary conditions [22] and also for homogeneous Dirichlet boundary conditions [8].

3.1. Test-problem. Replacing $D_{x_i x_i}$ by $D_{x_i}^2$ in \mathcal{M} yields a system of differential equations $\dot{U} = \tilde{\mathcal{M}}U$ which can be diagonalized. In [8] it is proved that asymptotic stability of $\dot{U} = \tilde{\mathcal{M}}U$ implies that of $\dot{U} = \mathcal{M}U$. Our numerical experiments indicate (although we do not have a rigorous proof) that such a property is likely to hold also for the numerical solution.

The system $\dot{U} = \tilde{\mathcal{M}}U$ can be decoupled into scalar linear differential equations

$$(3.1) \quad \dot{v} = -\left(\sum_{i,j=1}^m \alpha_{i,j} \lambda_i \lambda_j\right)v, \quad \lambda_i \in \mathbb{R} \ (i = 1, \dots, m).$$

where $i\lambda_i$ (with i the imaginary unit) represents an eigenvalue of D_{x_i} . As in Section 1.2 we assume that $\mathbb{A} = (\alpha_{i,j})_{i,j=1}^m$ is a symmetric positive definite matrix. The change

$$(3.2) \quad c_{i,j} = \alpha_{i,j} / \sqrt{\alpha_{i,i} \cdot \alpha_{j,j}}, \quad \mathcal{C} = (c_{i,j})_{i,j=1}^m > 0,$$

simplifies the scalar test problem (3.1) to

$$(3.3) \quad \dot{u} = -\left(\sum_{i=1}^m \lambda_i^2 + 2 \sum_{1 \leq i < j \leq m} c_{i,j} \lambda_i \lambda_j\right)u, \quad \lambda_i \in \mathbb{R} \ (i = 1, \dots, m).$$

The diagonal elements of the matrix $\mathcal{C} > 0$ satisfy $c_{i,i} = 1$, and the off-diagonal elements are bounded as $|c_{i,j}| < \sqrt{c_{i,i} \cdot c_{j,j}} = 1$ for $1 \leq i, j \leq m$, $i \neq j$.

3.2. Stability function. Applying an AMF-type W-method to (3.3) with

$$(3.4) \quad f_j(u) = -\lambda_j^2 u \quad (j = 1, \dots, m), \quad f_0(u) = \left(-2 \sum_{i < j} c_{i,j} \lambda_i \lambda_j\right) u,$$

yields a recursion $u_{n+1} = R(z, z_1, \dots, z_m)u_n$, where $R(z, z_1, \dots, z_m)$ is a rational function of the real variables

$$(3.5) \quad z = z_0 + \sum_{j=1}^m z_j, \quad z_j = -\tau \lambda_j^2, \quad z_0 = -2\tau \sum_{1 \leq i < j \leq m} c_{i,j} \lambda_i \lambda_j, \quad \tau > 0.$$

It is called the *linear stability function* of the method. For the AMF-type W-method, based on coefficients $(\mathcal{A}, L, b, \theta)$, this function is given by

$$(3.6) \quad R(z, z_1, \dots, z_m) = 1 + zb^\top (\Pi_m(\theta) I_s - L - z\mathcal{A})^{-1} \mathbf{1}$$

where $\mathbf{1} := (1, \dots, 1)^\top \in \mathbb{R}^s$. The expression $\Pi_m(\theta)$ depends on the choice of the AMF approximation (Section 2.2) and is given by

$$(3.7) \quad \begin{aligned} \text{(A)} \quad & \frac{1}{\Pi_m(\theta)} = \frac{1}{\Pi_m^*(\theta)} && \text{AMF-W-method,} \\ \text{(B)} \quad & \frac{1}{\Pi_m(\theta)} = \frac{1}{\Pi_m^*(\theta)} \left(1 + \frac{\theta z_0}{\Pi_m^*(\theta)}\right) && \text{PDE-W-method,} \\ \text{(C)} \quad & \frac{1}{\Pi_m(\theta)} = \frac{1}{\Pi_m^*(\nu)} \left(2 - \frac{1 - \theta z}{\Pi_m^*(\nu)}\right) && \text{AMFR-W-method,} \end{aligned}$$

where $\Pi_m^*(\theta) := \prod_{j=1}^m (1 - \theta z_j)$. Note that, for the case (C), the expression $\Pi_m(\theta)$ depends on the additional parameter $\nu > 0$. We also remark that the positive definiteness of the matrix \mathcal{C} implies that the real variable z , defined in (3.5), satisfies $z \leq 0$.

DEFINITION 3.1. *A numerical time integrator which, when applied to the test equation (3.3), yields the recursion $u_{n+1} = R(z, z_1, \dots, z_m)u_n$ with stability function (3.6), is called unconditionally stable for a given $m \geq 2$, if*

$$|R(z, z_1, \dots, z_m)| \leq 1$$

for all z, z_1, \dots, z_m of (3.5) and each matrix $\mathcal{C} > 0$.

3.3. Main result. To state our main result on unconditional stability, we will need some stability properties of the underlying Rosenbrock method $(\mathcal{A}, L, b, \theta)$. We denote by

$$(3.8) \quad R_\theta(z) = 1 + zb^T((1 - \theta z)I - L - z\mathcal{A})^{-1} \mathbf{1}, \quad z \in \mathbb{C},$$

the function (3.6), where $(1 - \theta z)$ is substituted for $\Pi_m(\theta)$. It is the stability function based on Dahlquist's test equation $\dot{u} = \lambda u$, $z = \tau \lambda$. We recall that the Rosenbrock method $(\mathcal{A}, L, b, \theta)$ is A_0 -stable, if its stability function (3.8) fulfils $|R_\theta(x)| \leq 1$ for all $x \leq 0$. This is one of the ingredients of our main result, which serves a key lemma for the stability statements.

LEMMA 3.2. *Consider an AMF-type W-method with stability function (3.6). Assume there exist $\theta_0 > 0$ and $\mu_m(\theta) > 0$ such that*

$$\begin{aligned} \text{(S1)} \quad & |R_\theta(z)| \leq 1 \quad \text{for all real } z \leq 0 \text{ and for all } \theta \geq \theta_0, \\ \text{(S2)} \quad & 0 < \frac{1}{\Pi_m(\theta)} \leq \frac{1}{1 - \mu_m(\theta)z} \quad \text{for } z, z_j \text{ given by (3.5) with } \mathcal{C} > 0. \end{aligned}$$

Then, the method is unconditionally stable for all θ satisfying $\mu_m(\theta) \geq \theta_0$.

Proof. Taking into account that $z \leq 0$, it follows from (S2) that

$$(3.9) \quad \frac{1}{\Pi_m(\theta)} = \frac{1}{1 - \mu z}$$

for some $\mu \geq \mu_m(\theta)$ that may depend on θ , z , and z_j , $j = 1, \dots, m$. Consequently, we have

$$R(z, z_1, \dots, z_m) = R_\mu(z),$$

and Assumption (S1) together with $\mu \geq \mu_m(\theta) \geq \theta_0$ yield the statement of the theorem. \square

The range of values for $\theta \geq \theta_0$ providing A_0 -stable methods (i.e., Assumption (S1)) is known for many Rosenbrock methods. Some results are collected in Table 1, where s denotes the number of stages, p the classical order, and for $p \geq 3$ also the reference to the coefficients of the methods is given.

TABLE 1
Parameter θ_0 of Assumption (S1) for some Rosenbrock methods

method	$s = p = 1$	$s = p = 2$	$s = p = 3$ [11, Thm.1]	$s = p = 4$ [10, Sect.6]
θ_0	$1/2$	$1/4$	$1/3$	$(3 + \sqrt{3})/12$

3.4. Verification of Assumption (S2). The value of $\mu_m(\theta)$, appearing in Assumption (S2), is the subject of the following three theorems.

THEOREM 3.3 (AMF-W-methods). *For the case (A) of (3.7) the Assumption (S2) is satisfied with*

$$\mu_m(\theta) = \frac{\theta}{m}.$$

Proof. The left inequality of Assumption (S2) is obvious, because $z_j < 0$ for $j = 1, \dots, m$. To prove the right inequality, we note that the positive definiteness of \mathcal{C} implies $|c_{i,j}| \leq 1$ for $i \neq j$, so that by the Cauchy–Schwarz inequality

$$\begin{aligned} z_0 + z_1 + \dots + z_m &= -\tau \sum_{i,j=1}^m c_{i,j} \lambda_i \lambda_j \geq -\tau \left(\sum_{j=1}^m |\lambda_j| \right)^2 \\ &\geq -\tau m \sum_{j=1}^m \lambda_j^2 = m(z_1 + \dots + z_m). \end{aligned}$$

This implies

$$\begin{aligned} \Pi_m^*(\theta) - (1 - \mu z) &\geq (1 - \theta(z_1 + \dots + z_m)) - (1 - \mu(z_0 + z_1 + \dots + z_m)) \\ &\geq (m\mu - \theta)(z_1 + \dots + z_m), \end{aligned}$$

which is non-negative for $\mu \leq \theta/m$. Hence, the right inequality of Assumption (S2) is satisfied with $\mu_m(\theta) = \theta/m$. \square

Note that the value $\mu_m(\theta)$ of Theorem 3.3 is optimal in the sense that the right inequality of Assumption (S2) is no longer satisfied with $\mu_m(\theta)$ that is larger than θ/m .

THEOREM 3.4 (PDE-W-methods). *For the case (B) of (3.7) the Assumption (S2) is satisfied with*

$$\mu_m(\theta) = \theta \quad \text{for } 2 \leq m \leq 3.$$

Proof. By [8, Theorem 5.2] the right inequality of Assumption (S2) is satisfied for all $\mu_m(\theta) \leq \theta$. The positivity of $\Pi_m(\theta)$, i.e., the left inequality of Assumption (S2), follows from [8, Formula (3.11)] for $m = 2$, and from [8, Theorem 5.3] for $m = 3$. \square

To get results on unconditional stability also for $m \geq 4$, one has to restrict the class of problems, i.e., one has to pose additional conditions on \mathcal{C} . Sufficient as well as necessary conditions are discussed in [8, Remark 5.1].

For the verification of Assumption (S2) for AMFR-W-methods we consider the polynomial

$$(3.10) \quad g_m(x) = 2x \left(\frac{m-x}{m-1} \right)^{m-1} - 1,$$

and denote by κ_m the smallest positive zero of $g_m(x)$. These numbers are given in Table 2 for $2 \leq m \leq 9$. One can prove (see Lemma 7.1 of Section 7 below) that they satisfy

$$(3.11) \quad 0.2320 \leq \kappa_{m+1} < \kappa_m, \quad (m+1)\kappa_{m+1} > m\kappa_m.$$

TABLE 2
Values for κ_m , $2 \leq m \leq 9$, rounded up to 4 significant digits.

m	2	3	4	5	6	7	8	9
κ_m	0.2929	0.2680	0.2576	0.2519	0.2482	0.2457	0.2439	0.2425

THEOREM 3.5 (AMFR-W-methods). *For the case (C) of (3.7) the Assumption (S2) is satisfied with*

$$\mu_m(\theta) = \theta \quad \text{if } \nu \geq m\kappa_m\theta.$$

Proof. The identity

$$\frac{1}{1-\mu z} - \frac{1}{\Pi_m(\theta)} = \frac{1}{1-\mu z} \left(1 - \frac{1-\mu z}{\Pi_m^*(\nu)} \right)^2 + \frac{(\mu-\theta)z}{\Pi_m^*(\nu)^2}$$

implies that the right inequality of Assumption (S2) is satisfied for all $\mu_m(\theta)$ satisfying $\mu_m(\theta) \leq \theta$ (independent of the choice of ν).

The positivity of $\Pi_m(\theta)$ (left inequality of Assumption (S2)) is equivalent to $2\Pi_m^*(\nu) - (1-\theta z) > 0$, and, using the notation $y_j = \sqrt{\nu\tau}\lambda_j$, can be written as

$$D := 2 \prod_{j=1}^m (1 + y_j^2) - 1 - \frac{\theta}{\nu} \sum_{i,j=1}^m c_{i,j} y_i y_j > 0.$$

Using $|c_{i,j}| \leq 1$, we obtain the lower bound

$$(3.12) \quad D \geq 2 \prod_{j=1}^m (1 + y_j^2) - 1 - \frac{\theta}{\nu} \left(\sum_{j=1}^m |y_j| \right)^2.$$

It follows from Lemma 7.2 below that this lower bound is non-negative, if $\nu \geq m\kappa_m\theta$, and that it can be equal to 0 only if $y_1 = \dots = y_m = y$ for some $y \neq 0$. However, in this case the inequality in (3.12) is strict. This completes the proof of the theorem. \square

For the natural choice $\nu = \theta$ of the additional parameter we have unconditional stability for all $\mathcal{C} > 0$ in dimensions $m = 2$ and $m = 3$, because $m\kappa_m < 1$ for $m \leq 3$. For $m \geq 4$, one has the option of either choosing $\nu \geq m\kappa_m\theta > \theta$ or restricting the class of problems (as it is necessary for the case (B)).

3.5. Unconditional stability of AMF-type W-methods. Inserting the values of $\mu_m(\theta)$ from Section 3.4 into the main theorem we get the following result on unconditional stability of AMF-type W-methods.

THEOREM 3.6. *Consider a W-method $(\mathcal{A}, L, b, \theta)$ and assume that the underlying Rosenbrock method is A_0 -stable for all $\theta \geq \theta_0$. Then we have unconditional stability in dimension m for the*

- AMF-W-method, if $\theta \geq m\theta_0$;
- PDE-W-method, if $\theta \geq \theta_0$ and $2 \leq m \leq 3$;
- AMFR-W-method, if $\theta \geq \theta_0$ and $\nu \geq m\kappa_m\theta$ (with κ_m from Table 2).

Remark 3.7. The analysis of unconditional stability of some standard schemes for parabolic problems with mixed derivatives and with order of consistency one or two (the Craig–Sneyd scheme [3], Modified Craig–Sneyd scheme [22] and the Hundsdorfer and Verwer schemes [20, 22]) in the case of periodic boundary conditions and some general finite difference discretizations for the mixed derivatives was carried out in [22]. The results there obtained for the case of the so-called Hundsdorfer–Verwer scheme [22, Theorem 2.8] are the same as the ones here given in Theorem 3.6 for the one-stage AMFR-W-method with $\theta = 1/2$. In fact the bounds in [22, Table 1, for (2.18)] coincide with our values for $\nu_m = m\kappa_m\theta$ in Table 2 when $\theta = 1/2$ and $m \geq 2$.

4. AMF-type W-methods for non-autonomous differential equations.

Considering time t as an independent variable, and augmenting (1.2) with $\dot{t} = 1$, the autonomous equation (2.1)–(2.2) yields for $y = (t, U)^\top$ the system

$$(4.1) \quad \dot{y}(t) = \begin{pmatrix} \dot{t} \\ \dot{U} \end{pmatrix} = \sum_{j=0}^m f_j(y) = \begin{pmatrix} 1 \\ F_0(t, U) \end{pmatrix} + \sum_{j=1}^m \begin{pmatrix} 0 \\ F_j(t, U) \end{pmatrix}.$$

Here, all mixed derivatives and possibly a non-stiff reaction term $G(t, U)$ are assumed to be collected in $F_0(t, U)$. The corresponding splitting for the full Jacobian is then given by

$$(4.2) \quad f'(y_n) = \sum_{j=0}^m \begin{pmatrix} 0 & 0 \\ \partial_t F_j(t_n, U_n) & \partial_U F_j(t_n, U_n) \end{pmatrix}.$$

In the equations (2.3) we set

$$(4.3) \quad \tilde{K}_i = \begin{pmatrix} \tau\rho_i \\ K_i \end{pmatrix}, \quad \rho_i \in \mathbb{R}, \quad i = 1, \dots, s,$$

so that for each stage ($i = 1, \dots, s$) we have

$$(4.4) \quad \begin{aligned} (I - \theta\tau W) \begin{pmatrix} \tau\rho_i \\ K_i \end{pmatrix} &= \tau \begin{pmatrix} 1 \\ F(t_n + c_i\tau, U_n + \sum_{j=1}^{i-1} a_{ij}K_j) \end{pmatrix} + \sum_{j=1}^{i-1} \ell_{ij} \begin{pmatrix} \tau\rho_j \\ K_j \end{pmatrix}, \\ \begin{pmatrix} t_{n+1} \\ U_{n+1} \end{pmatrix} &= \begin{pmatrix} t_n \\ U_n \end{pmatrix} + \sum_{i=1}^s b_i \begin{pmatrix} \tau\rho_i \\ K_i \end{pmatrix} \end{aligned}$$

with

$$(4.5) \quad \rho = (\rho_i)_{i=1}^s = (I - L)^{-1} \mathbb{1}, \quad c = (c_i)_{i=1}^s = \mathcal{A}\rho.$$

Observe that order of consistency one for W-methods implies $b^T \rho = 1$, so that $t_{n+1} = t_n + \tau$ as expected. We use the notations

$$(4.6) \quad A_{n,j} := \partial_U F_j(t_n, U_n), \quad a_{n,j} = \partial_t F_j(t_n, U_n), \quad j = 0, 1, \dots, m,$$

to describe the approximation of W for the three cases of Subsection 2.2:

- (A) For the AMF-W-methods (case (A)), the choice for $(I - \tau\theta W)$ in (4.4) is obtained by neglecting the Jacobian terms corresponding to the mixed derivatives, i.e.,

$$(I - \theta\tau W)^{-1} = \prod_{j=m}^1 \begin{pmatrix} 1 & 0 \\ -\theta\tau a_{n,j} & (I - \tau\theta A_{n,j}) \end{pmatrix}^{-1}.$$

By performing the calculations in (4.4) we see that the stages are computed one after the other (for $i = 1, \dots, s$) by the formula

$$\begin{aligned} K_i^{(0)} &= \tau F(t_n + c_i\tau, U_n + \sum_{j=1}^{i-1} a_{ij}K_j) + \sum_{j=1}^{i-1} \ell_{ij}K_j, \\ (4.7) \quad (I - \theta\tau A_{n,j})K_i^{(j)} &= K_i^{(j-1)} + \theta\rho_i\tau^2 a_{n,j}, \quad (j = 1, \dots, m) \\ K_i &= K_i^{(m)}. \end{aligned}$$

The numerical solution after one step is then given by

$$(4.8) \quad U_{n+1} = U_n + \sum_{i=1}^s b_i K_i.$$

Remark 4.1. An alternative that can be more efficient in some cases, in particular in the absence of mixed derivatives in the elliptic operator, is to include the non-stiff reaction terms in one or in several terms of the directional splitting.

- (B) For the PDE-W-methods (case (B)), the choice for $(I - \tau\theta W)$ in (4.4) is

$$\begin{aligned} (4.9) \quad (I - \theta\tau W)^{-1} &= P_m(\theta)^{-1} \left(I + \theta\tau \begin{pmatrix} 0 & 0 \\ a_{n,0} & A_{n,0} \end{pmatrix} P_m(\theta)^{-1} \right), \\ P_m(\theta) &:= \prod_{j=m}^1 \begin{pmatrix} 1 & 0 \\ -\theta\tau a_{n,j} & (I - \theta\tau A_{n,j}) \end{pmatrix}. \end{aligned}$$

The stages of the PDE-W method $(\mathcal{A}, L, b, \theta)$ are computed as follows:

$$\begin{aligned} K_i^{(0)} &= \tau F(t_n + c_i\tau, U_n + \sum_{j=1}^{i-1} a_{ij}K_j) + \sum_{j=1}^{i-1} \ell_{ij}K_j, \\ (I - \theta\tau A_{n,j})K_i^{(j)} &= K_i^{(j-1)} + \theta\rho_i\tau^2 a_{n,j}, \quad (j = 1, \dots, m) \\ (4.10) \quad \hat{K}_i^{(0)} &= K_i^{(0)} + \theta\tau A_{n,0}K_i^{(m)} + \theta\rho_i\tau^2 a_{n,0}, \\ (I - \theta\tau A_{n,j})\hat{K}_i^{(j)} &= \hat{K}_i^{(j-1)} + \theta\rho_i\tau^2 a_{n,j}, \quad (j = 1, \dots, m) \\ K_i &= \hat{K}_i^{(m)}, \end{aligned}$$

with advancing solution after one step given by (4.8).

- (C) For the AMFR-W-methods of Subsection 2.2 (case (C)), the choice for $(I - \tau\theta W)$ in (4.4) is, with $P_m(\nu)$ as in (4.9),

$$\begin{aligned} (I - \theta\tau W)^{-1} &= P_m(\nu)^{-1} \left(2I - \left(I - \theta\tau \begin{pmatrix} 0 & 0 \\ \partial_t F & \partial_U F \end{pmatrix} \right) P_m(\nu)^{-1} \right), \\ \partial_t F &:= \partial_t F(t_n, U_n), \quad \partial_U F := \partial_U F(t_n, U_n). \end{aligned}$$

Hence, for $i = 1, 2, \dots, s$, we compute K_i from:

$$\begin{aligned}
 (4.11) \quad K_i^{(0)} &= \tau F(t_n + c_i \tau, U_n + \sum_{j=1}^{i-1} a_{ij} K_j) + \sum_{j=1}^{i-1} \ell_{ij} K_j, \\
 (I - \nu \tau A_{n,j}) K_i^{(j)} &= K_i^{(j-1)} + \nu \rho_i \tau^2 a_{n,j}, \quad (j = 1, \dots, m) \\
 \hat{K}_i^{(0)} &= 2K_i^{(0)} + \theta \rho_i \tau^2 \partial_t F(t_n, U_n) - (I - \theta \tau \partial_U F(t_n, U_n)) K_i^{(m)}, \\
 (I - \nu \tau A_{n,j}) \hat{K}_i^{(j)} &= \hat{K}_i^{(j-1)} + \nu \rho_i \tau^2 a_{n,j}, \quad (j = 1, \dots, m) \\
 K_i &= \hat{K}_i^{(m)}.
 \end{aligned}$$

The numerical solution after one step is then computed from (4.8).

5. Numerical experiments. This section is intended to illustrate the performance of some AMF-type methods presented in Section 2.2 in relation with classical ADI schemes like the Hundsdorfer–Verwer scheme [19, 20, 22], when constant time step sizes are used. To this aim, the time integration of a linear diffusion model with constant coefficients in three and four spatial dimensions ($m = 3, 4$) and the 2D Heston model ($m = 2$) from financial option pricing will be considered. Particular attention will be paid to the unconditional stability, the temporal order of convergence observed and the efficiency in terms of CPU time versus global errors at the end-point in the ℓ^2 -norm. All calculations below were performed with a desktop computer (3,3 GHz Intel Core i5 processor) employing a Fortran code. Some of the corresponding codes can be found at <http://www.unige.ch/~hairer/preprints.html>.

5.1. Time integrators.

HV is an extension of the Douglas scheme [4] and termed *Hundsdorfer–Verwer* scheme in [22, Formula (1.4)]. Parameters are $\mu = 1/2$ to have classical order 2, and $\theta > 0$ to be selected for stability requirements.

$$\begin{aligned}
 (5.1) \quad Y_0 &= U_n + \tau F(t_n, U_n), \\
 Y_j &= Y_{j-1} + \theta \tau (F_j(t_{n+1}, Y_j) - F_j(t_n, U_n)), \quad j = 1, \dots, m, \\
 \tilde{Y}_0 &= Y_0 + \mu \tau (F(t_{n+1}, Y_m) - F(t_n, U_n)), \\
 \tilde{Y}_j &= \tilde{Y}_{j-1} + \theta \tau (F_j(t_{n+1}, \tilde{Y}_j) - F_j(t_{n+1}, Y_m)), \quad j = 1, \dots, m, \\
 U_{n+1} &= \tilde{Y}_m.
 \end{aligned}$$

This scheme is unconditionally stable whenever $\theta \geq 0.2929$, $\theta \geq 0.4020$ and $\theta \geq 0.5152$ for $m = 2$, $m = 3$ and $m = 4$, respectively (see [22, Table 1]). For $2 \leq m \leq 4$ we shall consider $\theta = (3 + \sqrt{3})/6$, $\theta = 0.4020$ and $\theta = 0.5152$, respectively. For the case $m = 2$, the chosen value for $\theta = (3 + \sqrt{3})/6$ is larger than the corresponding lower bound for unconditional stability. This choice has been motivated by the fact that it ensures unconditional stability for 2D convection-diffusion problems without mixed derivatives [25] and has been recently considered in applications to 2D and 3D models in Finance [12, 13].

PDE-W1 is the 1-stage PDE-W-method $(\mathcal{A}, L, b, \theta)$ with coefficients

$$(5.2) \quad \mathcal{A} = L = 0, \quad b = 1.$$

The stability parameter is $\theta = 1/2$. This method has only 1 stage, but it is of order 2 since (2.4) is fulfilled.

AMFR-W1 is the 1-stage AMFR-W-method $(\mathcal{A}, L, b, \theta, \nu)$ with coefficients (5.2), where we have chosen $\nu = \theta = 1/2$ for $m \leq 3$ and $\nu = 4\kappa_4\theta$, $\theta = 1/2$ for $m = 4$ (with $\kappa_4 = 0.2576$) to have order 2 and to meet the stability bounds given in Theorem 3.6.

AMF-W2 is the 2-stage AMF-W-method $(\mathcal{A}, L, b, \theta)$ with coefficients taken from the book by Hundsdorfer & Verwer [20, p. 400]

$$(5.3) \quad \mathcal{A} = \begin{pmatrix} 0 & 0 \\ 2/3 & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 \\ -4/3 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 5/4 \\ 3/4 \end{pmatrix}.$$

The method is of order 3 if (2.4) is fulfilled and $\theta = (3 + \sqrt{3})/6$, otherwise it is order two. We have chosen $\theta = (3 + \sqrt{3})/6$ for $m \leq 3$ and $\theta = 1$ for $m = 4$ to ensure stability according the stability bounds given in Theorem 3.6. For the kind of problems under consideration the assumption (2.4) is violated due to the presence of mixed derivatives.

PDE-W2 is the 2-stage PDE-W-method $(\mathcal{A}, L, b, \theta)$ in [8] based on the coefficients (5.3). The stability parameter is $\theta = (3 + \sqrt{3})/6$. This method has only 2 stages, but it is of order 3 since (2.4) is fulfilled.

AMFR-W2 is the 2-stage AMFR-W-method $(\mathcal{A}, L, b, \theta, \nu)$ with coefficients (5.3), where we have chosen $\nu = \theta = (3 + \sqrt{3})/6$ for $m \leq 3$ and $\nu = 4\kappa_4\theta$, $\theta = (3 + \sqrt{3})/6$ for $m = 4$ (with $\kappa_4 = 0.2576$) to meet the stability bounds given in Theorem 3.6. It is of order 3 since (2.4) is fulfilled.

5.2. Linear diffusion equation with constant coefficients. We consider linear diffusion partial differential equations in three and four spatial dimensions in such a way that mixed derivatives of the exact solution are present. Our aim is to illustrate numerically the stability results provided for AMF-type W-methods in Section 3.

For our numerical experiments we consider the diffusion partial differential equation with linear constant coefficients and mixed derivative terms

$$(5.4) \quad \partial_t u = \sum_{i,j=1}^m \alpha_{i,j} \partial_{x_i x_j}^2 u + g(t, \vec{x})$$

for $\vec{x} \in (0, 1)^m$, $t \in [0, 1]$, where $g(t, \vec{x})$ is selected in such way that

$$(5.5) \quad u(t, \vec{x}) = u_e(t, \vec{x}) := e^t \left(4^m \prod_{j=1}^m x_j (1 - x_j) + \kappa \sum_{j=1}^m \left(x_j + \frac{1}{j+2} \right)^2 \right)$$

is the exact solution of (5.4). We impose the initial condition $u(0, \vec{x}) = u_e(0, \vec{x})$ and Dirichlet boundary conditions. Here, we consider the cases $m = 3, 4$. If $\kappa = 0$ we have homogeneous boundary conditions, but when $\kappa = 1$ we get non-homogeneous time-dependent Dirichlet conditions. Furthermore, we take $\alpha_{i,i} = 1$, $1 \leq i \leq m$, and $\alpha_{i,j} = \alpha$, for $i \neq j$, where $\alpha > 0$ is a parameter which will be selected in order to illustrate the stability of the AMF-type methods introduced in Section 2.2 (see also Section 4). In all cases, α will be chosen so that the second order differential operator is elliptic.

We apply the MOL approach on a uniform grid with meshwidth $\Delta x_i = 1/(N + 1)$, $1 \leq i \leq m$, with $N = 128$ for $m = 3$ and $N = 40$ if $m = 4$. Hence, the following semi-discretized system with corresponding dimension N^m

$$(5.6) \quad \dot{U} = \mathcal{M}U + G(t) + b(t)$$

is obtained, where \mathcal{M} is given in (1.5), D_{x_i} and $D_{x_i x_i}$ are the differentiation matrices corresponding to the first and second order central differences in each spatial direction, $G(t)$ denotes the discretization of the term $g(t, \vec{x})$ and $b(t)$ stores the terms due to non-homogeneous boundary conditions. Note that the differential equation (5.6) is of the form (1.2)-(1.3). Observe that the exact solution (5.5) is a polynomial of degree 2 in each spatial variable so that the global errors come only from the time discretization. AMF-type W-methods will be applied to (5.6) with fixed step size $\tau = 2^{-j}$, $2 \leq j \leq 11$, as detailed in Section 4.

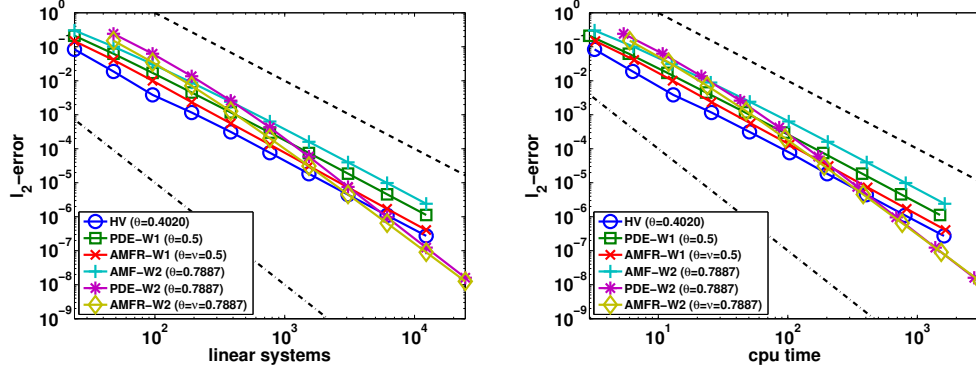


FIG. 1. 3D Linear model (5.4)-(5.5) with $\alpha = 0.9$, homogeneous boundary conditions ($\kappa = 0$) and $\Delta x_i = 1/129$, $1 \leq i \leq 3$. Error vs Linear Systems (left). Error vs CPU Time (right). Dashed straight lines with slopes two and three, respectively, are included to compare the temporal orders of convergence.

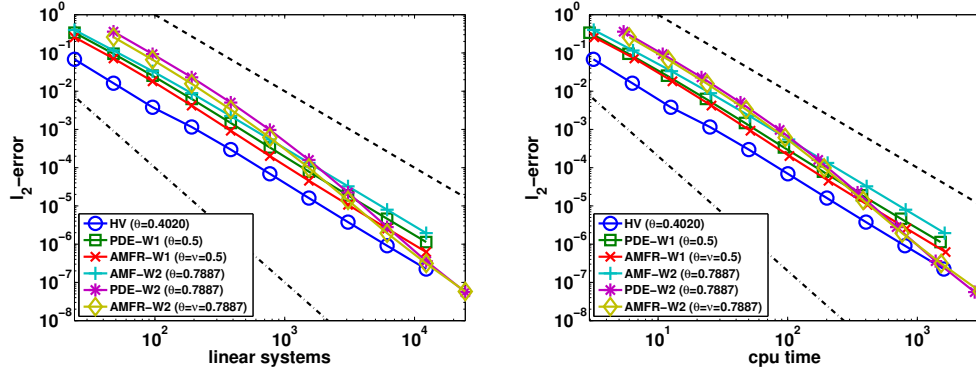


FIG. 2. 3D Linear model (5.4)-(5.5) with $\alpha = 0.9$, time dependent boundary conditions ($\kappa = 1$) and $\Delta x_i = 1/129$, $1 \leq i \leq 3$. Error vs Linear Systems (left). Error vs CPU Time (right).

5.3. Numerical illustration. The time integration of (5.6) for $m = 3$ and $m = 4$ spatial dimensions with the methods of Section 5.1 is summarized in this section. Figures 1 and 2 deal with the 3-dimensional case, whereas Figures 3 and 4 correspond to the case $m = 4$. The global errors are plotted in relation to both the number of linear system calls which is proportional to the number of time steps (to check the temporal order of the current method) and the CPU time in seconds (to measure the efficiency of each integrator). Each figure contains dashed straight lines with slopes two and three, respectively, to compare the temporal orders of convergence for the methods under consideration.

For the elliptic operator in (5.4), we take diffusion parameters $\alpha_{i,j} = \alpha$, for $i \neq j$, with $\alpha = 0.9$. Note that for the case of 4 spatial dimensions the necessary condition for stability of PDE-W-methods [8, Remark 5.1] is violated. In order to meet this condition we also take $\alpha = 0.7$ when $m = 4$. Under this stability assumption, the numerical results for $m = 3$ with $\alpha = 0.9$ (see Figures 1 and 2) are similar to those obtained for $m = 4$ with $\alpha = 0.7$ (Figure 4).

For the case $m = 3$ in Figures 1 and 2, HV, PDE-W1, AMFR-W1 and AMF-W2 are seen to be second order methods, whereas PDE-W2 and AMFR-W2 attain order

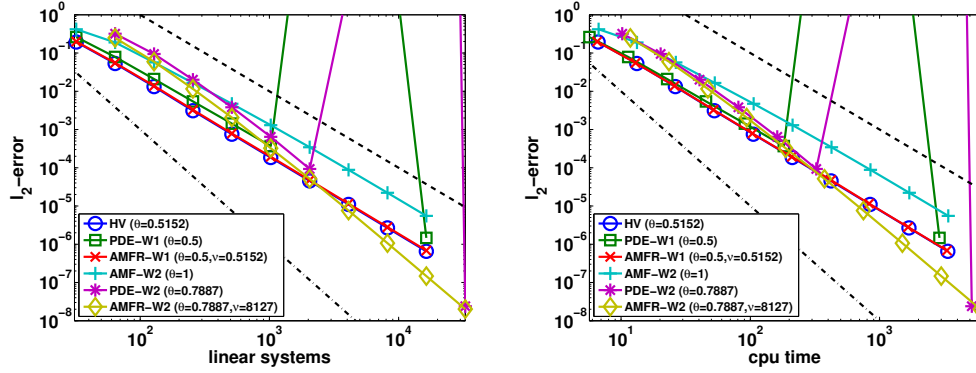


FIG. 3. 4D Linear model (5.4)-(5.5) with $\alpha = 0.9$, homogeneous boundary conditions ($\kappa = 0$) and $\Delta x_i = 1/41$, $1 \leq i \leq 4$. Error vs Linear Systems (left). Error vs CPU Time (right).

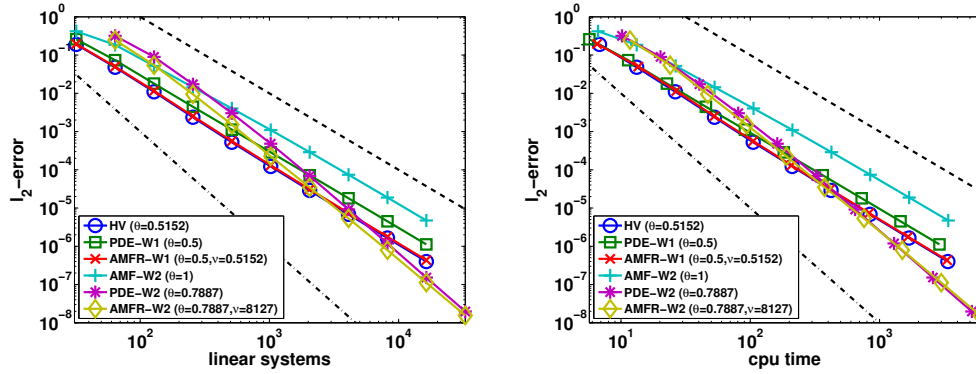


FIG. 4. 4D Linear model (5.4)-(5.5) with $\alpha = 0.7$, homogeneous boundary conditions ($\kappa = 0$) and $\Delta x_i = 1/41$, $1 \leq i \leq 4$. Error vs Linear Systems (left). Error vs CPU Time (right).

three when $\kappa = 0$ (homogeneous BCs). For $\kappa = 1$ the order of convergence of these two latter methods lies around 2.5. It is observed that **HV** is among the most efficient methods, although both **PDE-W2** and **AMFR-W2** are competitive candidates when high accuracy is required.

The order reduction phenomenon due to time dependent Dirichlet BCs in the time integration of parabolic PDEs by means of Rosenbrock or Runge-Kutta methods has been extensively reported and studied by several authors, e.g. [28, 29]. For AMF-type W-methods the order reduction is not completely understood and requires the study of the local truncation error and of the error propagation with estimates that are uniform in the space discretization. This is an interesting, challenging problem for future research.

For the 4-dimensional case, similar considerations as above correspond to the plots presented with $\alpha = 0.7$ (Figure 4). For $\alpha = 0.9$ the necessary condition for stability of PDE-W-methods [8, Remark 5.1] is not fulfilled and, as a matter of fact, both **PDE-W1** and **PDE-W2** perform in an unstable way in this case (see Figure 3). For the remaining methods, the selected values for the parameters θ and ν ensure stability according to Theorem 3.6 and the observed temporal orders of convergence are similar to those obtained for $m = 3$. Furthermore, in Figure 3 it is seen that again **AMFR-W2** overtakes **HV** when medium-high accuracy is needed.

We note that the **PDE-W2** and **AMFR-W2** methods are less efficient for time-dependent, non-homogeneous Dirichlet boundary conditions. Such boundary conditions can be avoided by a transformation to homogeneous boundary conditions as explained in [8, Section 4.4] for 2D-problems ($m = 2$). Here, we develop the idea for an arbitrary number of variables.

5.4. Transformation to homogeneous boundary conditions. The idea is to construct a function $\widehat{u}(t, x_1, \dots, x_m)$ which interpolates for fixed t the values at the boundary of the domain, and then to solve numerically the differential equation for the difference $w(t, x_1, \dots, x_m) = u(t, x_1, \dots, x_d) - \widehat{u}(t, x_1, \dots, x_m)$. For a rectangular domain it is proved in Lemma 7.4 below that this interpolant function \widehat{u} can be recursively constructed by taking $u^{[0]} := u$ (the values of u are only needed on the boundary of the spatial domain) and

$$\begin{cases} q_j &:= \left(\frac{x_j - 1}{0 - 1} \right) u_{|x_j=0}^{[j-1]} + \left(\frac{x_j - 0}{1 - 0} \right) u_{|x_j=1}^{[j-1]}, \\ u^{[j]} &:= u^{[j-1]} - q_j, \end{cases} \quad 1 \leq j \leq m,$$

$$\widehat{u} := \sum_{j=1}^m q_j,$$

where $u_{|x_k=x^*}^{[j]}$ stands for the evaluation of $u^{[j]}$ at a point $(x_1, \dots, x_m)^T \in \overline{\Omega}$ with $x_k = x^*$, $1 \leq k \leq m$. In the particular case of the PDE problem (5.4)-(5.5), it is not difficult to check that this interpolation process gives

$$\widehat{u}(t, \vec{x}) = \kappa e^t \sum_{j=1}^m \left(x_j + \frac{1}{j+2} \right)^2$$

in such a way that the PDE for $w = u - \widehat{u}$ reduces to (5.4)-(5.5) with $\kappa = 0$, i.e., exactly to the case of homogeneous boundary conditions. In order to avoid the analytic calculation of the elliptic operator acting on the interpolant, the homogenization of the problem can be achieved by applying the spatial discretization of the elliptic operator to the interpolant function. In this situation some additional spatial errors could be introduced, but they are of similar size to those ones involved in the discretization of the original problem.

5.5. The Heston problem. The Heston problem [18] is a two-dimensional extension of the well-known Black-Scholes equation from financial option pricing theory. The problem admits a semi-closed analytical expression for its solution [18, p. 330-331], which has not been used in our numerical experiments below. The results obtained in the experiments on this problem show that the proposed AMF-type schemes also perform satisfactorily on PDEs with variable coefficients, and they can be easily applied on practical models that involve mixed derivative terms.

This model predicts the fair price of a call option $u(s, v, t)$ at time $t > 0$, when the asset price is $s > 0$ and $v > 0$ represents its variance, by the following partial differential equation

$$(5.7) \quad \begin{aligned} \partial_t u &= \frac{1}{2} s^2 v \partial_{ss}^2 u + \rho \sigma s v \partial_{sv}^2 u + \frac{1}{2} \sigma^2 v \partial_{vv}^2 u \\ &+ (r_d - r_f) s \partial_s u + \kappa(\eta - v) \partial_v u - r_d u. \end{aligned}$$

Here t represents the days left until what it is called *maturity time* $T > 0$, so $t \in [0, T]$, $s > 0$, $v > 0$. The parameter $\kappa > 0$ is the mean-reversion rate and $\eta > 0$ is the long-term mean, r_d and r_f represent the domestic and foreign interest rates, respectively, $\sigma > 0$ is the volatility of the variance and $\rho \in [-1, 1]$ measures the correlation between the two variables s and v . The details of the derivation of the PDE (5.7) from the corresponding stochastic model can be seen in [18]. Naturally, maximum values for the spatial variables $(s, v) \in [0, S] \times [0, V]$

are prefixed and in the case of a *European call option*, the following boundary conditions are imposed

$$(5.8) \quad \begin{aligned} s = 0 : \quad & u(0, v, t) = 0, \quad t \in [0, T] \\ s = S : \quad & \partial_s u(S, v, t) = e^{-r_f t}, \quad t \in [0, T] \\ v = V : \quad & u(s, V, t) = s e^{-r_f t}, \quad t \in [0, T]. \end{aligned}$$

Moreover, the initial condition

$$(5.9) \quad u(s, v, 0) = \max(0, s - K)$$

is considered, where $K > 0$ is the *strike price* of the option, i.e., the price that the holder can buy the asset for when the option expires.

The values for the PDE parameters have been experimentally adjusted in many different practical situations. Here we will consider three different cases. The first one is the set of values proposed by [1],

$$(5.10) \quad \kappa = 1.5, \eta = 0.04, \sigma = 0.3, \rho = -0.9, r_d = 0.025, r_f = 0, K = 100,$$

so that the boundary conditions are time-independent. In the second case, given in [2],

$$(5.11) \quad \kappa = 3, \eta = 0.12, \sigma = 0.04, \rho = 0.6, r_d = 0.01, r_f = 0.04, K = 100,$$

the boundary conditions are time-dependent with a small volatility σ and the problem becomes more advection-dominated near the border $v = 0$. Finally we also consider a time-dependent case with a larger volatility

$$(5.12) \quad \kappa = 1.5, \eta = 0.02, \sigma = 0.62, \rho = -0.67, r_d = 0.01, r_f = 0.02, K = 100.$$

In all the cases (5.10)-(5.12) above $S = 3000$ and $V = 15$ are taken, whereas the code performs the time integration until $T = 1$.

We apply the MOL approach on this model on a non-uniform spatial mesh following the ideas given in [21], since it is known that uniform spatial grids are not efficient on it. The reason is that the initial condition (5.9) is not smooth at $s = K$ and that for v close to 0 the PDE becomes advection-dominated. So we build a rectangular non-uniform grid

$$s_0 = 0 < s_1 < \dots < s_{n_1} = S, \quad v_0 = 0 < v_1 < \dots < v_{n_2} = V,$$

where many more points are close to $s = K$ and $v = 0$ than in the rest of the domain. We must take into account that, due to the boundary conditions (5.8), finite difference approximations are only applied at the nodes (s_i, v_j) with $1 \leq i \leq n_1$ and $0 \leq j \leq n_2 - 1$. At each node of this grid, the partial derivatives of the PDE (5.7) are approximated by the corresponding finite difference formulation given in detail in [21]. Roughly speaking, in the case of the derivatives $\partial_{ss}^2 u$, $\partial_{vv}^2 u$ and $\partial_s u$, second-order central differences are applied. However, due to a change in the direction of the advection for v , different formulations are used to approximate $\partial_v u$ when $0 \leq v_j \leq 1$ and $v_j > 1$. Finally, the mixed derivative $\partial_{sv}^2 u$ is approximated by second-order central differences for the first partial derivative in each spatial direction.

Adding the initial and boundary conditions (5.8)-(5.9) and putting all the finite differences together at each spatial point, we arrive at the following linear semi-discrete initial value problem of dimension $n_1 \cdot n_2$ of type (1.2)-(1.3)

$$(5.13) \quad \dot{U} = F(t, U) = \sum_{j=0}^2 F_j(t, U), \quad U(0) = U_0, \quad t \in [0, T]$$

where

$$(5.14) \quad F_0(t, U) = A_0 U + g_0 e^{-r_f t} - r_d U, \quad F_j(t, U) = A_j U + g_j e^{-r_f t}, \quad j = 1, 2.$$

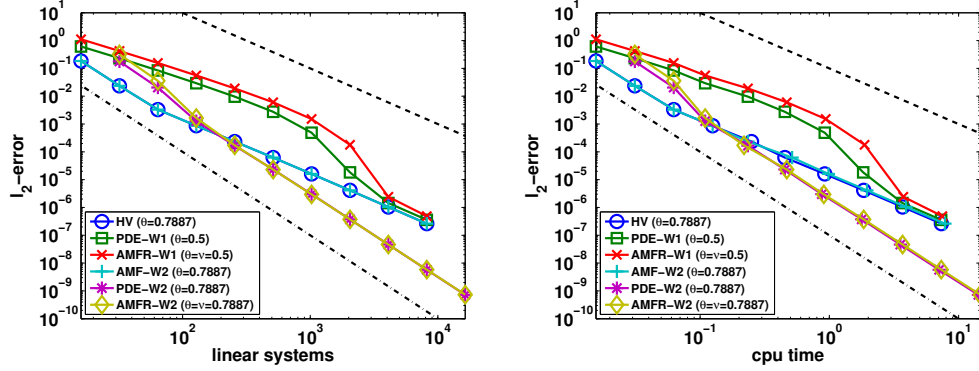


FIG. 5. Heston problem, case (5.10) with $n_1 = 200$ and $n_2 = 100$. Error vs Linear Systems (left). Error vs CPU Time (right).

$F_0(t, U)$ represents the splitting term corresponding to the mixed derivatives plus the (non-stiff) reaction, $\{g_j\}_{j=0}^2$ are constant vectors that come from the time-dependent boundary conditions (5.8) and the constant matrices A_1 and A_2 have simple structures

$$A_1 = \text{diag}(A_1^{(0)}, A_1^{(1)}, \dots, A_1^{(n_2-1)}), \quad A_2 = \tilde{A} \otimes I_{n_1},$$

where each submatrix $A_1^{(k)}$ is a tridiagonal matrix of dimension n_1 and \tilde{A} has dimension n_2 with only five non-zero diagonals. The constant matrix A_0 of dimension $n_1 \cdot n_2$ has nine non-zero bands (parallel to the main diagonal) that are non-consecutive but it is never used in the AMF (or ADI) factorizations. We mention that in [21] the splitting (5.13)-(5.14) is not applied in this way, since the reaction term $G(U) = -r_d U$ is included in the directional terms in the following way $F_j(t, U) = A_j U + g_j e^{-r_f t} - (r_d/2)U$, $j = 1, 2$. This does not imply any significant change in the numerical results below.

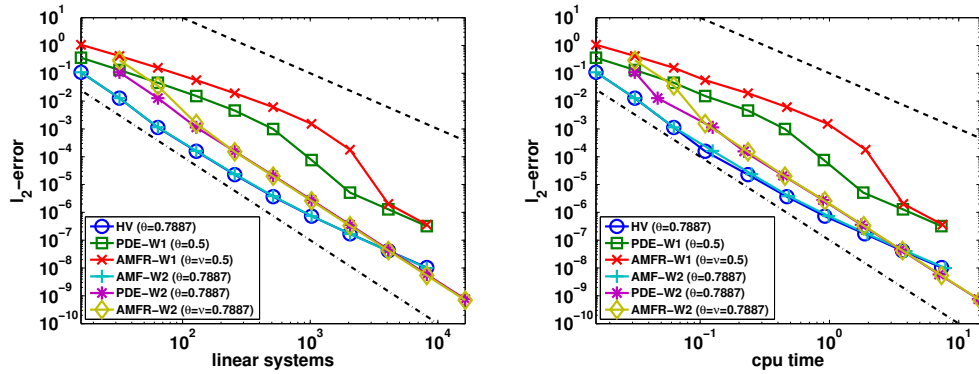


FIG. 6. Heston problem, case (5.11) with $n_1 = 200$ and $n_2 = 100$. Error vs Linear Systems (left). Error vs CPU Time (right).

Figures 5-7 show the results for the three cases (5.10)-(5.12), respectively, of the Heston problem with $n_1 = 200$ and $n_2 = 100$. Corresponding results for dimension $n_1 = 400$ and $n_2 = 200$ are presented in Figures 8-10. The time integrations have been carried out for $\tau = 2^{-j}$, $2 \leq j \leq 11$, and the global errors have been measured in the ℓ^2 -norm with respect

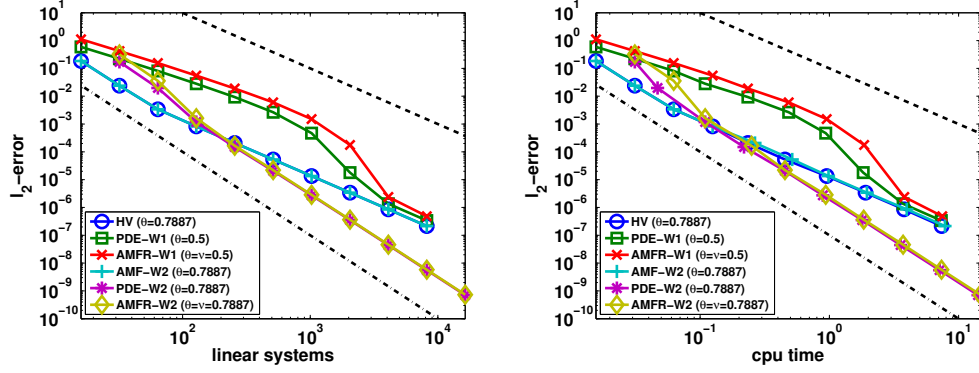


FIG. 7. Heston problem, case (5.12) with $n_1 = 200$ and $n_2 = 100$. Error vs Linear Systems (left). Error vs CPU Time (right).

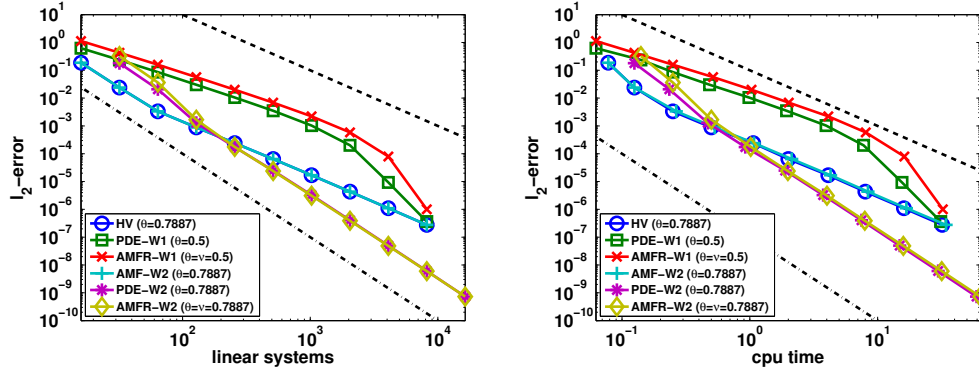


FIG. 8. Heston problem, case (5.10) with $n_1 = 400$ and $n_2 = 200$. Error vs Linear Systems (left). Error vs CPU Time (right).

to a reference solution at $T = 1$, obtained with the DOP853 code [14] at a very stringent tolerance. For the dimension $n_1 = 200$ and $n_2 = 100$, it can be nicely observed in Figures 5–7 that all methods confirm the achieved orders on the previous constant coefficient PDE (5.4), i.e., order around two for **HV**, **AMF-W2**, **PDE-W1**, **AMFR-W1** and order close to three for **AMFR-W2** and **PDE-W2**, but with the important difference that for these two latter methods the order three is maintained even in the case of time-dependent boundary conditions. Regarding the efficiency, it can be appreciated that the higher order methods, **PDE-W2** and **AMFR-W2**, are the most efficient in all cases (5.10)–(5.12). Nevertheless, in the case (5.11) **HV** and **AMF-W2** are also very competitive. Analogous considerations are applied to the dimension $n_1 = 400$ and $n_2 = 200$ in Figures 8–10, where it is also observed that the order for **PDE-W1** and **AMFR-W1** lies around 1.5 for large stepsizes.

6. Conclusions. Based on W-methods for the numerical solution of initial value problems in ordinary differential equations (ODEs), three different families of AMF-type methods have been proposed for the time integration of parabolic partial differential equations with mixed derivatives discretized in space via finite differences. These families mainly differ in the choice of the W-matrix. For the first family, denoted as AMF-W-methods, the corresponding W-choice is directional (ADI-type) and is an order-zero approximation to the true

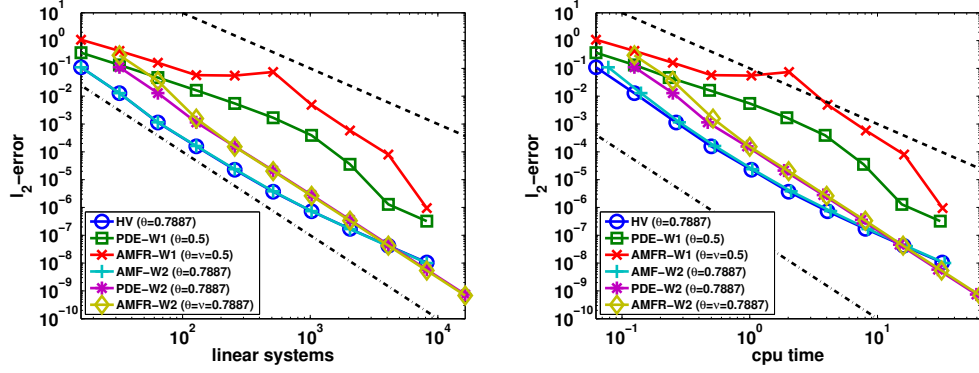


FIG. 9. Heston problem, case (5.11) with $n_1 = 400$ and $n_2 = 200$. Error vs Linear Systems (left). Error vs CPU Time (right).

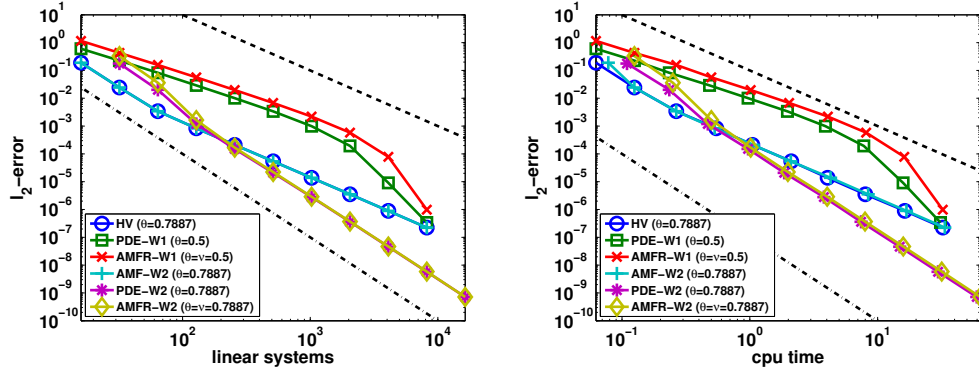


FIG. 10. Heston problem, case (5.12) with $n_1 = 400$ and $n_2 = 200$. Error vs Linear Systems (left). Error vs CPU Time (right).

ODE-Jacobian. The second one, denoted as PDE-W-methods, was previously introduced in [8] and represents an alternative to produce W -matrices with first order of approximation to the ODE-Jacobian. The third family, denoted as AMFR-W-methods also provides W -matrices with first order of approximation to the ODE-Jacobian, but allows the introduction of free parameter ν to improve the stability properties of the methods and it is based on applying some kind of refinement to the stages of the first family of methods.

An analysis of unconditional stability for these families on linear problems with constant coefficients has been provided. Both AMF-W- and AMFR-W-methods are unconditionally stable regardless of the spatial dimension m at the expense of possibly increasing the stability parameters (θ, ν) of the particular method. This aspect is shared with other classical ADI methods, like the Craig–Sneyd, Hundsdorfer–Verwer and the modified Craig–Sneyd schemes [22] whose temporal order of convergence is at most two. For PDE-W-methods, unconditional stability is only possible whenever $m \leq 3$, as it happens for the second order Craig–Sneyd scheme.

On the other hand, for the same number of implicit stages, the implementation of PDE-W- and AMFR-W-methods requires a similar computational cost, and this is about twice the cost associated to AMF-W-methods. Despite the lack of unconditional stability for PDE-W-methods in dimension $m \geq 4$, in case of stability, the numerical experiments provided show

similar performances for both PDE-W- and AMFR-W-methods.

The practical relevance of the methods has also been demonstrated by means of the 2D Heston model from financial option pricing, showing that both PDE-W- and AMFR-W-methods are good candidates to obtain temporal orders of convergence three. In some cases they outperform other classical ADI schemes like the Hundsdorfer–Verwer scheme [19, 20, 22], which has only order two.

7. Appendix.

LEMMA 7.1. *Let κ_m be the smallest positive zero of the polynomial*

$$(7.1) \quad g_m(x) = 2x \left(\frac{m-x}{m-1} \right)^{m-1} - 1.$$

These numbers satisfy (for $m \geq 2$)

$$(7.2) \quad \kappa_\infty \leq \kappa_{m+1} < \kappa_m, \quad (m+1)\kappa_{m+1} > m\kappa_m,$$

where $\kappa_\infty \approx 0.23196$ is the smallest positive zero of $g_\infty(x) = 2x \exp(1-x) - 1$.

Proof. Since $g_m(0) = -1$, $g_m(1) = 1$, and $g'_m(x) > 0$ for $x \in (0, 1)$, there exists a unique $\kappa_m \in (0, 1)$ satisfying $g_m(\kappa_m) = 0$.

Applying the well-known inequality (consequence of Bernoulli's inequality)

$$\left(1 + \frac{a}{m-1} \right)^{m-1} < \left(1 + \frac{a}{m} \right)^m$$

with $a = 1 - x$ yields $g_m(x) < g_{m+1}(x)$ for $x \in (0, 1)$. Consequently, we have $g_{m+1}(\kappa_m) > 0$, which implies $\kappa_{m+1} < \kappa_m$. Moreover, the sequence $\{\kappa_m\}$ converges for $m \rightarrow \infty$ to a zero of $g_\infty(x) = 2x \exp(1-x) - 1$, which gives the lower bound for all κ_m .

To prove the right inequality of (7.2), we check that $g_m\left(\frac{m+1}{m}x\right) > g_{m+1}(x)$, for all $m \geq 2$ and all $0 < x < \kappa_2 < 1/2$. This implies $g_m\left(\frac{m+1}{m}\kappa_{m+1}\right) > 0$ and thus also $m\kappa_m < (m+1)\kappa_{m+1}$. Its proof follows from

$$\frac{g_{m+1}(x) + 1}{g_m\left(\frac{m+1}{m}x\right) + 1} = \left(1 - \frac{1-2x}{m^2 - (m+1)x} \right)^{m-1} \left(\frac{m+1-x}{m+1} \right) < 1$$

because the modulus of each of the factors is smaller than 1 for $0 < x < 1/2$. \square

LEMMA 7.2. *Let $m \geq 2$. If $\delta \leq 1/(m\kappa_m)$ then we have*

$$(7.3) \quad f(y_1, \dots, y_m) := 2 \prod_{j=1}^m (1 + y_j^2) - 1 - \delta \left(\sum_{j=1}^m y_j \right)^2 \geq 0$$

for all $y_j \geq 0$, $j = 1, \dots, m$. Moreover, equality holds in (7.3) if and only if $y_1 = \dots = y_m = y$ for some $y \neq 0$.

Proof. From Lemma 7.1 and Table 2 we know that $m\kappa_m > 1/2$ for all $m \geq 2$, so that $\delta < 2$. To find the minimum of $f(y_1, \dots, y_m)$ we compute

$$(7.4) \quad \frac{\partial f}{\partial y_i}(y_1, \dots, y_m) = \frac{4y_i}{1 + y_i^2} \prod_{j=1}^m (1 + y_j^2) - 2\delta \sum_{j=1}^m y_j = 0.$$

For a critical point of $f(y_1, \dots, y_m)$ the expression $4y_i/(1 + y_i^2)$ has to be independent of i . Observe that $a/(1 + a^2) = b/(1 + b^2)$ implies $a = b$ or $ab = 1$. Denoting $y_1 = y$, all other components of an extremum have to be either equal to y or equal to $1/y$.

We shall prove that all components of an extremum are equal to y . Assume, by contradiction, that there is at least one component equal to $1/y$. Denoting by $1 \leq p < m$ the

number of components that are equal to y , we then have, because of $\delta < 2$,

$$\begin{aligned} \frac{\partial f}{\partial y_1}(y_1, \dots, y_m) &= 4\left(y + \frac{1}{y}\right)(1 + y^2)^{p-1}\left(1 + \frac{1}{y^2}\right)^{m-p-1} - 2\delta\left(py + (m-p)\frac{1}{y}\right) \\ &> 4\left(y + \frac{1}{y}\right)(1 + (p-1)y^2 + (m-p-1)\frac{1}{y^2}) - 4\left(py + (m-p)\frac{1}{y}\right) \\ &\geq 4\left((p-1)y^3 + (m-p-1)\frac{1}{y^3}\right) \geq 0. \end{aligned}$$

This contradicts (7.4) and implies that all components of an extremum have to be equal.

For all y_j equal to y , we write the function (7.3) as

$$(7.5) \quad f(y) = 2(1 + y^2)^m - 1 - \delta m^2 y^2.$$

For a critical point its derivative has to vanish,

$$(7.6) \quad f'(y) = 4my(1 + y^2)^{m-1} - 2\delta m^2 y = 0.$$

For $\delta m \leq 2$ the only critical point is $y = 0$, for which $f(0) = 1 \geq 0$. For $\delta m > 2$ we have a further critical point, denoted by y^* , which is implicitly defined by $2(1 + y^2)^{m-1} - \delta m = 0$. The value of $f(y^*)$ is

$$f(y^*) = (1 + y^2)\delta m - 1 - \delta m^2 y^2 = \delta m^2 - 1 + \delta m(1 - m)\left(\frac{\delta m}{2}\right)^{1/(m-1)}.$$

In (7.5) we have first substituted $2(1 + y^2)^{m-1}$ by δm , and then we have substituted y^2 by $(\delta m/2)^{1/(m-1)} - 1$. The condition $f(y^*) \geq 0$ becomes

$$\left(\frac{1 - \delta m^2}{\delta m(1 - m)}\right)^{m-1} \geq \frac{\delta m}{2} \quad \text{or} \quad 2x\left(\frac{m-x}{m-1}\right)^{m-1} \geq 1$$

with the new variable $x = 1/(\delta m) < 1/2$. It follows from the definition of κ_m and from the proof of Lemma 7.1 that this inequality holds if $\kappa_m \leq x \leq 1/2$, which translates into $2/m \leq \delta \leq 1/(m\kappa_m)$. This proves the estimate, if the minimum of $f(y_1, \dots, y_m)$ is attained in the interior of the domain.

On the border of $\{y_j \geq 0; j = 1, \dots, m\}$, where $y_j = 0$ for some j , the same argument can be applied with reduced m . The statement follows in this case from

$$\delta \leq \frac{1}{m\kappa_m} < \frac{1}{(m-1)\kappa_{m-1}} < \dots < \frac{1}{2\kappa_2}.$$

which is a consequence of Lemma 7.1. \square

Remark 7.3. A proof of the statement of Lemma 7.2 can be found in [22, Theorem 2.8, Appendix A]. The present proof, however, is more direct.

LEMMA 7.4. *Let $u = u(t, \vec{x})$ be a function defined for $t \geq 0$ and $\vec{x} = (x_1, \dots, x_m)^T \in \overline{\Omega}$, with $\Omega := (0, 1)^m$. For all $t \geq 0$ and $\vec{x} \in \overline{\Omega}$ let $u^{[0]} := u$, and define recursively for $j = 1, 2, \dots, m$ (using the notation of Section 5.4)*

$$(7.7) \quad \begin{cases} q_j &:= \left(\frac{x_j - 1}{0 - 1}\right)u_{|x_j=0}^{[j-1]} + \left(\frac{x_j - 0}{1 - 0}\right)u_{|x_j=1}^{[j-1]}, \\ u^{[j]} &:= u^{[j-1]} - q_j, \end{cases} \quad 1 \leq j \leq m,$$

and $\hat{u} := \sum_{j=1}^m q_j.$

Then it holds that $\hat{u}|_{\partial\Omega} = u|_{\partial\Omega}$.

Proof. From (7.7) we have for all $1 \leq j \leq m$ that $q_{j|_{x_j=0,1}} = u_{|_{x_j=0,1}}^{[j-1]}$, and hence

$$(7.8) \quad u_{|_{x_j=0,1}}^{[j]} = 0, \quad (j = 1, \dots, m).$$

Assume, by induction on j , that $u_{|_{x_k=0,1}}^{[j]} = 0$ for $1 \leq k \leq j \leq m-1$. It follows from (7.8) that $u_{|_{x_{j+1}=0,1}}^{[j+1]} = 0$, and from the definition of q_{j+1} that $q_{j+1|_{x_k=0,1}} = u_{|_{x_k=0,1}}^{[j]}$ for $1 \leq k \leq j$. This implies that

$$u_{|_{x_k=0,1}}^{[j+1]} = u_{|_{x_k=0,1}}^{[j]} - q_{j+1|_{x_k=0,1}} = 0, \quad (k = 1, \dots, j).$$

Therefore we have that $u_{|\partial\Omega}^{[m]} = 0$ and this concludes the proof since $u^{[m]} = u - \hat{u}$. \square

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