W-methods and Approximate Matrix Factorization for parabolic PDEs with mixed derivative terms

S. González-Pinto and D. Hernández-Abreu

Abstract In this chapter W-methods are combined with the Approximate Matrix Factorization technique (AMF) in alternating direction implicit (ADI) sense for the time integration of parabolic partial differential equations with mixed derivatives in the elliptic operator, previously discretized in space by means of Finite Differences. Three different families of AMF-type W-methods are introduced and their unconditional stability is analized regardless of the spatial dimension. To this aim, a scalar test equation is presented and it is shown to be relevant for the class of problems under consideration when either periodic or homogeneous Dirichlet boundary conditions are imposed. Numerical results comparing the proposed AMF-type W-methods and some classical ADI schemes in the literature for $2 \leq m \leq 4$ space dimensions are presented.

1 ADI and W-methods

This chapter deals with the time integration of parabolic partial differential equations (PDEs) with mixed derivative terms discretized by means of the method of lines (MoL). On an m-dimensional box, which for ease of presentation we take $\Omega = (0,1)^m \subset \mathbb{R}^m$, and for $t > 0$ we consider the PDE problem

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$$\begin{aligned}
&\partial_t u = \textstyle\sum_{i,j=1}^m \alpha_{i,j}(t,\mathbf{x})\,\partial^2_{x_i x_j} u + \sum_{j=1}^m \eta_j(t,\mathbf{x})\partial_{x_j} u + g(t,\mathbf{x},u)\\
&\qquad \mathbf{x} = (x_1,\ldots,x_m)^\top \in \Omega, \quad t \in (0,T],\\
&u(t,\mathbf{x}) = \beta(t,\mathbf{x}), \quad (t,\mathbf{x}) \in (0,T] \times \partial\Omega,\\
&u(0,\mathbf{x}) = u_0(\mathbf{x}), \quad \mathbf{x} \in \Omega,
\end{aligned} \tag{1}$$

where $\partial\Omega$ denotes the boundary of Ω ($\bar{\Omega} = \Omega \cup \partial\Omega$), $g(t,\mathbf{x},u)$ stands for the reaction terms, $\eta_j(t,\mathbf{x})$ corresponds to advection terms on each space variable and the diffusion terms are those corresponding to the coefficient matrix $\mathscr{A} = (\alpha_{i,j}(t,\mathbf{x}))_{i,j=1}^m$, which is assumed to be symmetric and positive definite for each $(t,\mathbf{x}) \in [0,T] \times \bar{\Omega}$. In the sequel $\mathscr{A} > 0$ indicates that $\mathscr{A}$ is a positive definite matrix. The PDE problem is provided with an initial condition and Dirichlet boundary conditions.

With a space discretization of (1) by means of Finite Differences (or Finite Volumes) large systems of Ordinary Differential Equations (ODEs) arise

$$\dot{U} = F(t,U), \quad U(0) = U_0, \quad t \in [0,T], \tag{2}$$

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. Inspired by the Alternating Direction Implicit (ADI) approach [23, 2], the function $F(t,U)$ is typically split as

$$F(t,U) = \sum_{j=0}^m F_j(t,U), \tag{3}$$

where for each $j = 1,\ldots,m$, $F_j(t,U)$ contains the terms corresponding to space derivatives with respect to x_j (including boundary conditions). Here, it is assumed that $F_0(t,U)$ includes the terms corresponding to the mixed derivatives and their respective boundary conditions, as well as the discretization of the reaction terms, which are assumed to be non-stiff or mildly stiff.

Alternating Direction Implicit schemes, in the absence of mixed derivatives, were proposed by Peaceman, Rachford, and Douglas (see [23] and [2]) in order to reduce the computational cost in the solution of the arising linear systems to the level of one dimensional problems (with matrices having a banded structure with small bandwidths). Craig and Sneyd [1] then came up with a second order scheme for parabolic problems with mixed derivatives. More recently, other ADI schemes of order two have become popular for the time integration of parabolic problems with mixed derivatives, in particular in the context of applications in financial mathematics. Examples of such schemes are the *Hundsdorfer-Verwer* (HV) method [16, 17, 19]

$$
\begin{aligned}
Y_0 &= U_n + \tau F(t_n, U_n),\\
Y_j &= Y_{j-1} + \theta\tau\big(F_j(t_{n+1}, Y_j) - F_j(t_n, U_n)\big), \quad j = 1,\dots,m,\\
\widetilde{Y}_0 &= Y_0 + \mu\tau\big(F(t_{n+1}, Y_m) - F(t_n, U_n)\big),\\
\widetilde{Y}_j &= \widetilde{Y}_{j-1} + \theta\tau\big(F_j(t_{n+1}, \widetilde{Y}_j) - F_j(t_{n+1}, Y_m)\big), \quad j = 1,\dots,m,\\
U_{n+1} &= \widetilde{Y}_m,
\end{aligned}
\tag{4}
$$

with $\mu = 1/2$ to get classical order two (and $\theta > 0$ for stability), and the *modified Craig-Sneyd* (MCS) scheme [19, 20]

$$
\begin{aligned}
Y_0 &= U_n + \tau F(t_n, U_n),\\
Y_j &= Y_{j-1} + \theta\tau\big(F_j(t_{n+1}, Y_j) - F_j(t_n, U_n)\big), \quad j = 1,\dots,m,\\
\widehat{Y}_0 &= Y_0 + \sigma\tau\big(F_0(t_{n+1}, Y_m) - F_0(t_n, U_n)\big),\\
\widetilde{Y}_0 &= \widehat{Y}_0 + \mu\tau\big(F(t_{n+1}, Y_m) - F(t_n, U_n)\big),\\
\widetilde{Y}_j &= \widetilde{Y}_{j-1} + \theta\tau\big(F_j(t_{n+1}, \widetilde{Y}_j) - F_j(t_n, U_n)\big), \quad j = 1,\dots,m,\\
U_{n+1} &= \widetilde{Y}_m,
\end{aligned}
\tag{5}
$$

with parameters $\sigma = \theta$ and $\mu = \frac{1}{2} - \theta$ to get order two and $\theta > 0$. The original second order Craig-Sneyd scheme [1] is obtained from (5) when $\mu = 0$ and $\sigma = \theta = \frac{1}{2}$. Above, $\tau > 0$ stands for the time stepsize to advance from (t_n, U_n) to (t_{n+1}, U_{n+1}).

Both schemes (4) and (5) are extensions of the Douglas scheme [2], which is obtained by considering just the first two lines of either methods, but this latter method is only order one when $F_0 \neq 0$. The HV scheme has been recently considered together with space discretizations of order 4 in [3] and applied to stochastic volatility models in financial option pricing in [4]. Compact schemes of order 4 in space based on both the MCS and the HV schemes have been also recently treated in [13, 14].

In this chapter our focus is on W-methods ([27], [12, 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 ODE. W-methods do not require the solution of nonlinear systems and they allow the use of non-exact approximations for the Jacobian of the vector field, providing both a high classical order and good stability properties.

Considering time t as an independent variable, and augmenting (2) with $\dot{t} = 1$ yields for $y = (t, U)^\top$ an autonomous system

$$
\dot{y} = f(y), \quad y(0) = y_0, \quad t \in [0, T]. \tag{6}
$$

The splitting (3) leads to a splitting of the form

$$\dot{y}(t) = f(y) = \sum_{j=0}^{m} f_j(y) = \begin{pmatrix} 1 \\ F_0(t,U) \end{pmatrix} + \sum_{j=1}^{m} \begin{pmatrix} 0 \\ F_j(t,U) \end{pmatrix}, \tag{7}$$

for which the corresponding splitting for the full Jacobian is then given by

$$\partial_y f(y_n) = \sum_{j=0}^{m} \partial_y f_j(y_n) = \sum_{j=0}^{m} \begin{pmatrix} 0 & 0 \\ \partial_t F_j(t_n,U_n) & \partial_U F_j(t_n,U_n) \end{pmatrix}. \tag{8}$$

Now, for the autonomous problem (6), let y_n be a numerical approximation to $y(t)$ at t_n. Then, with a stepsize $\tau > 0$, the numerical approximation y_{n+1} provided by a $s-$stage W-method at $t_{n+1} = t_n + \tau$ is defined by

$$\begin{aligned} (I - \theta\tau W)\tilde{K}_i &= \tau f\Big(y_n + \sum_{j=1}^{i-1} a_{i,j}\tilde{K}_j\Big) + \sum_{j=1}^{i-1} \ell_{i,j}\tilde{K}_j, \quad i = 1,2,\dots,s, \\ y_{n+1} &= y_n + \sum_{i=1}^{s} b_i\tilde{K}_i. \end{aligned} \tag{9}$$

The matrix W is arbitrary, but it is intended to approximate $\partial_y f(y_n)$. For $W = \partial_y f(y_n)$ we obtain the underlying ROW or Rosenbrock method. It is characterized by the coefficients (A,L,b,θ), where $A = (a_{i,j})_{j<i}$, $L = (\ell_{i,j})_{j<i}$ and $b = (b_i)_i$. The coefficient matrix $A(I-L)^{-1}$ and the weight vector $b^T(I-L)^{-1}$ define the underlying explicit Runge-Kutta method associated to the W-method (see, e.g., [9]).

In the literature, several options for the selection of the matrix W have been considered. Some methods up to order of consistency four under the assumption

$$W - \partial_y f(y_n) = \mathscr{O}(\tau), \qquad \tau \to 0, \tag{10}$$

have been introduced in [5, 9, 22, 25]. A more general situation where the commutator satisfies

$$[W, \partial_y f(y_n)] := W\partial_y f(y_n) - \partial_y f(y_n)W = \mathscr{O}(\tau), \qquad \tau \to 0, \tag{11}$$

was studied in [10] and some families of third order methods under such assumption were presented. The construction of efficient W-methods of order ≥ 3 in the general setting $W - \partial_y f(y_n) = \mathscr{O}(1)$ is a demanding task due to the high number of order conditions to be satisfied, see e.g. [12, 21]. In [24] some W-methods of order four and six stages have been built. It is worth to mention that the assumptions in (10) and (11) are in ODE sense, since negative powers of the space resolutions are present in the Jacobian matrices and in their approximations W.

In this chapter time integrators that can be applied to general problems of the form (1) are considered, although the emphasis is on a stability analysis that gives insight into the linear diffusion problem

$$\partial_t u = \sum_{i,j=1}^{m} \alpha_{i,j}\, \partial^2_{x_i x_j} u \tag{12}$$

with homogeneous Dirichlet boundary conditions and a constant positive definite coefficient matrix $\mathscr{A} = (\alpha_{i,j})_{i,j=1}^m$ so that the right-hand side represents an elliptic operator. A standard central finite difference discretization yields $\dot{U} = \mathscr{M}U$, where

$$\begin{aligned}\mathscr{M} &= \sum_{i=1}^{m} \alpha_{i,i}(I_{n_{x_m}} \otimes \ldots \otimes D_{x_i x_i} \otimes \ldots \otimes I_{n_{x_1}}) \\ &\quad + 2 \sum_{1\le i<j\le m} \alpha_{i,j}(I_{n_{x_m}} \otimes \ldots \otimes D_{x_j} \otimes \ldots \otimes D_{x_i} \otimes \ldots \otimes I_{n_{x_1}}),\end{aligned} \tag{13}$$

where I_p denotes the identity matrix of dimension p and $D_{x_i x_i}$ and D_{x_i} are banded differentiation matrices approaching the second and first order spatial derivatives, respectively, placed in the $(m-i+1)$th position of the tensor product. For the usual second order central discretization $D_{x_i x_i}$ and D_{x_i} are tridiagonal matrices with entries $(1,-2,1)/\Delta x_i^2$ and $(-1,0,1)/(2\Delta x_i)$, respectively, where $\Delta x_i = 1/(n_{x_i}+1)$ is the spacing in the x_i direction.

The analysis of unconditional stability on linear diffusion problems with constant coefficients for the schemes (4)-(5) in the case of periodic boundary conditions and some general finite difference discretizations for the mixed derivatives was carried out in [19]. From [19, Table 1] we borrow the following Table 1 indicating the values of $\theta \ge \theta_0$ for which the schemes (4)-(5) are unconditionally stable when applied to problems of the form (12). We also point out that the second order Craig-Sneyd scheme (obtained from (5) with $\mu = 0$ and $\sigma = \theta = \frac{1}{2}$) is unconditionally stable whenever $m = 2,3$, but not for $m \ge 4$.

m	2	3	4	5	6	7	8	9
HV (4)	0.293	0.402	0.515	0.630	0.745	0.860	0.975	1.091
MCS (5)	0.333	0.462	0.593	0.726	0.860	0.994	1.128	1.262

Table 1 Values of $\theta \ge \theta_0$ providing unconditional stability for the schemes (4) and (5), respectively, on the problem (12).

In Section 2 three different options to produce W-methods based on the Approximate Matrix Factorization (AMF), see e.g. [28, 17], for the time integration of (2)-(3) are introduced. These schemes are obtained in terms of the selection of the preconditioner $(I-\theta\tau W)$ in (9) and they slightly differ in computational cost, stability properties and consistency order (in ODE sense). However, the computational costs are quite reasonable, since very few function evaluations and linear systems solves with small bandwidth per integration step are required. In Section 3 the unconditional stability for these AMF-type W-methods on linear parabolic problems with mixed derivatives and constant coefficients (12) is analyzed.

2 W-methods based on AMF-type splitting

To solve the linear equations in (9) we set

$$\tilde{K}_i = \begin{pmatrix} \tau\rho_i \\ K_i \end{pmatrix}, \quad \rho_i \in \mathbb{R}, \quad i = 1,\dots,s. \tag{14}$$

According to (8), the matrix W approximating $\partial_y f(y_n)$ will be required to have the structure

$$W = \begin{pmatrix} 0 & \mathbf{0} \\ \times & \mathbf{X} \end{pmatrix}.$$

Then, from (9) and (7), for each stage $(i = 1,\dots,s)$ we deduce that

$$\begin{aligned} (I-\theta\tau W)\begin{pmatrix} \tau\rho_i \\ K_i \end{pmatrix} &= \left[\tau\begin{pmatrix} 1 \\ F(t_n + c_i\tau, U_n + \sum_{j=1}^{i-1} a_{ij}K_j) \end{pmatrix} + \sum_{j=1}^{i-1} \ell_{ij}\begin{pmatrix} \tau\rho_j \\ K_j \end{pmatrix}\right], \\ \begin{pmatrix} t_{n+1} \\ U_{n+1} \end{pmatrix} &= \begin{pmatrix} t_n \\ U_n \end{pmatrix} + \sum_{i=1}^{s} b_i \begin{pmatrix} \tau\rho_i \\ K_i \end{pmatrix}, \end{aligned} \tag{15}$$

with

$$\rho = (\rho_i)_{i=1}^s = (I-L)^{-1}\mathbf{1}, \quad c = (c_i)_{i=1}^s = A\rho. \tag{16}$$

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

$$A_{n,j} := \partial_U F_j(t_n, U_n), \quad a_{n,j} = \partial_t F_j(t_n, U_n), \quad j = 0,1,\dots,m. \tag{17}$$

Next, based on W-methods for the numerical solution of initial value problems in ordinary differential equations (ODEs), three different families of AMF-type methods will be proposed. 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 ODE-Jacobian. The second one, denoted as PDE-W-methods, was introduced in [7] 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 a free parameter to improve the stability properties of the methods and it is based on applying linear refinements to the stages of the first family of methods.

2.1 AMF-W methods

In this case the choice for $(I-\tau\theta W)$ in (15) is based on the Approximate Matrix Factorization, but neglecting in it the Jacobian terms corresponding to the mixed derivatives, i.e.,

$$(I-\theta\tau W)=\prod_{j=1}^{m}\begin{pmatrix}1 & 0\\ -\theta\tau a_{n,j} & (I-\tau\theta A_{n,j})\end{pmatrix}. \tag{18}$$

Here, and in the rest of the chapter, the product of matrices is defined as $\prod_{j=1}^{m}M_j=M_m\ldots M_1$.

By performing the calculations in (15) it is not difficult to check that the stages are computed one after the other (for $i=1,\ldots,s$) by the formula

$$\begin{aligned}K_i^{(0)} &= \tau F(t_n+c_i\tau, U_n+\textstyle\sum_{j=1}^{i-1}a_{ij}K_j)+\sum_{j=1}^{i-1}\ell_{ij}K_j\\ (I-\theta\tau A_{n,j})K_i^{(j)} &= K_i^{(j-1)}+\theta\rho_i\tau^2 a_{n,j}, \quad (j=1,\ldots,m)\\ K_i &= K_i^{(m)}.\end{aligned} \tag{19}$$

The numerical solution after one step is then given by

$$U_{n+1}=U_n+\sum_{i=1}^{s}b_iK_i. \tag{20}$$

2.2 PDE-W methods

PDE-W-methods were introduced in [7, Section 5] and they represent a modification of the AMF-W method (19) so that (10) is satisfied. Observe that $\partial_y f_0(y_n)$ has large positive and negative eigenvalues, so that an application of $\big(I-\theta\tau\partial_y f_0(y_n)\big)^{-1}$ would imply a step size restriction as for explicit time integrators. Moreover, $\partial_y f_0(y_n)$ is not a banded matrix with small band-width. Then, the idea is to approximate the AMF factor

$$\Big(I-\theta\tau\partial_y f_0(y_n)\Big)^{-1} \approx I+\theta\tau\partial_y f_0(y_n)\prod_{j=1}^{m}\big(I-\theta\tau\partial_y f_j(y_n)\big)^{-1}. \tag{21}$$

We then have $\big(I-\theta\tau\partial_y f_0(y_n)\big)^{-1}\approx I+\theta\tau\partial_y f_0(y_n)$, but before applying the operator $\partial_y f_0(y_n)$ the large eigenvalues are damped by applying successively $\big(I-\theta\tau\partial_y f_j(y_n)\big)^{-1}$, $1\le j\le m$. Hence, with the notation (17), PDE-W-methods are obtained with the following choice in (15)

$$
\begin{aligned}
(I-\theta\tau W)^{-1} = P_m^{-1}\left(I+\theta\tau\begin{pmatrix} 0 & 0 \\ a_{n,0} & A_{n,0}\end{pmatrix} P_m^{-1}\right),\\
P_m := \prod_{j=1}^{m}\begin{pmatrix} 1 & 0 \\ -\theta\tau a_{n,j} & (I-\theta\tau A_{n,j})\end{pmatrix}.
\end{aligned}
\tag{22}
$$

The stages of the PDE-W method (A,L,b,θ) are computed for $i=1,\dots,s$, as follows:

$$
\begin{aligned}
K_i^{(0)} &= \tau F(t_n+c_i\tau, U_n+\textstyle\sum_{j=1}^{i-1} a_{ij}K_j)+\sum_{j=1}^{i-1}\ell_{ij}K_j\\
(I-\theta\tau A_{n,j})K_i^{(j)} &= K_i^{(j-1)}+\theta\rho_i\tau^2 a_{n,j}, \qquad (j=1,\dots,m)\\
\hat{K}_i^{(0)} &= K_i^{(0)}+\theta\tau A_{n,0}K_i^{(m)}+\theta\rho_i\tau^2 a_{n,0}\\
(I-\theta\tau A_{n,j})\hat{K}_i^{(j)} &= \hat{K}_i^{(j-1)}+\theta\rho_i\tau^2 a_{n,j}, \qquad (j=1,\dots,m)\\
K_i &= \hat{K}_i^{(m)},
\end{aligned}
\tag{23}
$$

with advancing solution after one step given by (20).

2.3 AMFR-W methods

The AMFR-W methods have been recently introduced in [6] and they are based on the iteration

$$
(I-\mu\tau V)(x^{(p)}-x^{(p-1)}) = \tilde{d}-(I-\theta\tau J)x^{(p-1)}, \quad p=1,2,3,\dots \tag{24}
$$

to solve linear systems of the form,

$$
(I-\theta\tau J)x=\tilde{d}, \quad \theta>0, \quad \tau>0. \tag{25}
$$

The convergence of this iteration for an arbitrary initial approximation $x^{(0)}$ is determined by the spectral radius ($\mathfrak{p}$) of the matrix $\mathscr{P}$ below,

$$
\mathscr{P}=\tau(I-\mu\tau V)^{-1}(\theta J-\mu V), \quad \mathfrak{p}(\mathscr{P})<1.
$$

In [8, Sections 3-5] the authors followed this approach to derive some W-methods and other kind of AMF-W methods (see Theorems 5 and 11 in [8]) based on one- or two-stage ROW methods with orders of consistency two and three, respectively. Only two iterations per stage and $x^{(0)}=0$ are needed to recover the full order of convergence of the underlying ROW method in both cases. Here, we follow the same approach for any W-method applied to parabolic problems with mixed derivatives, but treating the Jacobian for the mixed derivatives in an explicit way, i.e., it is not included in the AMF-factorization. It is also important to remark that this iteration introduces a new parameter μ, that will allow to improve the stability properties of the method.

The second iteration (which is a refinement of the first approximation $x^{(1)}$) in (24) by taking as initial guess $x^{(0)} = 0$ gives

$$x^{(2)} = (I - \theta\tau W)^{-1}\tilde{d},$$

where

$$(I - \theta\tau W)^{-1} = (I - \mu\tau V)^{-1}\left(2I - (I - \theta\tau J)(I - \mu\tau V)^{-1}\right). \tag{26}$$

It should be observed that this approach implies

$$J - W = \mathscr{O}(\tau), \quad \tau \to 0, \quad \forall\,\mu,\,\forall\,V.$$

The AMFR-W method can be seen as a refined AMF-W method and it is obtained from (15) with the choice made in (26) and (27)

$$\begin{aligned} I - \mu\tau V &= \prod_{j=1}^{m}\begin{pmatrix} 1 & 0 \\ -\mu\tau a_{n,j} & (I - \mu\tau A_{n,j}) \end{pmatrix}, \\ J &= \begin{pmatrix} 0 & 0 \\ \partial_t F(t_n, U_n) & \partial_U F(t_n, U_n) \end{pmatrix}. \end{aligned} \tag{27}$$

For a given ROW (A, L, b, θ), the corresponding AMFR-W method (A, L, b, θ, μ) is then given by the following formulation. For $i = 1, 2, \ldots, s$, compute K_i from:

$$\begin{aligned} K_i^{(0)} &= \tau F(t_n + c_i\tau, U_n + \textstyle\sum_{j=1}^{i-1} a_{ij}K_j) + \sum_{j=1}^{i-1}\ell_{ij}K_j \\ (I - \mu\tau A_{n,j})K_i^{(j)} &= K_i^{(j-1)} + \mu\rho_i\tau^2 a_{n,j}, \quad (j = 1, \ldots, m) \\ \hat{K}_i^{(0)} &= 2K_i^{(0)} + \theta\rho_i\tau^2\partial_t F(t_n, U_n) - (I - \theta\tau\partial_U F(t_n, U_n))K_i^{(m)}, \\ (I - \mu\tau A_{n,j})\hat{K}_i^{(j)} &= \hat{K}_i^{(j-1)} + \mu\rho_i\tau^2 a_{n,j}, \quad (j = 1, \ldots, m) \\ K_i &= \hat{K}_i^{(m)}. \end{aligned} \tag{28}$$

The numerical solution after one step is then computed from (20).

Remark 1. For the same number of 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.

3 Stability

The study of stability for W-methods gets complicated due to the fact that the matrices W and $\partial_y f(y_n)$ do not need to commute. In this section a scalar test equation is proposed that is relevant for a large class of partial differential equations for which the dominant part is an elliptic operator with constant coefficients endowed either with periodic boundary conditions [19] or homogeneous Dirichlet boundary conditions [7]. An analysis of unconditional stability for the families of methods presented in Section 2 on linear problems with constant coefficients is provided below. This stability analysis comprises some results that can also be found in [7, 6]. Both AMF-W- and AMFR-W-methods will be seen to be unconditionally stable regardless of the spatial dimension m at the expense of possibly increasing the stability parameters 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 [19] 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.

A standard second-order central space discretization of (12) leads to the linear ordinary differential equation

$$\dot{U} = \mathscr{M} U, \qquad U(0) = U_0, \tag{29}$$

where $\mathscr{M}$ is given by (13). The difficulty of studying the stability of time integrators lies in the fact that the differentiation matrices D_{x_i} =TriDiag$(-1,0,1)/(2\Delta x_i)$ and $D_{x_i x_i}$ =TriDiag$(1,-2,1)/\Delta x_i^2$ do not commute.

Theorem 1. *If the coefficient matrix $\mathscr{A} = (\alpha_{ij})_{i,j=1}^m$ in (12) is positive definite, then the system (29) is asymptotically stable.*

Proof. The main idea is to approximate $D_{x_i x_i}$ by $D_{x_i}^2$ and to study the resulting defect. The matrix $\mathscr{M}$ can be split as $\mathscr{M} = \mathscr{M}_0 + \sum_{i=1}^m \mathscr{M}_i$ with

$$\begin{aligned} \mathscr{M}_i &= \alpha_{i,i}(I_{n_{x_m}} \otimes \ldots \otimes \left(D_{x_i x_i} - D_{x_i}^2\right) \otimes \ldots \otimes I_{n_{x_1}}), \qquad i = 1,\ldots,m, \\ \mathscr{M}_0 &= \sum_{i,j=1}^m \alpha_{i,j}(I_{n_{x_m}} \otimes \ldots \otimes D_{x_j} \otimes \ldots \otimes D_{x_i} \otimes \ldots \otimes I_{n_{x_1}}). \end{aligned}$$

First, we observe the relation

$$D_{x_i x_i} = D_{x_i}^2 - \frac{\Delta x_i^2}{4} D_{x_i x_i}^2 - \frac{1}{2\Delta x_i^2} \operatorname{Diag}(1,0,\ldots,0,1),$$

which implies that the logarithmic norm of the defect $D_{x_i x_i} - D_{x_i}^2$ is negative for $i = 1,\ldots,m$.

Secondly, if we let v_i be an eigenvector of D_{x_i} (recall that the eigenvectors form an orthogonal base of $\mathbb{C}^{n_{x_i}}$, $n_{x_i} = 1/\Delta x_i - 1$) with eigenvalue $\mathrm{i}\lambda_i$, then $v_m \otimes \ldots \otimes v_1$ is an eigenvector of $\mathscr{M}_0$ corresponding to the eigenvalue

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

This proves the asymptotic stability of the system (29). □

Motivated by Theorem 1 we replace $D_{x_ix_i}$ by $D_{x_i}^2$ in $\mathscr{M}$, so that the system (29) can be decoupled into scalar linear ODEs of the form

$$\dot{u} = -\Big(\sum_{i,j=1}^{m} \alpha_{i,j}\lambda_i\lambda_j\Big)u, \quad \lambda_i \in \mathbb{R}\ \ (i=1,\dots,m) \tag{30}$$

where $\mathrm{i}\lambda_i$ represents an eigenvalue of D_{x_i} and $\mathscr{A} = (\alpha_{i,j})_{i,j=1}^m$ is a symmetric positive definite matrix. Let us now consider the change

$$\lambda_i \leftrightarrow \lambda_i\sqrt{\alpha_{i,i}}, \quad c_{i,j} = \alpha_{i,j}/\sqrt{\alpha_{i,i}\cdot\alpha_{j,j}}, \quad \mathscr{C} = (c_{i,j})_{i,j=1}^m > 0, \tag{31}$$

which reduces the scalar test problem (30) to

$$\dot{u} = -\Big(\sum_{i=1}^{m}\lambda_i^2 + 2\sum_{1\le i<j\le m} c_{i,j}\lambda_i\lambda_j\Big)u, \quad \lambda_i \in \mathbb{R}\ \ (i=1,\dots,m). \tag{32}$$

Observe that the diagonal elements of the matrix $\mathscr{C} > 0$ 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 $1 \le i,j \le m$, $i \neq j$.

Now, applying an AMF-type W-method to (32) with the splitting

$$F_j(t,u) = -\lambda_j^2 u\ (j=1,\dots,m), \quad F_0(t,u) = \left(-2\sum_{i<j} c_{i,j}\lambda_i\lambda_j\right)u, \tag{33}$$

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

$$z = z_0 + \sum_{j=1}^{m} z_j, \quad z_0 = -2\tau\sum_{1\le i<j\le m} c_{i,j}\lambda_i\lambda_j, \quad z_j = -\tau\lambda_j^2,\ 1\le j\le m, \quad \tau>0. \tag{34}$$

This rational function is called the *linear stability function* of the method. For an AMF-type W-method based on the coefficients (A,L,b,θ), it is given by

$$R(z,z_1,\dots,z_m) = 1 + zb^\top\big(\tilde{\Pi}_m(\theta)\,I - L - zA\big)^{-1}\mathbf{1} \tag{35}$$

where $\mathbf{1} := (1,\dots,1)^\top \in \mathbb{R}^s$ and for each AMF approximation (18), (22) and (26)-(27) in section 2, it holds that

$$\text{(A)} \qquad \frac{1}{\tilde{\Pi}_m(\theta)} = \frac{1}{\Pi_m(\theta)}, \qquad \text{for AMF-W-methods,}$$

$$\text{(B)} \qquad \frac{1}{\tilde{\Pi}_m(\theta)} = \frac{1}{\Pi_m(\theta)}\left(1 + \frac{\theta z_0}{\Pi_m(\theta)}\right), \qquad \text{for PDE-W-methods,}$$

$$\text{(C)} \qquad \frac{1}{\tilde{\Pi}_m(\theta)} = \frac{1}{\Pi^*_m(\mu,\theta)}, \qquad \text{for AMFR-W-methods,}$$

$$\text{where} \quad \Pi_m(\theta) := \textstyle\prod_{j=1}^m (1-\theta z_j), \qquad \frac{1}{\Pi^*_m(\mu,\theta)} := \frac{1}{\Pi_m(\mu)}\left(2 - \frac{1-\theta z}{\Pi_m(\mu)}\right). \tag{36}$$

Of course, in case (C), the AMF factor $\tilde{\Pi}_m(\theta)$ depends on the additional parameter $\mu > 0$.

It should be also noticed from (34) that $z \le 0$, for all $\lambda_j \in \mathbb{R}$, $\tau > 0$, because of the positive definiteness of the matrix $\mathscr{C}$.

Definition 1. A time integrator which, when applied to the test equation (32), yields the recursion $u_{n+1} = R(z, z_1, \ldots, z_m)u_n$ with stability function (35), is called unconditionally stable for a given $m \ge 2$, if

$$|R(z, z_1 \ldots, z_m)| \le 1$$

for all $z, z_1 \ldots, z_m$ of (34) and each matrix $\mathscr{C} > 0$.

The unconditional stability properties of AMF-type W-methods rely on the linear stability of the underlying ROW method (A, L, b, θ), whose linear stability function is obtained from (35) by replacing the AMF factor $\tilde{\Pi}_m(\theta)$ by $1-\theta z$. Hence, it is given by

$$R_\theta(z) = 1 + zb^T\left((1-\theta z)I - L - zA\right)^{-1}\mathbf{1}, \quad z \in \mathbb{C}. \tag{37}$$

The ROW-method (A, L, b, θ) is A_0-stable when its stability function (37) fulfils

$$|R_\theta(x)| \le 1, \quad \text{for all } x \le 0.$$

The range of values for $\theta \ge \theta_0$ providing A_0-stable methods is known for many Rosenbrock methods. The most simple one-stage W-method is given by, (see e.g. [17, p. 398])

$$\left(I - \theta\tau W\right)(y_{n+1} - y_n) = \tau f(y_n). \tag{38}$$

It is of classical order 1, and for $\theta = 1/2$ reaches order 2 if (10) holds. Its stability function is

$$R_\theta(z) = 1 + \frac{z}{1-\theta z}, \tag{39}$$

and the method is A_0-stable whenever $\theta \ge 1/2$.

For two-stage methods, there is a two-parameter family of W-methods of order ≥ 2 (see [17, p. 400]) with free parameters θ, b_2 and coefficients given by

$$b_1 = 2 - b_2, \qquad a_{21} = \frac{1}{2b_2}, \qquad \ell_{21} = -\frac{1}{b_2}. \tag{40}$$

It is not difficult to check that the stability function for the methods (40) only depends on the stability parameter θ and is given by

$$R_\theta(z) = 1 + \frac{2z}{1-\theta z} + \frac{z(z-2)}{2(1-\theta z)^2} \tag{41}$$

and A_0-stability is obtained as long as $\theta \geq 1/4$.

On the other hand, a family of 3-stage W-methods of order ≥ 3 under the special assumption (11) was studied in [10, Theorem 1]. There it was shown that, under the assumption (11), there exist two three-parametric families of 3-stage W-methods of order three, with free parameters a_{32}, a_{21} and θ, satisfying $a_{32}a_{21} \neq 0$, whose coefficients are given by

$$\begin{aligned}
&b_3 = \frac{1}{6a_{32}a_{21}}, \qquad \ell_{21} = ra_{21}, \qquad \ell_{32} = \frac{6}{r}a_{32},\\
&a_{31}^2 + (-a_{21} + 2a_{32} + 2ra_{32}a_{21})\,a_{31} + \left[a_{32}(a_{32} + a_{21}(-3 + 2ra_{32}) + a_{21}^2(6/r + 9 + r^2 a_{32}))\right] = 0,\\
&b_2 = \frac{3/2 - b_3(a_{31} + a_{32})}{a_{21}}, \qquad \ell_{31} = -\frac{3 + b_2\ell_{21} + b_3\ell_{32}}{b_3}, \qquad b_1 = 3 - (b_2 + b_3).
\end{aligned} \tag{42}$$

and $r = -3 \pm \sqrt{3}$. All the methods in (42) have the same stability function (depending only on θ), which is given by

$$R_\theta(z) = 1 + \frac{3z}{1-\theta z} + \frac{3z(z-2)}{2(1-\theta z)^2} + \frac{z(z^2-6z+6)}{6(1-\theta z)^3}. \tag{43}$$

In this case, A_0-stability is obtained for $\theta \geq 1/3$. It must also be observed that there do not exist 3-stage W-methods of order 3 without any restriction on W [27].

Further, a one-parameter family of four-stage fourth-order ROW-methods with the classical Kutta's 3/8-rule method as underlying explicit Runge-Kutta method was introduced in [9, Section 6]. Its coefficients (9) are given by $A = \widetilde{A}\Gamma^{-1}$, $L = I_4 - \Gamma^{-1}$ and $b^T = \widetilde{b}^T\Gamma^{-1}$, with

$$\Gamma = \begin{pmatrix} 1 & 0 & 0 & 0\\ -\frac{4}{3} & 1 & 0 & 0\\ -\frac{2(-1-2\theta+12\theta^2)}{3(-1+4\theta)(-1+6\theta)} & -\frac{2(1-6\theta+12\theta^2)}{(-1+4\theta)(-1+6\theta)} & 1 & 0\\ \frac{24\theta(-1+3\theta)}{(-1+4\theta)(-1+6\theta)} & \frac{6(1-6\theta+12\theta^2)}{(-1+4\theta)(-1+6\theta)} & -6 & 1 \end{pmatrix}, \tag{44}$$

$$\widetilde{A} = \begin{pmatrix} 0 & 0 & 0 & 0\\ \frac{1}{3} & 0 & 0 & 0\\ -\frac{1}{3} & 1 & 0 & 0\\ 1 & -1 & 1 & 0 \end{pmatrix}, \qquad \widetilde{b}^T = \left(\tfrac{1}{8}, \tfrac{3}{8}, \tfrac{3}{8}, \tfrac{1}{8}\right)^T.$$

The associated linear stability function is then given by

$$R_\theta(z) = 1 + \frac{q_1 z}{1-\theta z} + \frac{q_2 z}{(1-\theta z)^2} + \frac{q_3 z}{(1-\theta z)^3} + \frac{q_4 z}{(1-\theta z)^4}, \qquad \text{with}$$

$$q_1 = \frac{96\theta^2-42\theta+5}{(4\theta-1)(6\theta-1)}, \qquad q_3 = \frac{(21-138\theta+288\theta^2-14z+120\theta z-276\theta^2 z+2z^2-19\theta z^2+45\theta^2 z^2)}{(3(4\theta-1)(6\theta-1))},$$
$$q_2 = \frac{210\theta^2 z-432\theta^2-90\theta z+198\theta+10z-27}{3(4\theta-1)(6\theta-1)}, \; q_4 = \frac{(z-6)(z-4)\left(24\theta^2 z-24\theta^2-10\theta z+12\theta+z-2\right)}{24(4\theta-1)(6\theta-1)}, \tag{45}$$

and A_0-stability is obtained whenever $\theta \geq (3+\sqrt{3})/12$.

The A_0-stability properties of the methods (38), (40), (42) and (44) above are collected in Table 2, where s denotes the number of stages, and they have order of consistency $p \geq s$.

method	$s=1$	$s=2$	$s=3$ (42)	$s=4$ (44)
θ_0	$1/2$	$1/4$	$1/3$	$(3+\sqrt{3})/12$

Table 2 Values of $\theta \geq \theta_0$ for some $s-$stage A_0-stable ROW methods (A, L, b, θ) of order $p \geq s$.

Observe that the linear stability functions (35) for the different AMF options (36) are obtained from (39)-(45) by replacing the factor $1-\theta z$ for the corresponding AMF factor $\tilde{\Pi}_m(\theta)$.

The following assumption (46) is the main ingredient to prove unconditional stability for AMF-type W-methods. It relates the stability of such a method with the A_0-stability of the underlying ROW method. Here, θ^* is some constant which may depend on θ and m.

$$0 < \frac{1}{\tilde{\Pi}_m(\theta)} \leq \frac{1}{1-\theta^* z}, \quad \theta^* \geq 0, \quad \forall \mathscr{C} > 0, \quad \forall z, z_1 \ldots, z_m \text{ in (34).} \tag{46}$$

Theorem 2. *Assume that the ROW method (A, L, b, θ) is A_0-stable for any $\theta \geq \theta_0 > 0$, and consider an AMF-type W-method with stability function given by (35)-(36). If for the given θ (and μ in case (C)) (46) holds with $\theta^* \geq \theta_0$, then the AMF-type W-method is unconditionally stable.*

Proof. Since $z \leq 0$, taking into account (46) and the mean value theorem, it holds that

$$\frac{1}{\tilde{\Pi}_m(\theta)} = \frac{1}{1-\nu z} \tag{47}$$

for some $\nu \geq \theta^*$ that may depend on θ, z, and z_j, $j = 1, \ldots, m$. Therefore,

$$R(z, z_1 \ldots, z_m) = R_\nu(z).$$

Now, the proof is concluded from the A_0-stability of the ROW method together with $\nu \geq \theta^* \geq \theta_0$. □

Theorem 2 will be considered in forthcoming subsections in order to show unconditional stability for the AMF-type W-methods presented in section 2. The application of this result will depend on whether the assumption (46) is fulfilled for such methods.

3.1 Stability of AMF-W-methods

Theorem 3. *For the stability function of the AMF-W-method (35)-(36)-(A) we have that (46) holds with $\theta^* = m^{-1}\theta > 0$.*

Proof. The left inequality in (46) is trivial. To show the one on the right, let us define the vector

$$v := (|y_1|, |y_2|, \ldots, |y_m|)^T, \qquad \text{with } y_j = \sqrt{\theta\tau}\lambda_j, \quad 1 \le j \le m.$$

Since $|c_{i,j}| \le 1$, $1 \le i, j \le m$, it then holds that

$$\begin{aligned} \tilde{\Pi}_m(\theta) - (1 - m^{-1}\theta z) &= \textstyle\prod_{j=1}^m (1 + y_j^2) - 1 - m^{-1} \sum_{i,j=1}^m c_{i,j} y_i y_j \\ &\ge (1 + \textstyle\sum_{j=1}^m y_j^2) - 1 - m^{-1} \sum_{i,j=1}^m |y_i|\,|y_j| \\ &= \textstyle\sum_{j=1}^m y_j^2 - m^{-1} (\sum_{j=1}^m |y_j|)^2 \\ &\ge \|v\|_2^2 - m^{-1} m \|v\|_2^2 = 0, \end{aligned}$$

where the last inequality above follows from the Cauchy-Schwarz inequality.

□

Observe that the value $\theta^* = m^{-1}\theta$ given in Theorem 3 is optimal since a right inequality as in (46) for other θ^* such that $0 \le \theta^* < m^{-1}\theta$ cannot be obtained.

Corollary 1. *Assume that the ROW method (A, L, b, θ) is A_0-stable for any $\theta \ge \theta_0 > 0$. Then, the AMF-W method (A, L, b, θ) (19)-(20) is unconditionally stable as long as $\theta \ge m\theta_0$.*

Proof. It follows directly from Theorems 2 and 3. □

The previous result allows to show the unconditional stability of several important AMF-W methods considered in the literature.

Theorem 4. *Consider a family of s-stage consistent AMF-W methods (A, L, b, θ) (19)-(20).*

1. *For $s = 1$, the methods are unconditionally stable as long as $\theta \ge m/2$.*
2. *For $s = 2$ and order of consistency at least two for the underlying ROW methods, the corresponding AMF-W methods are unconditionally stable as long as $\theta \ge m/4$.*
3. *For $s = 3$, the AMF-W methods with coefficients given in (42) are unconditionally stable as long as $\theta \ge m/3$.*

4. *For $s=4$, the AMF-W methods based on the Kuttas's 3/8-rule with coefficients given in (44) are unconditionally stable as long as $\theta \geq m\theta_0$, with $\theta_0 = (3+\sqrt{3})/12$.*

Proof. The θ-values that provide A_0-stability for the family of s-stage consistent ROW methods (A, L, b, θ), with $\theta \geq \theta_0$, are given in Table 2. The proof now follows from Corollary 1. □

3.2 Stability of PDE-W-methods

The properties of unconditional stability of PDE-W-methods were studied in [7], where it was seen that there exist unconditionally stable methods for $m = 2,3$ but not for $m \geq 4$ on arbitrary linear parabolic problems with constant coefficients (12). Anyhow, let us first show that the right inequality in (46) holds with $\theta^* = \theta$ for all $m \geq 2$.

Theorem 5. *Let $\lambda_i \in \mathbb{R}$, $1 \leq i \leq m$, and assume that $\mathscr{C} = (c_{i,j})_{i,j=1}^m$ (with $c_{i,i} = 1$) is positive definite. With z_i of (34) and $z = z_0 + z_1 + \ldots + z_m$, then the AMF factor $\tilde{\Pi}_m(\theta)$ (with $\theta \geq 0$) given by (36)-(B) satisfies*

$$\frac{1}{\tilde{\Pi}_m(\theta)} \leq \frac{1}{1-\theta z}. \tag{48}$$

Proof. Let us take $w_i = -\theta z_i$ for $0 \leq i \leq m$, in such a way that $w_0 \in \mathbb{R}$, $w_i \geq 0$, $1 \leq i \leq m$, satisfy $1 + w_0 + \sum_{i=1}^m w_i > 0$. Then (48) is equivalent to show that

$$\frac{1}{\prod_{i=1}^m (1+w_i)} \left(1 - \frac{w_0}{\prod_{i=1}^m (1+w_i)}\right) \leq \frac{1}{1 + w_0 + \sum_{i=1}^m w_i}.$$

Let us define $P_m := \prod_{i=1}^m (1+w_i) \geq 1$ and $S_m := \sum_{i=1}^m w_i \geq 0$. Then, it is not difficult to check that

$$\frac{1}{P_m}\left(1 - \frac{w_0}{P_m}\right) - \frac{1}{1+w_0+S_m} = \frac{-\left(w_0 + \frac{1}{2}(1+S_m-P_m)\right)^2 + \frac{1}{4}(1+S_m+P_m)^2 - P_m^2}{P_m^2(1+w_0+S_m)}.$$

In order to show that this expression is non positive, observe that

$$\frac{1}{4}(1+S_m+P_m)^2 - P_m^2 = \frac{1}{4}\Big(1+S_m+3P_m\Big)\Big(1+S_m-P_m\Big) \leq 0$$

since $P_m \geq 1 + S_m$. This concludes the proof. □

The stability analysis of PDE-W-methods also requires the positivity of $\tilde{\Pi}_m(\theta)$ so that the left inequality in (46) is fulfilled. However, this condition can only be satisfied for all positive definite matrices $\mathscr{C}$ as long as $m = 2,3$. To see this, we rewrite the condition $\tilde{\Pi}_m(\theta) > 0$ as

$$\prod_{j=1}^{m}(1+y_j^2)-\sum_{i\neq j}c_{i,j}y_iy_j>0 \qquad \text{for all } y_i\in\mathbb{R}. \tag{49}$$

Considering the change $y_i=\sqrt{\theta\tau}\lambda_i$, this inequality becomes equivalent to the positivity of the factor $\tilde{\Pi}_m(\theta)$ of (36)-(B). Unconditionl stability for PDE-W-methods then requires (49) to hold for all positive definite matrices $\mathscr{C}$. However, it turns out that this is true in dimensions $m=2,3$, but not in general for $m\geq 4$. Observe that for $m=2$, (49) follows immediately since $|c_{1,2}|<1$. For $m=3$, we have the following result.

Theorem 6. *Assume that $\mathscr{C}=(c_{i,j})_{i,j=1}^{3}$ is positive definite, with $c_{i,i}=1$ for all i. Then, (49) holds with $m=3$.*

Proof. First observe that $|c_{i,j}|<\sqrt{c_{i,i}\cdot c_{j,j}}=1$ $(1\leq i,j\leq 3,\ \ i\neq j)$. Then, for all $y_j\in\mathbb{R}$

$$\begin{aligned}\textstyle\prod_{j=1}^{3}(1+y_j^2)-\sum_{i\neq j}c_{i,j}y_iy_j &\geq 1+\textstyle\sum_{j=1}^{3}y_j^2+\sum_{i<j}y_i^2y_j^2-\sum_{i\neq j}|y_i||y_j|\\ &\geq -2+\textstyle\sum_{j=1}^{3}y_j^2+\sum_{i<j}(|y_i||y_j|-1)^2.\end{aligned}$$

Let us now consider the function

$$f(y_1,y_2,y_3)=-2+(y_1^2+y_2^2+y_3^2)+(y_1y_2-1)^2+(y_1y_3-1)^2+(y_2y_3-1)^2,$$

with $y_1,y_2,y_3\geq 0$. It is then seen that the critical points of $f(y_1,y_2,y_3)$ fulfil $y_1=y_2=y_3$, and the minimum value of f is $f(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}})=\frac{1}{4}>0$. □

Remark 2. The previous result for dimension $m=3$ is not true in higher dimensions, i.e., (49) does not hold for arbitrary positive definite matrices $\mathscr{C}=(c_{i,j})_{i,j=1}^{m}$, with $c_{i,i}=1$ $(1\leq i\leq m)$ whenever $m\geq 4$. This can be seen by taking $y_j=y\geq 0$ $(1\leq j\leq m)$ in (49) and considering

$$f(y)=(1+y^2)^m-Sy^2, \qquad S=\sum_{i\neq j}c_{i,j}.$$

If $S\geq m$, $f(y)$ attains a minimum at the point $y^*\geq 0$, with

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

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

$$S=\sum_{i\neq j}c_{i,j}<m\left(\frac{m}{m-1}\right)^{m-1}. \tag{50}$$

Hence (50) is a necessary condition for (49).

Remark 3. A sufficient condition for (49) to hold in dimension $m \geq 4$ is that the matrix $2I - \mathscr{C}$ is positive semi-definite. In fact, expanding the product in (49) and neglecting the fourth and higher order terms shows that (49) holds if

$$y_1^2 + \ldots + y_m^2 - \sum_{i \neq j} c_{i,j} y_i y_j \geq 0, \tag{51}$$

and, since $c_{i,i} = 1$, this is equivalent to $2I - \mathscr{C} \geq 0$.

The stability of PDE-W-methods in dimension $m \geq 2$ can be now established under the assumption (49).

Corollary 2. *Assume that the ROW method (A, L, b, θ) is A_0-stable for any $\theta \geq \theta_0 > 0$. If (49) holds, then the PDE-W method (A, L, b, θ) (23)-(20) is unconditionally stable as long as $\theta \geq \theta_0$.*

Proof. (46) follows from Theorem 5 and assumption (49). Now the proof is a consequence of Theorem 2 with $\theta^* = \theta$. □

Theorem 7. *Consider a family of s-stage consistent PDE-W methods (A, L, b, θ) (23)-(20). Under the assumption (49),*

1. *for $s = 1$, the methods are unconditionally stable as long as $\theta \geq 1/2$.*
2. *For $s = 2$ and order of consistency at least two for the underlying ROW methods, the corresponding PDE-W methods are unconditionally stable as long as $\theta \geq 1/4$.*
3. *For $s = 3$, the PDE-W methods with coefficients given in (42) are unconditionally stable as long as $\theta \geq 1/3$.*
4. *For $s = 4$, the PDE-W methods based on the Kuttas's 3/8-rule with coefficients given in (44) are unconditionally stable as long as $\theta \geq (3 + \sqrt{3})/12$.*

Proof. The proof now follows from Corollary 2 and the θ-values in Table 2 that provide A_0-stability for the family of s-stage consistent ROW methods (A, L, b, θ), with $\theta \geq \theta_0$. □

3.3 Stability of AMFR-W-methods

For each integer $m \geq 2$ let us consider the polynomial

$$g_m(x) = 2x\left(\frac{m - x}{m - 1}\right)^{m-1} - 1, \tag{52}$$

and denote by κ_m the smallest positive zero of $g_m(x)$. These numbers play a relevant role in the stability analysis for AMFR-W-methods as Theorems 8 and 9 below reflect. We first state a Lemma showing some properties of these zeros.

Lemma 1. *1. Let* $g(x) := 2x\exp(1-x)-1$*, with* $x \geq 0$*. Then*

$$g(x) > 0 \iff x \in (\kappa^*, \mathscr{K}^*), \quad \text{with } \kappa^* = 0.2319\ldots, \; \mathscr{K}^* = 2.6783\ldots \tag{53}$$

2. Let $g_m(x) := 2x\left(\frac{m-x}{m-1}\right)^{m-1} - 1$*, with* $x \in [0,m]$*,* $m \in \mathbb{N}$*,* $m \geq 2$*. Then*

$$g_m(x) > 0 \iff x \in (\kappa_m, \mathscr{K}_m), \quad \text{with } \kappa^* < \kappa_m < \mathscr{K}_m < \mathscr{K}^*. \tag{54}$$

3. For all $m \in \mathbb{N}$*,* $m \geq 2$*, it holds that* $\kappa_{m+1} < \kappa_m$ *and* $\mathscr{K}_m < \mathscr{K}_{m+1}$*.*
4. For all $m \in \mathbb{N}$*,* $m \geq 2$*, it holds that*

$$(m+1)\kappa_{m+1} > m\kappa_m. \tag{55}$$

Proof. First, in order to prove items 1-3, we observe that the functions $g_m(x) = 2x\left(\frac{m-x}{m-1}\right)^{m-1} - 1$, $x \in [0,m]$, $m \geq 2$, fulfil $g_m(0) = g_m(m) = -1$, $g_m(1) = 1$ and $g'_m(x) > 0$, for $x \in (0,1)$, and $g'_m(x) < 0$, for $x \in (1,m)$. This shows that there exist real numbers $0 < \kappa_m < 1 < \mathscr{K}_m < m$ such that

$$g_m(x) > 0 \iff x \in (\kappa_m, \mathscr{K}_m).$$

Moreover, it is readily checked that $g_m(1/2) > 0$, for all $m \geq 2$. Hence, $\kappa_m < \frac{1}{2}$, for all $m \geq 2$.

Now, we observe that $g_{m+1}(x) > g_m(x)$, $\forall x \in (0,m)$, $x \neq 1$, and from here it holds that $g_{m+1}(\kappa_m) > 0$ and $g_{m+1}(\mathscr{K}_m) > 0$, which implies $\kappa_{m+1} < \kappa_m$ and $\mathscr{K}_m < \mathscr{K}_{m+1}$. To see that $g_{m+1}(x) > g_m(x)$, $\forall x \in (0,m)$, $x \neq 1$, it is enough to consider that

$$g_{m+1}(x) - g_m(x) = (2x)\left(\left(1 + \tfrac{1-x}{m}\right)^m - \left(1 + \tfrac{1-x}{m-1}\right)^{m-1}\right) > 0$$

since

$$\begin{aligned}\frac{\left(1+\frac{1-x}{m}\right)^m}{\left(1+\frac{1-x}{m-1}\right)^{m-1}} &= \left(1 - \tfrac{1-x}{m(m-x)}\right)^m \left(\tfrac{m-x}{m-1}\right) \\ &> \left(1 - (m)\tfrac{1-x}{m(m-x)}\right)\left(\tfrac{m-x}{m-1}\right) = 1\end{aligned}$$

for all $\forall x \in (0,m)$, $x \neq 1$, by virtue of the Bernoulli's inequality.

The proof of items 1-3 is concluded taking into account that the function $g(x) = (2x)\exp(1-x) - 1$ is the pointwise limit of $g_m(x)$ as $m \to \infty$, for all $x \geq 0$.

To prove item 4, we shall next check that $g_m\left(\frac{m+1}{m}x\right) > g_{m+1}(x)$, for all $m \geq 2$ and $x \in (0, \frac{1}{2})$. Hence, the proof of item 4 follows just by evaluating this inequality at $x = \kappa_{m+1}$ and considering the property stated in item 2.

To see that $g_m\left(\frac{m+1}{m}x\right) > g_{m+1}(x)$, for all $m \geq 2$ and $x \in (0, \frac{1}{2})$, from a direct calculation we have that

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

with $h_m(x) = (m^2-1)\left(m^2-(m+1)x\right)^{m-1} - \left((m^2-1)-(m-1)x\right)^m$. Now we have for $m \geq 2$ and $x \in (0, \frac{1}{2})$ that

$$h_m(x) > ((m^2-1)-(m-1)x)\left\{\left(m^2-(m+1)x\right)^{m-1} - \left((m^2-1)-(m-1)x\right)^{m-1}\right\}$$

and the expression on the right hand side is positive since for all $x \in (0, \frac{1}{2})$ we have that $(m^2-(m+1)x) - ((m^2-1)-(m-1)x) = 1-2x > 0$. □

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
$\mathscr{K}_m$	1.7071	2	2.1572	2.2552	2.3223	2.3709	2.4079	2.4370

Table 3 Values for κ_m and $\mathscr{K}_m$ in Lemma 1, $2 \leq m \leq 9$, rounded up with 4 digits.

Theorem 8. *Let $m \geq 2$ be any given integer and $\theta > 0$. If $\mu \geq m\kappa_m\theta$ then for the stability function of the AMFR-W method (35)-(36)-(C) we have that (46) holds with $\theta^* = \theta$, i.e., for $\Pi_m^*(\mu,\theta)$ defined in (36)-(C), it holds that*

$$0 < \frac{1}{\Pi_m^*(\mu,\theta)} \leq \frac{1}{1-\theta z}, \quad \forall \mathscr{C} > 0, \quad \forall z, z_1 \ldots, z_m \text{ in (34).}$$

Proof. The inequality on the right follows immediately taking into account that

$$\frac{1}{1-\theta z} - \frac{1}{\Pi_m^*(\mu,\theta)} = \frac{1}{1-\theta z}\left(1 - \frac{1-\theta z}{\Pi_m(\mu)}\right)^2 \geq 0.$$

The positivity of $\Pi_m^*(\mu,\theta)$ is equivalent to show that $2\Pi_m(\mu) - (1-\theta z) > 0$, and considering the change of variables $y_j = \sqrt{\mu\tau}\lambda_j$, this can be written as

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

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

$$\mathscr{D} \geq 2\prod_{j=1}^{m}\left(1+y_j^2\right) - 1 - \frac{\theta}{\mu}\Big(\sum_{j=1}^{m}|y_j|\Big)^2. \tag{56}$$

It follows from Lemma 2 below that this lower bound is non-negative, if $\mu \geq m\kappa_m\theta$, and that it can be equal to 0 only if $y_1 = \ldots = y_m = y$ for some $y \neq 0$. However, in this latter case the inequality in (56) is strict. This completes the proof. □

Lemma 2. *Let $m \geq 2$ be any given integer and κ_m given by (54). If $\delta \leq \dfrac{1}{m\kappa_m}$ then it holds that*

$$2\prod_{j=1}^{m}(1+y_j^2)-1-\delta\left(\sum_{j=1}^{m}y_j\right)^2\geq 0,\quad \forall\, y_j\geq 0,\ 1\leq j\leq m. \tag{57}$$

Moreover, the equality can only hold if and only if $y_1=y_2=\ldots=y_m=y$, *for some* $y\neq 0$.

Proof. First observe from (53)-(54) that $m\kappa_m>\frac{1}{2}$, for all $m\geq 2$, and hence $\delta<2$. Let us now define, for $y_j>0$, $1\leq j\leq m$,

$$f(y_1,\ldots,y_m):=2\prod\nolimits_m-1-\delta\left(\sum\nolimits_m\right)^2,\ \text{ with }\ \prod\nolimits_m:=\prod\nolimits_{j=1}^{m}(1+y_j^2),\quad \sum\nolimits_m=\sum\nolimits_{j=1}^{m}y_j.$$

Since $\dfrac{\partial f}{\partial y_i}=\dfrac{4y_i}{1+y_i^2}\prod_m-2\delta\sum_m$, it follows that the components of a critical point $\mathbf{y}=(y_1,\ldots,y_m)$ for f must fulfil

$$\frac{y_i}{1+y_i^2}=\frac{\delta\sum_m}{2\prod_m},\quad 1\leq i\leq m.$$

Since $\dfrac{a}{1+a^2}=\dfrac{b}{1+b^2}$ implies $a=b$ or $ab=1$, a critical point $\mathbf{y}=(y_1,\ldots,y_m)$ for f must fulfil that

$$\forall i,j\in\{1,\ldots,m\},\ i\neq j: y_i=y_j\quad\text{or}\quad y_i=\frac{1}{y_j}.$$

We shall now see that all components y_j must be equal. To this aim, let us assume that a critical point $\mathbf{y}$ has m_1 components equal to $y>1$ and $m-m_1$ components equal to $\dfrac{1}{y}$, for a certain m_1, $1\leq m_1\leq m-1$. Then $\prod_m=(1+y^2)(1+\frac{1}{y^2})\hat{\prod}_m$ and $\sum_m=y+\frac{1}{y}+\hat{\sum}_m$, with

$$\hat{\prod}_m=\prod\nolimits_{k=1}^{m_1-1}(1+y^2)\prod\nolimits_{k=1}^{m-m_1-1}(1+\tfrac{1}{y^2})\geq 1+(m_1-1)y^2+(m-m_1-1)\tfrac{1}{y^2}$$

and

$$\hat{\sum}_m=\sum\nolimits_{k=1}^{m_1-1}y+\sum\nolimits_{k=1}^{m-m_1-1}\tfrac{1}{y}=(m_1-1)y+(m-m_1-1)\tfrac{1}{y}.$$

Since $\delta<2$, we would have

$$\begin{aligned}\frac{\partial f}{\partial y_i}(\mathbf{y}) &= \frac{4y}{1+y^2}\prod\nolimits_m-2\delta\sum\nolimits_m\\ &> 4\left(\frac{y}{1+y^2}\prod\nolimits_m-\sum\nolimits_m\right)\\ &\geq 4\left((m_1-1)y^3+(m-m_1-1)\tfrac{1}{y^3}\right)\geq 0,\end{aligned}$$

and hence $\dfrac{\partial f}{\partial y_i}(\mathbf{y})>0$, which contradicts that $\mathbf{y}$ is a critical point for f. Therefore, we must have $m_1=0$ or $m_1=m$, that is, a critical point for f must have equal components.

Let then $\mathbf{y} = (y, \dots, y) \in \mathbb{R}^m$ be such a critical point. It must then hold that

$$4y(1+y^2)^{m-1} - 2m\delta y = 0$$

and from here it is readily seen that for $\delta \leq \dfrac{2}{m}$ the only critical point is $(0, \dots, 0)$, for which $f(0, \dots, 0) = 1$. On the other hand, for $\delta > \dfrac{2}{m}$ there is also a nontrivial critical point $\mathbf{y} = (y, \dots, y) \in \mathbb{R}^m$ with

$$(1+y^2)^{m-1} = \frac{m\delta}{2}.$$

By making the change $\delta \leftrightarrow \kappa$, $\delta := \dfrac{1}{m \cdot \kappa}$, it is readily seen that $\dfrac{2}{m} < \delta \leq \dfrac{1}{m\kappa_m}$ gives $\kappa_m \leq \kappa < \dfrac{1}{2} (< \mathscr{K}_m)$. Hence, $\kappa \in [\kappa_m, \mathscr{K}_m)$.

Furthermore, using the fact that $(1+y^2)^m = \left(\dfrac{1}{2\kappa}\right)^{\frac{m}{m-1}}$, a simple calculation shows that

$$\begin{aligned} f(y, \dots, y) &= 2(1+y^2)^m - 1 - \frac{m}{\kappa} y^2 \\ &= 2(1+y^2)^m - 1 - \frac{m}{\kappa} \frac{(1+y^2)^m}{\frac{m\delta}{2}} + \frac{m}{\kappa} \\ &= \frac{1}{\kappa} \left(2\kappa(1+y^2)^m (1-m) + (m-\kappa) \right) \\ &= \frac{1}{(m-1)\kappa(2\kappa)^{\frac{1}{m-1}}} \left(-1 + (2\kappa)^{\frac{1}{m-1}} \left(\frac{m-\kappa}{m-1} \right) \right) \geq 0, \end{aligned}$$

by virtue of Lemma 1 since $\kappa \in [\kappa_m, \mathscr{K}_m)$.

Finally, an induction argument shows that $f(y_1, y_2, \dots, y_m) > 0$ in case that $y_j = 0$ for some $j \in \{1, 2, \dots, m\}$. In this case, it must be observed that from (55) it holds that

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

□

Remark 4. A natural option to select the additional parameter μ in AMFR-W-methods is $\mu = \theta$. In that case unconditional stability holds in dimensions $m = 2$ and $m = 3$, since $m\kappa_m < 1$ for $m \leq 3$. However, for $m \geq 4$, in order to guarantee unconditional stability one has to take $\mu \geq m\kappa_m\theta > \theta$.

Corollary 3. *Assume that the ROW method (A, L, b, θ) is A_0-stable for any $\theta \geq \theta_0 > 0$. Then, the AMFR-W method (A, L, b, θ, μ) (28)-(20) is unconditionally stable as long as $\mu \geq \kappa_m m\theta$, with $\theta \geq \theta_0$.*

Proof. From Theorem 8 we get $\theta^* = \theta$ in (46) as long as $\mu \geq \kappa_m m\theta$. The result then follows from Theorem 2. □

Theorem 9. *Consider a familiy of s-stage consistent ROW methods (A,L,b,θ). If $\mu \geq \kappa_m\, m\theta$ and $\theta \geq \theta_0$, then all consistent AMFR-W methods (A,L,b,θ,μ) are unconditionally stable*

1. *for $s = 1$ and $\theta_0 = 1/2$.*
2. *For $s = 2$ with order of consistency at least two as ROW method and $\theta_0 = 1/4$.*
3. *For $s = 3$, $\theta_0 = 1/3$ and the family of ROW methods with coefficients given in (42).*
4. *For $s = 4$, $\theta_0 = (3+\sqrt{3})/12$ and the family of ROW methods based on the Kuttas's 3/8-rule considered in (44).*

Proof. It follows from Corollary 3, taking into account that the θ-values that provide A_0-stability for the family of consistent ROW-methods (A,L,b,θ), with $\theta \geq \theta_0$, depending on the number of stages s, are given in Table 2. □

Remark 5. For all $m \geq 2$, the stability bounds in Table 1 for the Hundsdorfer-Verwer scheme (4) coincide with the corresponding ones given in Theorem 9 for the one-stage AMFR-W method with $\theta = 1/2$, that is, $\mu_m = m\kappa_m\theta$ with κ_m in Table 3.

4 Numerical experiments

The AMF-type W-methods of Section 2 will be compared to classical ADI schemes like the Hundsdorfer-Verwer and the modified Craig-Sneyd schemes (4)-(5) in 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 finance. Fixed stepsize integrations are considered in Figures 1-6 below so as to check unconditional stability and observe the temporal order of convergence in the ℓ^2-norm. The efficiency of the time integrators presented below is measured in relation to CPU time versus global errors. Moreover, each figure contains dashed straight lines with slopes two and three, respectively, to compare the temporal orders of convergence for the methods under consideration. Additional numerical experiments on the above-mentioned problems can also be found in [6].

HV is the method (4) with parameters $\mu = 1/2$ and $\theta > 0$ to be selected for stability requirements. The method is order two in ODE sense and it is unconditionally stable for $\theta \geq 1-\frac{\sqrt{2}}{2}$, $\theta \geq 0.4020$ and $\theta \geq 0.5152$ when $m = 2$, $m = 3$ and $m = 4$, respectively (see Table 1). For $2 \leq m \leq 4$ we shall consider $\theta = (3+\sqrt{3})/6$, $\theta = 0.4020$ and $\theta = 0.5152$, respectively.

MCS is the method (5) with parameters $\sigma = \theta$, $\mu = 1/2-\theta$ and $\theta > 0$ to be chosen for stability. This scheme is order two in ODE sense and it is unconditionally stable for $\theta \geq \frac{1}{3}$, $\theta \geq \frac{6}{13}$ and $\theta \geq \frac{54}{91}$ when $m = 2$, $m = 3$ and $m = 4$, respectively (see Table 1). For $2 \leq m \leq 4$ we shall consider $\theta = \frac{1}{3}$, $\theta = \frac{6}{13}$ and $\theta = \frac{54}{91}$, respectively.

AMFR-W1 is the 1-stage AMFR-W-method (A, L, b, θ, μ) with coefficients

$$A = L = 0, \quad b = 1. \tag{58}$$

where we have chosen $\mu = \theta = 1/2$ for $m \leq 3$ and $\mu = 4\kappa_4\theta$, $\theta = 1/2$ for $m = 4$ (with $\kappa_4 = 0.2576$) to meet the stability bounds given in Theorem 9. This method is order two in ODE sense.

AMF-W2 is the 2-stage AMF-W-method (A, L, b, θ) with coefficients taken from [17, p. 155]

$$A = \begin{pmatrix} 0 & 0 \\ 2/3 & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 \\ -4/3 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 5/4 \\ 3/4 \end{pmatrix}. \tag{59}$$

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 4. The method is only order two in ODE sense since (10) is not satisfied.

PDE-W2 is the 2-stage PDE-W-method (A, L, b, θ) based on the coefficients (59) and stability parameter $\theta = (3+\sqrt{3})/6$. This method has only 2 stages, but it is of order three in ODE sense since (10) is fulfilled.

AMFR-W2 is the 2-stage AMFR-W-method (A, L, b, θ, μ) with coefficients (59), where we have chosen $\mu = \theta = (3+\sqrt{3})/6$ for $m \leq 3$ and $\mu = 4\kappa_4\theta$, $\theta = (3+\sqrt{3})/6$ for $m = 4$ (with $\kappa_4 = 0.2576$) to meet the stability bounds given in Theorem 9. The method is order three in ODE sense.

4.1 Linear diffusion equation with constant coefficients

In order to illustrate the stability results for AMF-type W-methods in Section 3 let us consider the linear diffusion reaction partial differential equation with constant coefficients and mixed derivative terms

$$\partial_t u = \sum_{i,j=1}^{m} \alpha_{i,j}\, \partial^2_{x_i x_j} u + g(t, \mathbf{x}), \qquad \mathbf{x} \in (0,1)^m, \; t \in (0,1], \tag{60}$$

with $g(t, \mathbf{x})$ chosen such that

$$u(t, \mathbf{x}) = u_e(t, \mathbf{x}) := \mathrm{e}^t \left(\prod_{j=1}^m x_j(1-x_j) + \kappa \sum_{j=1}^m (x_j + \tfrac{1}{j+2})^2 \right) \tag{61}$$

is the exact solution of (60). The initial condition $u(0, \mathbf{x}) = u_e(0, \mathbf{x})$ and Dirichlet boundary conditions (BCs) are imposed. We restrict our attention to the cases $m =$

$3,4$. Observe that for $\kappa = 0$ we have homogeneous boundary conditions, but non-homogeneous time-dependent Dirichlet BCs are obtained when $\kappa = 1$. 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 W-methods introduced in Section 2. 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 $m = 4$. A semi-discretized system

$$\dot{U} = \mathscr{M}U + G(t) + b(t) \tag{62}$$

of dimension N^m is obtained, where $\mathscr{M}$ is given in (13), 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 reaction term $g(t, \mathbf{x})$ and $b(t)$ stores the terms due to non-homogeneous boundary conditions. From here, the differential equation (62) also takes the form (2)-(3). Observe that the exact solution (61) is e^t times a polynomial of degree 2 in each spatial variable so that the global errors come only from the time discretization. Now, AMF-type W-methods are applied to (62) with fixed stepsize $\tau = 2^{-j}$, $2 \leq j \leq 10$, as detailed in Section 2.

The time integrations of (62) for $m = 3$ and $m = 4$ spatial dimensions with the methods presented above are summarized in Figures 1-3 below. Figure 1 deals with the three-dimensional case, and Figures 2-3 correspond to the case $m = 4$. The global errors are plotted in relation to both the stepsize τ -to check the temporal order of the current method- and the CPU time in seconds -to measure the efficiency of each integrator-.

Regarding the elliptic operator in (60), we take diffusion parameters $\alpha_{i,j} = \alpha$, for $i \neq j$, with $\alpha = 0.9$. Observe that for the case of four spatial dimensions the necessary condition (50) for stability of PDE-W-methods (23) is not fulfilled. In order to meet this condition we also take $\alpha = 0.7$ when $m = 4$.

For the case $m = 3$ in Figure 1 the methods **HV**, **MCS**, **AMFR-W1** and **AMF-W2** are seen to be second order methods as expected, whereas **PDE-W2** and **AMFR-W2** attain order three when $\kappa = 0$ (homogeneous boundary conditions). For $\kappa = 1$ the order of convergence of these two latter methods is more irregular, and it seems to be two for larger stepsizes and around 2.5 for medium and small stepsizes.

On the other hand, for the four-dimensional case, when $\alpha = 0.9$ the necessary condition (50) for stability of PDE-W-methods is not fulfilled and, in fact, **PDE-W2** is unstable in this case, see Figure 2 (left). For the remaining methods, the selected values for the parameters θ and μ ensure stability according to Theorems 4 and 9 and the observed temporal orders of convergence are similar to those obtained when $m = 3$. When $\alpha = 0.7$ and $m = 4$, the stability requirements are satisfied for all the methods and this is illustrated in Figure 2 (right), where a convergence order around three is observed for the methods **AMFR-W2** and **PDE-W2** in case of homogeneous boundary conditions.

In order to make a more fair comparison of the performance of the methods in a constant time-step size framework, we have plotted in Figure 3 the global error versus the CPU time for the 4D-problem with $\alpha = 0.7$, both with homogeneous and time-dependent boundary conditions. We can observe that the **HV** is a good candidate despite being a second order method. This latter method is only outperformed by the **AMFR-W2** and **PDE-W2** methods when medium-high accuracies are required and homogeneous BCs are imposed. This could be explained by the fact that the **HV**-method has a reduced computational cost per integration step (similar to **AMFR-W1**) and it also possesses small error constants. For time dependent BCs it is possible to make a simple change in the PDE problem through multilinear interpolation (see e.g. [7]) in order to reduce the problem to homogeneous BCs, which is a more favorable situation for AMF-type W-methods.

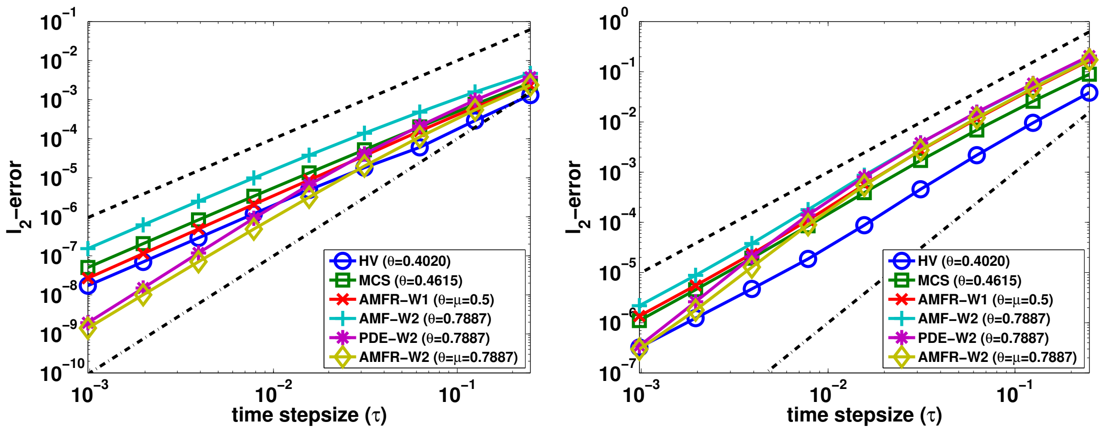

Fig. 1 3D Linear model (60)-(61) with $\alpha = 0.9$. Error vs Time stepsize in the case of homogeneous boundary conditions $\kappa = 0$ (left) and in the case of time-dependent boundary conditions $\kappa = 1$ (right). $\Delta x_i = 1/129$, $1 \leq i \leq 3$.

4.2 The Heston model

The Heston model [15] is a two-dimensional extension of the well-known Black-Scholes equation from financial option pricing theory. The results obtained in the experiments on this problem show that the proposed AMF-type schemes also perform correctly on PDEs with variable coefficients, and they can be easily applied on practical models that involve mixed derivatives 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

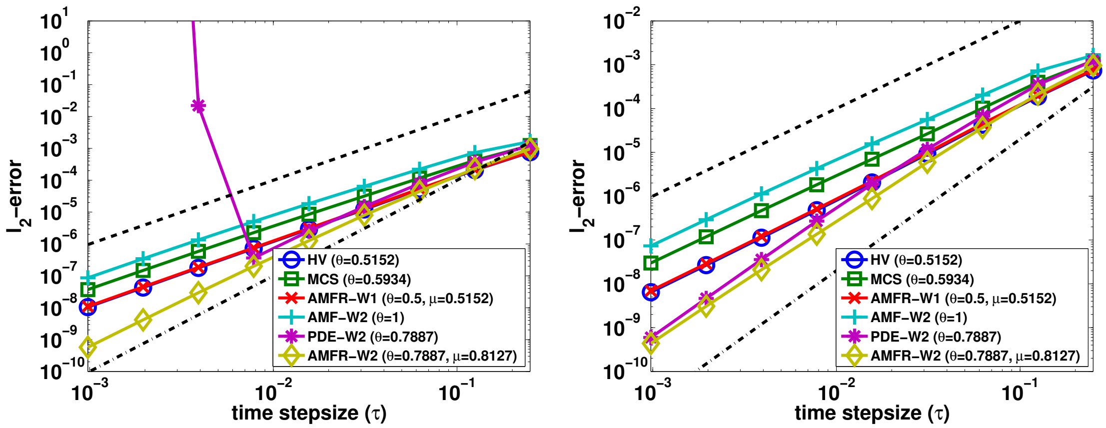

Fig. 2 4D Linear model (60)-(61) with homogeneous boundary conditions ($k=0$) and $\Delta x_i = 1/41$, $1 \leq i \leq 4$: $\alpha = 0.9$ (left) and $\alpha = 0.7$ (right). Error vs Time stepsize.

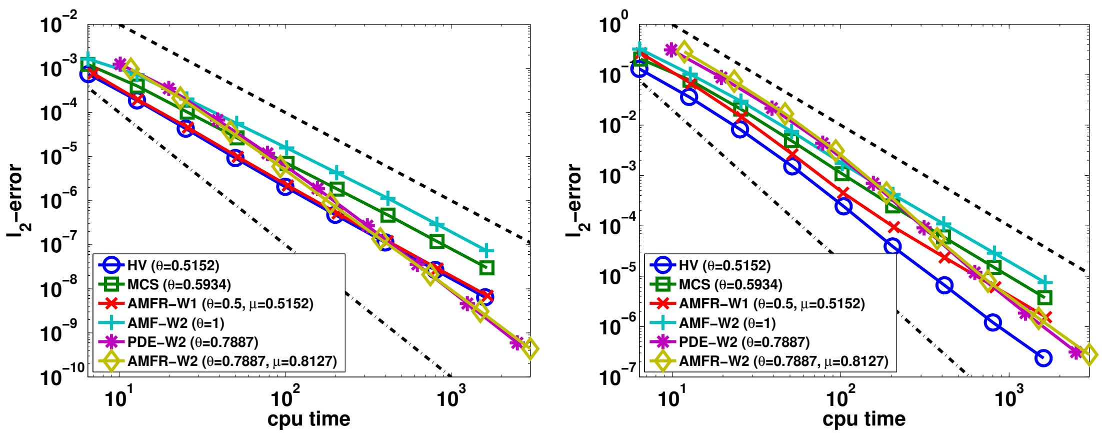

Fig. 3 4D Linear model (60)-(61) with $\alpha = 0.7$. Error vs CPU time, with homogeneous boundary conditions $k=0$ (left) and time-dependent boundary conditions $k=1$ (right). $\Delta x_i = 1/41$, $1 \leq i \leq 4$:

$$\partial_t u = \frac{1}{2} s^2 v\, \partial_{ss}^2 u + \rho \sigma s v\, \partial_{sv}^2 u + \frac{1}{2} \sigma^2 v\, \partial_{vv}^2 u \\ +(r_d - r_f) s\, \partial_s u + \kappa(\eta - v)\, \partial_v u - r_d u. \tag{63}$$

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 respectively the domestic and foreign interest rates, $\sigma > 0$ 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 this PDE (63) from the corresponding stochastic model can be seen in [15]. 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

$$\begin{aligned} s = 0: &\ u(0,v,t) = 0, \quad t \in [0,T] \\ s = S: &\ \partial_s u(S,v,t) = e^{-r_f t}, \quad t \in [0,T] \\ v = V: &\ u(s,V,t) = s e^{-r_f t}, \quad t \in [0,T] \end{aligned} \tag{64}$$

On the other hand, the initial condition

$$u(s,v,0) = \max(0, s-K) \tag{65}$$

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 in [26]

$$\kappa = 0.6067,\ \eta = 0.0707,\ \sigma = 0.2928,\ \rho = -0.7571,\ r_d = 0.03,\ r_f = 0, \tag{66}$$

in such a way that the boundary conditions are time-independent. Secondly the set of values in [29]

$$\kappa = 2.5,\ \eta = 0.06,\ \sigma = 0.5,\ \rho = -0.1,\ r_d = 0.0507,\ r_f = 0.0469, \tag{67}$$

is considered, such that the boundary conditions are time-dependent with a small correlation parameter ρ. Finally we also consider a time-dependent case with a larger correlation parameter

$$\kappa = 1.5,\ \eta = 0.02,\ \sigma = 0.62,\ \rho = -0.67,\ r_d = 0.01,\ r_f = 0.02. \tag{68}$$

In the case (66) the codes perform the time integration until $T = 3$, whereas $T = 0.25$ and $T = 1$ are considered in cases (67) and (68), respectively. In all cases, we take $K = 100$, $S = 30K$ and $V = 15$.

We apply the MOL approach on this model on a non-uniform spatial mesh following the ideas given in [18], since it is known that uniform spatial grids are not efficient on it, because the initial condition (65) has a differentiability problem at $s = K$ and that for v close to 0 the PDE becomes advection-dominated. So we build a rectangular non-uniform grid

$$s_0 = 0 < s_1 < \cdots < s_m = S, \quad v_0 = 0 < v_1 < \cdots < v_n = V$$

where there are many more points 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 (64), finite-differences approximations are only applied at the nodes (s_i, v_j) with $1 \le i \le m$ and

$0 \le j \le n-1$. At each node of this grid, the partial derivatives of the PDE (63) are approximated by the corresponding finite-difference formulation given in detail in [18]. Roughly speaking, in the case of the derivatives $\partial^2_{ss}u$, $\partial^2_{vv}u$ 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 $0 \le v_j \le 1$ and $v_j > 1$. Finally, the mixed derivative $(\partial^2_{sv}u)$ is approximated by second-order central differences for the first partial derivative at each spatial direction.

Adding the initial and boundary conditions (64)-(65) and putting all the finite differences together at each spatial point, we arrive at the following linear semi-discrete IVP of dimension $m \cdot n$ of type (2)-(3)

$$U'(t) = F(t,U) = \sum_{j=0}^{2} F_j(t,U), \quad U(0) = U_0, \quad t \in [0,T] \tag{69}$$

where

$$F_j(t,U) = A_j U + g_j e^{-r_f t}, \ (j=1,2), \quad F_0(t,U) = A_0 U + g_0 e^{-r_f t} - r_d U. \tag{70}$$

$F_0(t,U)$ represents the splitting term corresponding to the mixed derivatives together with the reaction part $G(U) = -r_d U$, whereas $F_j(t,U)$, $(j=1,2)$ corresponds to the directional splitting terms. $\{g_j\}_{j=0}^{2}$ are constant vectors that come from the time-dependent boundary conditions (64) and the constant matrices A_1 and A_2 have simple structures

$$A_1 = \mathrm{diag}(A_1^{(0)}, A_1^{(1)}, \ldots, A_1^{(n-1)}), \quad A_2 = \tilde{A} \otimes I_m$$

where each submatrix $A_1^{(k)}$ is a tridiagonal matrix of dimension m and $\tilde{A}$ has dimension n with only five non-zero diagonals. The constant matrix A_0 of dimension $n \cdot m$ 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 [18] the splitting (69)-(70) is not applied exactly in this way, since the reaction term $G(U)$ is included in the directional terms in the following way $F_j(t,U) = A_j U + g_j e^{-r_f t} - (r_d/2)U$, $j = 1,2$. However, this does not imply any significant change in the numerical results below in Figure 4-6.

Figures 4-6 show the results for the cases (66)-(68) of the Heston problem, respectively. The time integrations have been carried out for $\tau = 2^{-j}$, $2 \le j \le 10$, and the global errors have been measured with respect to a reference solution at the respective end-point T, obtained with the DOP853 code [11] with a very stringent tolerance. In Figures 4-6 it is observed that all methods confirm the achieved orders on the previous constant coefficient PDE (60), i.e, order around two for **HV**, **MCS**, **AMF-W2** and order three for **AMFR-W2** and **PDE-W2**, but with the important difference that in this case the order three is maintained even in the case of time-dependent BCs. The observed order for **AMFR-W1** and larger stepsizes lies around 1.5, and order two can be observed when very small stepsizes are considered. It is also noteworthy to observe that the global errors provided by **HV** and **AMF-W2** are very similar in the three cases.

Regarding the efficiency (plots in the right side) it can be appreciated that the higher order methods, **PDE-W2** and **AMFR-W2**, are the most efficient when medium or small errors are required. For low accuracy (2 or 3 significant digits) **HV**, **MCS** and **AMF-W2** are better.

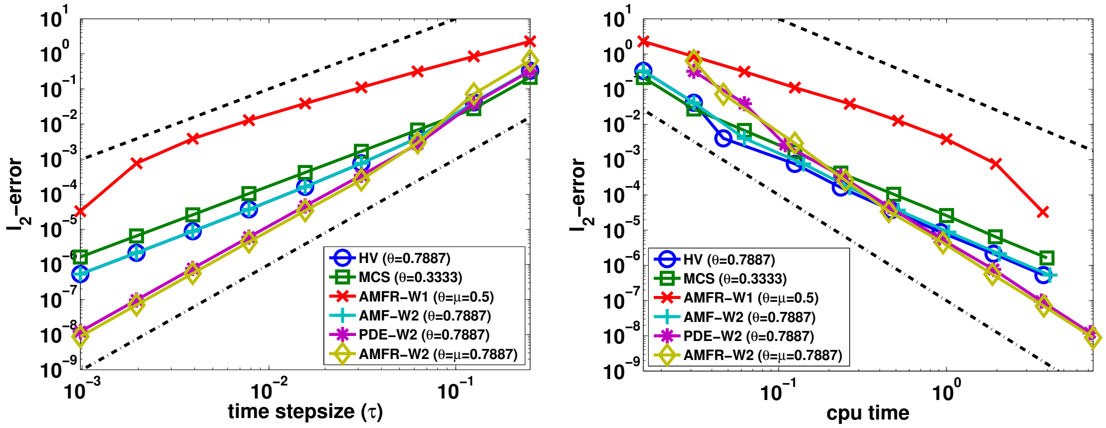

Fig. 4 Heston problem, case (66) with $m = 200$ and $n = 100$. Error vs Time Stepsize (left). Error vs CPU Time (right).

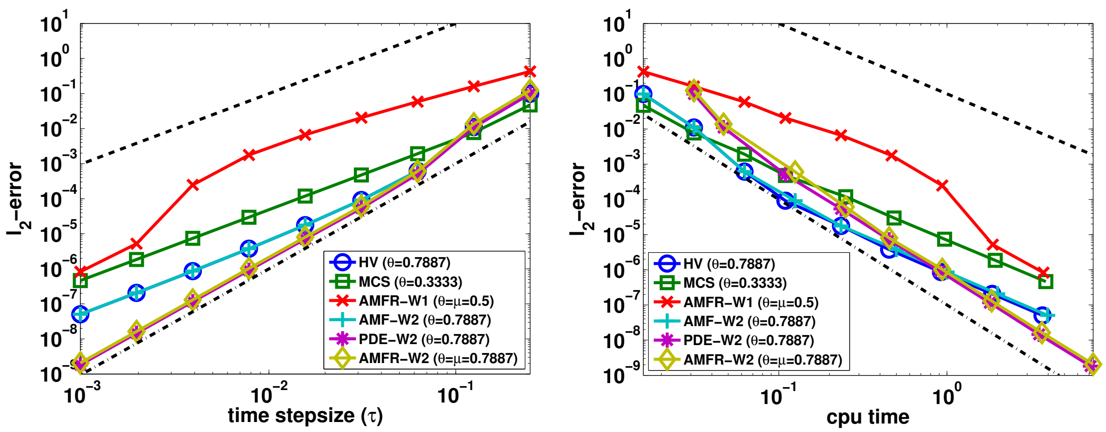

Fig. 5 Heston problem, case (67) with $m = 200$ and $n = 100$. Error vs Time Stepsize (left). Error vs CPU Time (right).

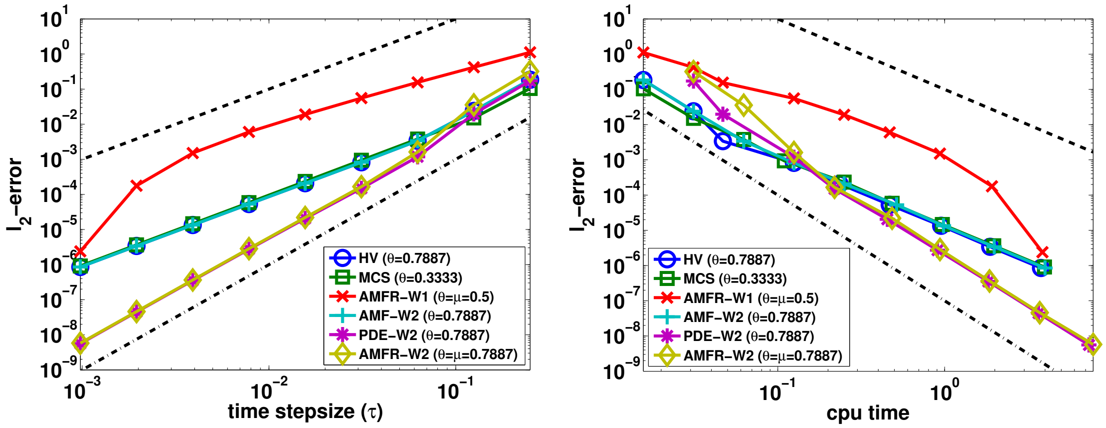

Fig. 6 Heston problem, case (68) with $m = 200$ and $n = 100$. Error vs Time Stepsize (left). Error vs CPU Time (right).

5 Conclusions and work in progress

According to the stability results presented and the numerical experiments carried out, it appears that AMF-type W-methods are an attractive option to deal with the time integration of parabolic problems when mixed derivatives are involved in the spatial elliptic operator and finite differences are considered for the spatial discretizations. These options are new regarding the classical approaches of Craig-Sneyd type or modified Douglas schemes, and the AMF-approach allows for higher orders of convergence (orders greater than two) according to numerical evidences. A full convergence analysis in the line of the one carried out in [20] for the modified Craig-Sneyd method is still lacking for the AMF-W-approach. This is being considered by the authors and their collaborators at present.

References

1. I. J. D. Craig and A. D. Sneyd. An alternating-direction implicit scheme for parabolic equations with mixed derivatives. *Comput. Math. Appl.*, 16(4):341–350, 1988.
2. J. Douglas, Jr. and H. H. Rachford, Jr. On the numerical solution of heat conduction problems in two and three space variables. *Trans. Amer. Math. Soc.*, 82:421–439, 1956.
3. B. Düring, M. Fournié and A. Rigal. High-order ADI schemes for convection-diffusion equations with mixed derivative terms. *In: Spectral and High Order Methods for Partial Differential Equations - ICOSAHOM'12, Gammarth, Tunisia, M. Azaez et al. (eds.)*: 217-226. Lecture Notes in Computational Science and Engineering 95, Springer, Berlin, Heidelberg, 2014.
4. B. Düring and J. Miles. High-order ADI scheme for option pricing in stochastic volatility models. *J. Comput. Appl. Math.*, 316: 109-121, 2017.
5. A. Gerisch and J. G. Verwer. Operator splitting and approximate factorization for taxis-diffusion-reaction models. *Appl. Numer. Math.*, 42(1-3):159–176, 2002. Ninth Seminar on

Numerical Solution of Differential and Differential-Algebraic Equations (Halle, 2000).
6. S. González Pinto, E. Hairer, D. Hernández Abreu and S. Pérez Rodríguez. AMF-type W-methods for parabolic PDEs with mixed derivatives. *SIAM J. Sci. Comput.*, 40(5):A2905–A2929, 2018.
7. S. González Pinto, E. Hairer, D. Hernández Abreu and S. Pérez Rodríguez. PDE-W-methods for parabolic problems with mixed derivatives. *Numer. Algor.*, 78:957–981, 2018.
8. S. González Pinto, D. Hernández Abreu and S. Pérez Rodríguez. Rosenbrock-type methods with inexact AMF for the time integration of advection diffusion reaction PDEs. *J. Comput. Appl. Math.*, 262:304–321, 2014.
9. S. González Pinto, D. Hernández Abreu and S. Pérez Rodríguez. W-methods to stabilize standard explicit Runge-Kutta methods in the time integration of advection-diffusion-reaction PDEs. *J. Comput. Appl. Math.*, 316:143-160, 2017.
10. S. González Pinto, D. Hernández Abreu, S. Pérez Rodríguez and R. Weiner. A family of three-stage third order AMF-W-methods for the time integration of advection diffusion reaction PDEs. *Appl. Math. Comp.*, 274:565–584, 2016.
11. E. Hairer, S.P. Norsett and G. Wanner. *Solving Ordinary Differential Equations I. Non Stiff Problems*. Springer Series in Computational Mathematics 8. Springer-Verlag, Berlin, 2nd revised edition, 1993.
12. E. Hairer and G. Wanner. *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*. Springer Series in Computational Mathematics 14. Springer-Verlag, Berlin, 2nd edition, 1996.
13. C. Hendricks, M. Ehrhardt, and M. Günther. High-order ADI schemes for diffusion equations with mixed derivatives in the combination technique. *Appl. Numer. Math.*, 101:36–52, 2016.
14. C. Hendricks, C. Heuer, M. Ehrhardt and M. Günther. High-order ADI finite difference schemes for parabolic equations in the combination technique with application in finance. *J. Comput. Appl. Math.*, 316: 175-194, 2017.
15. S. L. Heston. A closed form solution for options with stochastic volatility with applications to bonds and currency options. *The Review of Financial Studies* 6:2: 327–343, 1993.
16. W. Hundsdorfer. Accuracy and stability of splitting with stabilizing corrections. *Appl. Numer. Math.*, 42(1-3):213–233, 2002. Ninth Seminar on Numerical Solution of Differential and Differential-Algebraic Equations (Halle, 2000).
17. W. Hundsdorfer and J.G. Verwer. *Numerical solution of time-dependent advection-diffusion-reaction equations*, volume 33 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 2003.
18. K. J. in 't Hout and S. Foulon. ADI finite difference schemes for option pricing in the Heston model with correlation. *Int. J. Numer. Anal. Model.*, 7:2: 303–320, 2010.
19. K. J. in 't Hout and B. D. Welfert. Unconditional stability of second-order ADI schemes applied to multi-dimensional diffusion equations with mixed derivative terms. *Appl. Numer. Math.*, 59(3-4):677–692, 2009.
20. K.J. in 't Hout and M. Wyns. Convergence of the Modified Craig-Sneyd scheme for two-dimensional convection-diffusion equations with mixed derivative term. *J. Comput. Appl. Math.*, 296: 170-180, 2016.
21. T. Jax and G. Steinebach. Generalized ROW-type methods for solving semi-explicit DAEs of index-1. *J. Comput. Appl. Math.*, 316:213-228, 2017.
22. J. Lang and J. G. Verwer. W-methods in optimal control. *Numer. Math.*, 124(2):337–360, 2013.
23. D. W. Peaceman and H. H. Rachford, Jr. The numerical solution of parabolic and elliptic differential equations. *J. Soc. Indust. Appl. Math.*, 3:28–41, 1955.
24. A. Rahunanthan and D. Stanescu, *High-order W-methods*, J. Comput. Appl. Math. 233: 1798–1811, 2010.
25. J. Rang and L. Angermann. New Rosenbrock W-methods of order 3 for partial differential algebraic equations of index 1. *BIT*, 45(4):761–787, 2005.
26. W. Schoutens, E. Simons and J. Tistaert. A perfect calibration ! Now what ? *Wilmott Mag.*, March 2004, 66–78.

27. T. Steihaug and A. Wolfbrandt. An attempt to avoid exact Jacobian and nonlinear equations in the numerical solution of stiff differential equations. *Math. Comp.*, 33(146):521–534, 1979.
28. P. J. van der Houwen and B. P. Sommeijer. Approximate factorization for time-dependent partial differential equations. *J. Comput. Appl. Math.*, 128(1-2):447–466, 2001. Numerical analysis 2000, Vol. VII, Partial differential equations.
29. G. Winkler, T. Apel and U. Wystup. Valuation of options in Hestons stochastic volatility model using finite element methods. *In: Foreign Exchange Risk, eds. J. Hakala and U. Wystup, Risk Publ.*, 2002.