Interpolation preservation of AMF-W methods for linear diffusion problems

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Abstract

This article considers the numerical integration of linear diffusion problems in high space dimension by AMF-W methods. These are methods of the type ADI (alternating direction implicit). We focus on the treatment of general Dirichlet boundary conditions. New is the introduction of a property – interpolation preservation – which permits to extend convergence results for homogeneous boundary conditions to general time-dependent boundary conditions. Numerical experiments confirm the theoretical results.

Keywords: Parabolic partial differential equations, AMF-W methods, interpolation preservation, PDE-convergence, time-dependent Dirichlet boundary conditions.

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1 Introduction

A standard approach for solving evolution parabolic partial differential equations (PDEs) is the method of lines (MOL) which transforms the partial differential equation into a system of ordinary differential equations (ODE). Such an ODE is stiff and its numerical solution requires special time integrators. Moreover, for problems in more than two space dimensions, the dimension of the ODE is extremely large. For this reason we consider in this article AMF-W methods [24, 14], for which the implicitness is reduced to that for a sequence of problems in one space dimension.

Time integrators typically suffer from an order reduction and a loss of accuracy when time-dependent Dirichlet boundary conditions are considered compared to time-independent Dirichlet boundary conditions. This has been observed for Runge-Kutta methods and linearly implicit methods, e.g., in [1, 4, 5, 21, 22], and for several classes of splitting methods in, e.g. [2, 3, 6, 7, 8, 23], where some techniques to avoid or mitigate the order reduction have been proposed. For AMF-W methods the order reduction is documented in [11] and two alternatives for avoiding order reduction have been recently presented in [17, Sections 4.1 and 4.2] (see also [15, Section 5]).

A standard approach for avoiding order reduction is to search for a function $\widehat{u}(t, \mathbf{x})$ that interpolates the boundary conditions, so that the difference with the exact solution of the problem satisfies a PDE with an additional inhomogeneity, but has homogeneous boundary conditions. Such a technique is considered, e.g., in [9].

Outline of the paper. After describing the linear diffusion problems and their space discretisation by symmetric finite differences (Section 2), we introduce AMF-W methods in Section 3. These are linearly implicit time integrators, where implicitness appears only in one space direction, which is in the spirit of ADI (alternating direction implicit) type methods. We shortly present classical order conditions and the stability function of these methods. Section 4 emphasises on the treatment of Dirichlet boundary conditions by means of an expanded correction (see [17, Section 4.2] and [15, Section 5]) which avoids the order reduction due to time-dependent boundary conditions. Unlike other existing boundary correction techniques in the literature, the expanded correction consists of adding particular differential equations at the boundary grid points, in the spirit of the discretization at interior points, without any modification of the time integrator. Our theoretical investigation of this approach is based on a multi-dimensional interpolation of the boundary conditions (Section 5). The main convergence results are the topic of Section 6. We first collect known PDE-convergence results for time-independent Dirichlet boundary conditions (in the ℓ_2 and in the maximum norm), then we introduce the concept of interpolation preservation and we prove that it permits to extend PDE-convergence results for homogeneous boundary conditions to general time-dependent boundary conditions. This yields new insight into PDE-convergence for time-dependent Dirichlet boundary conditions in the ℓ_2 and in the maximum norm. Finally, Section 7 on numerical experiments confirms the theoretical statements of the present work.

2 Linear diffusion problem and its space discretization

This work is devoted to the numerical solution of linear diffusion problems

$$\begin{aligned} &u_t = u_{xx} + u_{yy} + C(t,x,y), \qquad t \in (0,T], \quad (x,y) \in \Omega = (a,b) \times (c,d), \\ &u(t,x,y) = \beta(t,x,y), \qquad (x,y) \in \partial\Omega, \\ &u(0,x,y) = g(x,y), \qquad (x,y) \in \Omega. \end{aligned} \tag{1}$$

with Dirichlet boundary conditions. We consider a uniform grid $\{(x_i,y_j)\,|\,i = 0,\ldots,N+1,\, j = 0,\ldots,M+1\}$ with spacings $\Delta x = (b-a)/(N+1)$ and $\Delta y = (d-c)/(M+1)$, and the solution approximations $U_{i,j}(t) \approx u(t,x_i,y_j)$. With the central differences $(1 \le i \le N,\ 1 \le j \le M)$

$$\delta_{xx}^2\, U_{i,j} = \frac{1}{\Delta x^2}\Big(U_{i-1,j} - 2U_{i,j} + U_{i+1,j}\Big), \qquad \delta_{yy}^2\, U_{i,j} = \frac{1}{\Delta y^2}\Big(U_{i,j-1} - 2U_{i,j} + U_{i,j+1}\Big), \tag{2}$$

and the notation $C_{i,j}(t) = C(t,x_i,y_j)$, we consider the system of ordinary differential equations (for $1 \le i \le N$ and $1 \le j \le M$)[1]

$$\dot U_{i,j} = \delta_{xx}^2\, U_{i,j} + \delta_{yy}^2\, U_{i,j} + C_{i,j}(t). \tag{3}$$

This equation requires functions $U_{i,j}$ for $(i,j) \in \partial\Omega$ which are not yet fixed. It is possible to define them as

$$U_{i,j}(t) = \beta(t,x_i,y_j), \qquad (i,j) \in \partial\Omega, \tag{4}$$

and to consider the system (3)-(4) as a differential-algebraic system of index 1. A direct application of AMF-W methods to the differential equation, when (4) is inserted into (3), leads to an order reduction (see [11] and [12]) and to a loss of accuracy in the case of time-dependent boundary conditions.

In the present article we concentrate on the situation where the missing values on the boundary are defined by differential equations. A straight-forward approach is to consider

$$\dot U_{i,j}(t) = \dot\beta(t,x_i,y_j), \qquad (i,j) \in \partial\Omega, \tag{5}$$

with initial values $\beta(0,x_i,y_j)$ from the boundary condition. Using the notation $B_{i,j}(t) = \beta(t,x_i,y_j)$ we can also consider the differential equation

$$\dot U_{i,j}(t) = \dot B_{i,j}(t) + \delta_{xx}^2\big(U_{i,j}(t) - B_{i,j}(t)\big) + \delta_{yy}^2\big(U_{i,j}(t) - B_{i,j}(t)\big), \qquad (i,j) \in \partial\Omega, \tag{6}$$

[1] In the following we write $(i,j) \in \Omega$ for $(x_i,y_j) \in \Omega$, i.e., for $1 \le i \le N$ and $1 \le j \le M$. Similarly, we write $(i,j) \in \partial\Omega$ for $(x_i,y_j) \in \partial\Omega$, i.e., when at least one relation among $i=0$, $i=N+1$, $j=0$, $j=M+1$ is satisfied.

with initial values as before. Here and throughout the article we use the convention that (for any grid function V_{ij})

$$\delta_{xx}^2 V_{ij} = 0 \quad \text{if} \quad i = 0 \quad \text{or} \quad i = N+1, \qquad \delta_{yy}^2 V_{ij} = 0 \quad \text{if} \quad j = 0 \quad \text{or} \quad j = M+1. \tag{7}$$

Note that at a vertex of Ω, the definition of $U_{i,j}$ reduces to that of (5), and hence it is possible to first compute the values corresponding to the four vertices of the rectangle. At a side, e.g., $i = 0$, we have a system of differential equations for $U_{0,j}$, $1 \le j \le M$. Note that for $(i,j) \in \partial\Omega$, the expression $U_{i,j}(t) - \beta(t, x_i, y_j)$ is an invariant of the differential equations (5) and (6).

Formulation in arbitrary space dimension. The main results of the present work are valid in arbitrarily high space dimension. On an m-dimensional hyperrectangle $\Omega = (a_1, b_1) \times \cdots \times (a_m, b_m)$ the problem is given by

$$\begin{aligned}
&u_t = u_{x_1x_1} + \cdots + u_{x_mx_m} + C(t, x_1, \ldots, x_m), \qquad (x_1, \ldots, x_m) \in \Omega,\\
&u(t, x_1, \ldots, x_m) = \beta(t, x_1, \ldots, x_m), \qquad (x_1, \ldots, x_m) \in \partial\Omega,\\
&u(0, x_1, \ldots, x_m) = g(x_1, \ldots, x_m), \qquad (x_1, \ldots, x_m) \in \Omega.
\end{aligned} \tag{8}$$

For the variable x_i we consider an equidistant grid $x_i^0 < x_i^1 < \cdots < x_i^{N_i+1}$ of the interval $[a_i, b_i]$ (with $x_i^0 = a_i$ and $x_i^{N_i+1} = b_i$). As in (2) we consider central difference operators $\delta_{x_jx_j}^2 V_{i_1,\ldots,i_m}$ and we make the convention (see (7)) that $\delta_{x_jx_j}^2 V_{i_1,\ldots,i_m} = 0$, if the jth component i_j is either 0 or $N_j + 1$. The resulting ordinary differential equation is then given for $(i_1, \ldots, i_m) \in \Omega$ (i.e., for $1 \le i_j \le N_j$, $j = 1, \ldots, m$) by

$$\dot{U}_{i_1,\ldots,i_m} = \left(\delta_{x_1x_1}^2 + \cdots + \delta_{x_mx_m}^2\right) U_{i_1,\ldots,i_m} + C_{i_1,\ldots,i_m}(t), \tag{9}$$

so that $U_{i_1,\ldots,i_m}(t)$ will be an approximation of $u(t, x_1^{i_1}, \ldots, x_m^{i_m})$. The corresponding approaches (5) and (6) to compute boundary values in the multidimensional case are respectively given by

$$\dot{U}_{i_1,\ldots,i_m}(t) = \dot{B}_{i_1,\ldots,i_m}(t), \tag{10}$$

and

$$\dot{U}_{i_1,\ldots,i_m}(t) = \dot{B}_{i_1,\ldots,i_m}(t) + \sum_{j=1}^{m} \delta_{x_jx_j}^2 \big(U_{i_1,\ldots,i_m}(t) - B_{i_1,\ldots,i_m}(t)\big), \tag{11}$$

whenever $(i_1, \ldots, i_m) \in \partial\Omega$, with $B_{i_1,\ldots,i_m}(t) = \beta(t, x_1^{i_1}, \ldots, x_m^{i_m})$.

3 AMF-W methods

Let $U_{n,ij}$ be an approximation of the solution $U_{ij}(t_n)$ of (3) at time $t_n = t_0 + n\tau$ (here, τ is the time step size). An application of an s-stage AMF-W method with parameters

$c_k, b_k, a_{kl}, \ell_{kl}, \rho_k, \theta$ and η is given for (i,j) in the interior of Ω by (see, e.g., [14])

$$\begin{aligned}
K^{(0)}_{k,ij} &= \tau\big(\delta^2_{xx} + \delta^2_{yy}\big)\Big(U_{n,ij} + \sum_{l=1}^{k-1} a_{kl}K_{l,ij}\Big) + \tau\, C_{ij}(t_n + c_k\tau) + \sum_{l=1}^{k-1} \ell_{kl}K_{l,ij},\\
K^{(1)}_{k,ij} - \theta\tau\delta^2_{xx}K^{(1)}_{k,ij} &= K^{(0)}_{k,ij} + \theta\rho_k\tau^2\dot{C}_{ij}(t_n + \eta\tau),\\
K_{k,ij} - \theta\tau\delta^2_{yy}K_{k,ij} &= K^{(1)}_{k,ij}
\end{aligned} \tag{12}$$

for $k = 1,\dots,s$, and the update formula

$$U_{n+1,ij} = U_{n,ij} + \sum_{k=1}^{s} b_k K_{k,ij}. \tag{13}$$

This formulation of the method is not yet complete. Due to the finite difference operators δ^2_{xx} and δ^2_{yy} also the values of $U_{n,ij}$ and that of $K_{k,ij}, K^{(1)}_{k,ij}$ are required on the border of Ω.

For homogeneous boundary conditions, i.e., $\beta(t,x,y) \equiv 0$, we not only put $U_{n,ij} = 0$ for $(i,j) \in \partial\Omega$, but we also put $K^{(0)}_{k,ij} = 0$, $K^{(1)}_{k,ij} = 0$, and $K_{k,ij} = 0$ for $(i,j) \in \partial\Omega$. The treatment of general time-dependent boundary conditions is postponed to Section 4.

3.1 Arbitrary space dimension

The extension of an AMF-W method to arbitrary space dimension is straight-forward. We use the abbreviation $\mathbf{i} = (i_1,\dots,i_m)$ for an m-dimensional index vector. For an s-stage AMF-W method we consider in the interior of Ω for $k = 1,\dots,s$

$$\begin{aligned}
K^{(0)}_{k,\mathbf{i}} &= \tau\big(\delta^2_{x_1x_1} + \cdots + \delta^2_{x_mx_m}\big)\Big(U_{n,\mathbf{i}} + \sum_{l=1}^{k-1} a_{kl}K_{l,\mathbf{i}}\Big) + \tau\, C_{\mathbf{i}}(t_n + c_k\tau) + \sum_{l=1}^{k-1} \ell_{kl}K_{l,\mathbf{i}},\\
K^{(1)}_{k,\mathbf{i}} - \theta\tau\delta^2_{x_1x_1}K^{(1)}_{k,\mathbf{i}} &= K^{(0)}_{k,\mathbf{i}} + \theta\rho_k\tau^2\dot{C}_{\mathbf{i}}(t_n + \eta\tau),\\
K^{(j)}_{k,\mathbf{i}} - \theta\tau\delta^2_{x_jx_j}K^{(j)}_{k,\mathbf{i}} &= K^{(j-1)}_{k,\mathbf{i}}, \qquad j = 2,\dots,m,
\end{aligned} \tag{14}$$

and with $K_{k,\mathbf{i}} = K^{(m)}_{k,\mathbf{i}}$ the update formula for the numerical solution is given by

$$U_{n+1,\mathbf{i}} = U_{n,\mathbf{i}} + \sum_{k=1}^{s} b_k K_{k,\mathbf{i}}. \tag{15}$$

For homogeneous boundary conditions, missing values on the border are defined by zero. The case of general time-dependent boundary conditions will be discussed in Section 4.2. We first recall the classical concepts of *order conditions* and the *stability function.*

3.2 Classical order conditions

Classical order p means that, for a fixed space discretisation, the local error is bounded by $\mathcal{O}(\tau^{p+1})$. Here, the constant involved in the $\mathcal{O}$-notation is allowed to depend on the space discretisation. In addition to the $s \times s$ matrices $A = (a_{kl})$ and $L = (\ell_{kl})$ we use the notation

$$\tilde{A} = A(I - L)^{-1}, \quad \tilde{b}^\top = b^\top (I - L)^{-1}, \quad \tilde{\Gamma} = \theta(I - L)^{-1}. \tag{16}$$

To get a certain order the parameter vectors $\rho = (\rho_k)$ and $c = (c_k)$ have to be given by $\rho = (I - L)^{-1}\mathbf{1}$ and $c = A\rho = \tilde{A}\mathbf{1}$. The classical order conditions (see [11] or [19, p. 114–117]) are then given for $p \leq 3$ by

$$\begin{array}{lll} \text{order } p = 1 & \iff & \tilde{b}^\top \mathbf{1} = 1. \\ \text{order } p = 2 & \iff & \tilde{b}^\top \mathbf{1} = 1 \quad \text{and} \quad \tilde{b}^\top (\tilde{A} + \tilde{\Gamma})\mathbf{1} = 1/2. \\ \text{order } p = 3 & \iff & \tilde{b}^\top \mathbf{1} = 1, \quad \tilde{b}^\top \tilde{A}\,\mathbf{1} = 1/2, \quad \tilde{b}^\top \tilde{\Gamma}\,\mathbf{1} = 0 \quad \text{and} \\ & & \quad \tilde{b}^\top c^2 = 1/3, \quad \tilde{b}^\top (\tilde{A} + \tilde{\Gamma})^2 \mathbf{1} = 1/6. \end{array}$$

The presentation of the convergence results of the present paper requires a subset of the order conditions for order 4. They are

$$\text{order } p = 4 \quad \Longrightarrow \quad \begin{array}{l} \tilde{b}^\top (\tilde{A} + \tilde{\Gamma})\,\tilde{\Gamma}\mathbf{1} = 0, \quad \tilde{b}^\top (\tilde{A} + \tilde{\Gamma})^3 \mathbf{1} = 1/24, \quad \tilde{b}^\top \tilde{\Gamma}\,(\tilde{A} + \tilde{\Gamma})\mathbf{1} = 0, \\ \tilde{b}^\top (\tilde{A} + \tilde{\Gamma})\, c^2 = 1/12, \quad \tilde{b}^\top c^3 = 1/4. \end{array} \tag{17}$$

3.3 Stability function

Applying the AMF-W method (14) to the test equation $\dot{U} = \lambda_1 U + \cdots + \lambda_m U$ and putting $z_j = \lambda_j \tau$ we get $U_{n+1} = R(z_1, \ldots, z_m)\, U_n$, where the stability function is given by

$$\begin{aligned} R(z_1, \ldots, z_m) &= 1 + b^\top P(z_1, \ldots, z_m)^{-1} \mathbf{1} \cdot (z_1 + \cdots + z_m), \qquad \text{with} \\ P(z_1, \ldots, z_m) &= \pi(z_1, \ldots, z_m) I - (z_1 + \cdots + z_m) A - L, \\ \pi(z_1, \ldots, z_m) &= (1 - \theta z_1) \cdots (1 - \theta z_m). \end{aligned} \tag{18}$$

Here, $P(z_1, \ldots, z_m)$ is a triangular matrix of dimension s. Since we consider only purely diffusion problems, we assume z_j to be real variables. The condition

$$-1 \leq R(z_1, \ldots, z_m) \leq 1, \qquad \text{for} \quad z_1, \ldots, z_m \leq 0 \tag{19}$$

is usually called A_0-stability. For optimal convergence orders we also consider the slightly stronger property

$$-1 \leq R(z_1, \ldots, z_m) \leq 1 - C_1 \frac{|z_1 + \cdots + z_m|}{\pi(z_1, \ldots, z_m)^2}, \qquad \text{for} \quad z_1, \ldots, z_m \leq 0, \tag{20}$$

where $C_1 > 0$ is some positive constant. A discussion of these stability requirements in terms of the coefficients of the AMF-W method is given in [12].

4 Treatment of time-dependent boundary conditions

For general Dirichlet boundary conditions there are several possibilities for defining $K_{k,ij}$ for $(i,j) \in \partial\Omega$. We discuss the approach based on the discretisation of (6) recently introduced in [17, Section 4.2] (see also [15, Section 5]). An alternative boundary correction approach based on the discretisation of (5) was also considered in [17, Section 4.1].

4.1 Expanded correction

"The general idea is always to treat boundary values as far as possible in the same way as the interior points." (Hundsdorfer & Verwer, 2003, p. 365)

Here we use the differential equation (6) on the boundary $\partial\Omega$ (see [17, Section 4.2] and [15, Section 5]). The differential equation (6) is formally equal to (3), where $C_{ij}(t)$ is replaced by

$$C_{ij}(t) = \dot{B}_{ij}(t) - \delta_{xx}^2 B_{ij}(t) - \delta_{yy}^2 B_{ij}(t), \qquad (i,j) \in \partial\Omega. \tag{21}$$

With the convention (7), this approach gives the formulas of (12) also for indices $(i,j) \in \partial\Omega$.

It is possible to first make the computations on the vertices, then independently on each side, and finally in the interior of the rectangle. It is interesting to note that for $(i,j) \in \partial\Omega$ the values only depend on the function $\beta(t,x,y)$ and on its time derivative.

4.2 Arbitrary space dimension

AMF-W methods are given in (14) for general space dimension m. The formulation is complete for homogeneous boundary conditions. For the case of inhomogeneous boundary conditions, K-values on the border $\partial\Omega$ are required. They depend on the kind of correction that is used.

For the expanded correction we use the formulas (14) not only in the interior of Ω, but also on its border. There, the function $C_{\mathbf{i}}(t)$ is given by

$$C_{\mathbf{i}}(t) = \dot{B}_{\mathbf{i}}(t) - \delta_{x_1 x_1}^2 B_{\mathbf{i}}(t) - \cdots - \delta_{x_m x_m}^2 B_{\mathbf{i}}(t), \qquad \mathbf{i} \in \partial\Omega, \tag{22}$$

with $B_{\mathbf{i}}(t) = \beta(t, x_1^{i_1}, \ldots, x_m^{i_m})$. In agreement with the convention (7) we set zero every expression $\delta_{x_j,x_j}^2 V_{\mathbf{i}}$, if the jth component of $\mathbf{i} = (i_1, \ldots, i_m)$ is either 0 or $N_j + 1$. As before we can start by computing the values $K_{k,\mathbf{i}}^{(j)}$ on the corners, then on the lines, on the faces, and so on. Finally, the method can be applied in the interior of Ω.

Remark 1. *(Explicit correction.)* An alternative approach for boundary correction considered in [17, Section 4.1] is based on applying the AMF-W method (14) to (5).

This just means that we have to remove all expressions containing $\delta^2_{x_jx_j}$ for some $j \in \{1,\dots,m\}$, and we have to use $\dot{B}_{\mathbf{i}}(t)$ instead of $C_{\mathbf{i}}(t)$, so that

$$K_{k,\mathbf{i}} = \tau \dot{B}_{\mathbf{i}}(t_n + c_k\tau) + \theta\rho_k\tau^2 \ddot{B}_{\mathbf{i}}(t_n + \eta\tau) + \sum_{l=1}^{k-1} \ell_{kl} K_{l,\mathbf{i}} \tag{23}$$

for $\mathbf{i} \in \partial\Omega$. The recursion is explicit and does not require any solution of linear systems. The numerical approximation $U_{n+1,\mathbf{i}}$ is then provided by the update formula (15). The application of (14) in the interior of Ω still requires the values of $K^{(j)}_{k,\mathbf{i}}$ on the boundary $\partial\Omega$. We put $K^{(m)}_{k,\mathbf{i}} = K_{k,\mathbf{i}}$, and we compute $K^{(m-1)}_{k,\mathbf{i}},\dots,K^{(1)}_{k,\mathbf{i}}$ recursively from the last line of (14).

5 Interpolation of Dirichlet boundary conditions

To get more symmetric formulas we treat in this section the m-dimensional hypercube $\Omega = (-1,1)^m$. This can be done without loss of generality. We consider Dirichlet boundary conditions $u(t,x_1,\dots,x_m) = \beta(t,x_1,\dots,x_m)$ on the border $(x_1,\dots,x_m) \in \partial\Omega$.

5.1 Multi-dimensional interpolation

In dimension $m = 1$ the linear interpolation of the boundary values is simply

$$\widehat{u}(t,x_1) = \tfrac{1}{2}\Big((1-x_1)\beta(t,-1) + (1+x_1)\beta(t,1)\Big). \tag{24}$$

In dimension $m = 2$ we consider the function

$$\begin{aligned}\widehat{u}(t,x_1,x_2) =& \tfrac{1}{2}\Big((1-x_1)\beta(t,-1,x_2) + (1+x_1)\beta(t,1,x_2) + (1-x_2)\beta(t,x_1,-1) + (1+x_2)\beta(t,x_1,1)\Big)\\ &- \tfrac{1}{4}\Big((1-x_1)(1-x_2)\beta(t,-1,-1) + (1+x_1)(1-x_2)\beta(t,1,-1)\\ &\qquad + (1-x_1)(1+x_2)\beta(t,-1,1) + (1+x_1)(1+x_2)\beta(t,1,1)\Big),\end{aligned}$$

which equals $\beta(t,x_1,x_2)$ on the border of Ω.

Lemma 1. *For the general case of m dimensions, consider the set $\mathcal{I} = \big\{\alpha = (\alpha_1,\dots,\alpha_m) \mid \alpha_i \in \{-1,0,1\}\big\} \setminus \{(0,\dots,0)\}$ and let $s(\alpha)$ be the number of non-zero elements of α. For a function $\beta(t,x_1,\dots,x_m)$, defined on $\partial\Omega$, we put*

$$\widehat{u}(t,x_1,\dots,x_m) = \sum_{\alpha\in\mathcal{I}} (-1)^{s(\alpha)+1} \Bigg(\prod_{\substack{j=1\\ \alpha_j\neq 0}}^{m} \Big(\frac{1+\alpha_j x_j}{2}\Big)\Bigg) \beta(t,x_1^\alpha,\dots,x_m^\alpha), \qquad x_j^\alpha = \begin{cases} -1 & \text{if } \alpha_j = -1\\ x_j & \text{if } \alpha_j = 0\\ +1 & \text{if } \alpha_j = 1.\end{cases} \tag{25}$$

This function interpolates the values $\beta(t,x_1,\dots,x_m)$ on the boundary.

Proof. Let $(x_1, \dots, x_m)$ be in $\partial\Omega$, e.g., $x_1 = 1$. The summands with $\alpha_1 = -1$ are all zero. The summand for $\alpha = (1, 0, \dots, 0)$ yields $\beta(t, x_1, \dots, x_m)$. The two summands for $\alpha = (1, \alpha_2, \dots, \alpha_m)$ and $\alpha = (0, \alpha_2, \dots, \alpha_m)$ (with at least one non-zero element among $\alpha_2, \dots, \alpha_m$) are identical but with opposite sign and thus vanish in the sum. A similar argument applies to other boundary points. $\square$

5.2 Interpolated grid functions

For each variable x_j we consider the equidistant grid-points $-1 = x_j^0 < x_j^1 < \dots < x_j^{N_j+1} = 1$ in the interval $[-1, 1]$. We let $U_{i_1,\dots,i_m}(t)$ be an approximation to $U(t, x_1^{i_1}, \dots, x_m^{i_m})$. The discrete analogue of (25) is then

$$U_{i_1,\dots,i_m}(t) = \sum_{\alpha\in\mathcal{I}} (-1)^{s(\alpha)+1} \left(\prod_{\substack{j=1 \\ \alpha_j \neq 0}}^{m} \left(\frac{1 + \alpha_j x_j^{i_j}}{2} \right) \right) U_{i_1^\alpha,\dots,i_m^\alpha}(t), \qquad i_j^\alpha = \begin{cases} 0 & \text{if } \alpha_j = -1 \\ i_j & \text{if } \alpha_j = 0 \\ N_j + 1 & \text{if } \alpha_j = 1. \end{cases} \tag{26}$$

As in the continuous case, $U_{i_1,\dots,i_m}$ interpolates the values on the boundary. Note that $U_{i_1^\alpha,\dots,i_m^\alpha}$ is the function value on the face of the hyperrectangle given by $x_j \in [-1, 1]$ if $\alpha_j = 0$, by $x_j = -1$ if $\alpha_j = -1$, and by $x_j = 1$ if $\alpha_j = 1$. Grid functions satisfying (26) are called *interpolated grid functions*. Later on, we will omit the dependence on t of the grid functions when it is not relevant. The set of all such grid functions is defined as

$$\mathcal{V}_m = \left\{ (V_{i_1,\dots,i_m}) \;\middle|\; V_{i_1,\dots,i_m} \text{ satisfies } (26) \right\}. \tag{27}$$

Lemma 2 (properties of $\mathcal{V}_m$)**.** *It holds*

- *for every m, the set $\mathcal{V}_m$ is a linear space,*
- *if $U_{i_1,\dots,i_m} \in \mathcal{V}_m$, then also $V_{i_1,\dots,i_m} = \partial^2_{x_j x_j} U_{i_1,\dots,i_m} \in \mathcal{V}_m$,*
- *if $U_{i_1,\dots,i_m} - \theta\tau\partial^2_{x_j x_j} U_{i_1,\dots,i_m} = V_{i_1,\dots,i_m}$, then $V_{i_1,\dots,i_m} \in \mathcal{V}_m$ if and only if $U_{i_1,\dots,i_m} \in \mathcal{V}_m$.*

Proof. The fact that $\mathcal{V}_m$ is a linear space of finite dimension is obvious.

For the second statement, consider an index vector $(i_1, \dots, i_m)$ that corresponds to the grid point $(x_1^{i_1}, \dots, x_m^{i_m}) \equiv (x_1, \dots, x_m)$. We then have

$$\begin{aligned} V_{i_1,\dots,i_m} = \partial^2_{x_l x_l} U_{i_1,\dots,i_m} &= \sum_{\alpha\in\mathcal{I}} (-1)^{s(\alpha)+1} \partial^2_{x_l x_l} \left[\left(\prod_{\substack{j=1 \\ \alpha_j \neq 0}}^{m} \left(\frac{1 + \alpha_j x_j}{2} \right) \right) U_{i_1^\alpha,\dots,i_m^\alpha} \right] \\ &= \sum_{\alpha\in\mathcal{I}} (-1)^{s(\alpha)+1} \left(\prod_{\substack{j=1 \\ \alpha_j \neq 0}}^{m} \left(\frac{1 + \alpha_j x_j}{2} \right) \right) \partial^2_{x_l x_l} U_{i_1^\alpha,\dots,i_m^\alpha}. \end{aligned}$$

The last equality is seen as follows. For $\alpha_l = 0$ the product is independent of x_l and can be moved outside the operator $\partial_{x_l x_l}$. For $\alpha_l \neq 0$ the second difference of the expression in square brackets vanishes, and we also have $\partial^2_{x_l x_l} U_{i_1^\alpha,\dots,i_m^\alpha} = 0$.

Since $\theta\tau$ is real and positive and the eigenvalues of $\partial_{x_l x_l}$ are negative, the linear mapping $U \mapsto (I - \theta\tau\partial_{x_l x_l})U$ is bijective on the vector space of all $\{U = (U_{i_1,\dots,i_m})\,;\, i_j = 0,\dots,N_j+1, j = 1,\dots,m\}$. As a consequence of the first two statements, the subspace $\mathcal{V}_m$ is invariant under this mapping. Therefore, its restriction to the subspace $\mathcal{V}_m$ is also bijective, which completes the proof of the lemma. □

6 PDE-convergence of AMF-W methods

Without loss of generality we consider the m-dimensional hypercube $\Omega = (-1,1)^m$ and Dirichlet boundary conditions $u(t, x_1, \dots, x_m) = \beta(t, x_1, \dots, x_m)$ on the border $(x_1, \dots, x_m) \in \partial\Omega$. We let $\widehat{u}(t, x_1, \dots, x_m)$ be the interpolation (25), which defines a smooth function in Ω and agrees with $\beta(t, x_1, \dots, x_m)$ on $\partial\Omega$. At the grid points we denote the interpolated values by $\widehat{U}_{i_1,\dots,i_m}(t) = \widehat{u}(t, x_1^{i_1}, \dots, x_m^{i_m})$. If $U_{i_1,\dots,i_m}(t)$ denotes the solution of the differential equation (9), then the function

$$\widetilde{U}_{i_1,\dots,i_m}(t) = U_{i_1,\dots,i_m}(t) - \widehat{U}_{i_1,\dots,i_m}(t) \tag{28}$$

has homogeneous Dirichlet boundary conditions $\widetilde{U}_{i_1,\dots,i_m}(t) = 0$ for $(i_1, \dots, i_m) \in \partial\Omega$, and satisfies the differential equation

$$\dot{\widetilde{U}}_{i_1,\dots,i_m} = \big(\delta^2_{x_1x_1} + \dots + \delta^2_{x_mx_m}\big)\,\widetilde{U}_{i_1,\dots,i_m} + C_{i_1,\dots,i_m}(t) + \widehat{C}_{i_1,\dots,i_m}(t), \tag{29}$$

with the additional inhomogeneity $\widehat{C}_{i_1,\dots,i_m}(t)$ defined by

$$\dot{\widehat{U}}_{i_1,\dots,i_m} = \big(\delta^2_{x_1x_1} + \dots + \delta^2_{x_mx_m}\big)\,\widehat{U}_{i_1,\dots,i_m} - \widehat{C}_{i_1,\dots,i_m}(t). \tag{30}$$

In addition to the numerical approximation $U_{n,i_1,\dots,i_m}$ of (12) (with the boundary condition treated either by the explicit correction or by the expanded correction) we let $\widetilde{U}_{n,i_1,\dots,i_m}$ be the numerical approximation (with the same AMF-W method) for (29) and homogeneous Dirichlet boundary conditions. We also put $\widehat{U}_{0,i_1,\dots,i_m} = \widehat{U}_{i_1,\dots,i_m}(0)$. The differences $\widehat{U}_{n,i_1,\dots,i_m} = U_{n,i_1,\dots,i_m} - \widetilde{U}_{n,i_1,\dots,i_m}$ then satisfy (using the abbreviation $\mathbf{i} = (i_1, \dots, i_m)$ for the multi-index)

$$\begin{aligned}
&\widehat{K}^{(0)}_{k,\mathbf{i}} = \tau\big(\delta^2_{x_1x_1} + \dots + \delta^2_{x_mx_m}\big)\Big(\widehat{U}_{n,\mathbf{i}} + \sum_{l=1}^{k-1} a_{kl}\widehat{K}_{l,\mathbf{i}}\Big) - \tau\,\widehat{C}_{\mathbf{i}}(t_n + c_k\tau) + \sum_{l=1}^{k-1} \ell_{kl}\widehat{K}_{l,\mathbf{i}},\\
&\widehat{K}^{(1)}_{k,\mathbf{i}} - \theta\tau\delta^2_{x_1x_1}\widehat{K}^{(1)}_{k,\mathbf{i}} = \widehat{K}^{(0)}_{k,\mathbf{i}} - \theta\rho_k\tau^2\dot{\widehat{C}}_{\mathbf{i}}(t_n + \eta\tau),\\
&\widehat{K}^{(j)}_{k,\mathbf{i}} - \theta\tau\delta^2_{x_jx_j}\widehat{K}^{(j)}_{k,\mathbf{i}} = \widehat{K}^{(j-1)}_{k,\mathbf{i}}, \qquad j = 2, \dots, m,
\end{aligned} \tag{31}$$

$\widehat{K}_{k,\mathbf{i}} = \widehat{K}^{(m)}_{k,\mathbf{i}}$, for $k = 1, \dots, s$, and the update formula

$$\widehat{U}_{n+1,\mathbf{i}} = \widehat{U}_{n,\mathbf{i}} + \sum_{k=1}^{s} b_k\widehat{K}_{k,\mathbf{i}}. \tag{32}$$

These formulas can be considered as the discretisation of the equation (30) by the AMF-W method, where the boundary conditions are treated in the same way as for $U_{n,\mathbf{i}}$. We note that $\widehat{U}_{0,\mathbf{i}}$ is an interpolated grid function, and that by Lemma 2 also $\widehat{C}_{\mathbf{i}}(t)$ are interpolated grid functions.

Optimal order of convergence in the Euclidean norm is known for AMF-W methods in the case of time-independent Dirichlet boundary conditions (see [11] for $m = 2$ and [12] for $m \geq 2$). We therefore know optimal estimates for the global error $\widetilde{U}_n - \widetilde{U}(t_n)$ (see Section 6.1 below), which corresponds to homogeneous Dirichlet boundary conditions. Because of

$$U_n - U(t_n) = \big(\widetilde{U}_n - \widetilde{U}(t_n)\big) + \big(\widehat{U}_n - \widehat{U}(t_n)\big), \tag{33}$$

estimates for the global error $U_n - U(t_n)$ (with general Dirichlet boundary conditions) can thus be obtained from estimates for $\widehat{U}_n - \widehat{U}(t_n)$, which depend only on $\beta(t, x_1, \ldots, x_m)$ and not on initial conditions.

6.1 PDE-convergence for time-independent boundary conditions

An AMF-W method is called *PDE-convergent* of order p, if the global error satisfies

$$\|U_n - U(t_n)\| \leq C\tau^p \qquad \text{for} \quad 0 \leq t_n = n\tau \leq T, \tag{34}$$

where the constant C is independent of the space discretisation. The order of PDE-convergence can depend on the chosen norm.

Euclidean norm. For real vectors $U = (U_{i_1,\ldots,i_m})$ and $V = (V_{i_1,\ldots,i_m})$ (where $i_j = 0, \ldots, N_j + 1$) and for the grid spacing $\Delta x_i = 2/(N_i + 1)$ we consider the weighted inner product and the induced ℓ_2 norm

$$\|U\|_2 = \sqrt{\langle U, U\rangle}, \qquad \langle U, V\rangle_2 = \Delta x_1 \cdots \Delta x_m \sum_{i_1=0}^{N_1+1} \cdots \sum_{i_m=0}^{N_m+1} U_{i_1,\ldots,i_m} V_{i_1,\ldots,i_m}. \tag{35}$$

The following convergence statements, taken from the publications [11] and [12], assume that the time step size satisfies $\tau \geq c_0 \max(\Delta x_1^2, \ldots, \Delta x_m^2)$ for some $c_0 > 0$.

Theorem 1. *Consider the s-stage AMF-W method (14) applied to (9) in space dimension $m \geq 2$ with time-independent Dirichlet boundary conditions. Assume that*

- *the classical conditions for order p ($p \leq 3$) hold,*
- *the stability condition (19) holds if $p = 1$ or $p = 2$, condition (20) holds if $p = 3$,*

then the AMF-W method is PDE-convergent of order p in the Euclidean norm.

It is conjectured in [12] that the statement of this theorem does not hold for order $p = 4$, and it is proved there that an order higher than 3 can be achieved.

Theorem 2. *Consider the s-stage AMF-W method (14) applied to (9) in space dimension $m \geq 2$ with time-independent Dirichlet boundary conditions. Assume that*

- *the classical conditions for order $p = 3$ and the five order conditions (17) hold,*

- *the stability condition* (20) *holds,*

then the AMF-W method is PDE-convergent of order $p^* = 3.25$ in the Euclidean norm. Here, convergence of order p^* means convergence of order $p - \epsilon$, for all $\epsilon > 0$.

Maximum norm. Convergence results in the maximum norm $\|U\|_\infty = \max\{|U_{i_1,\ldots,i_m}|\,;\, 0 \le i_j \le N_i + 1\}$ are much more difficult to obtain, even for homogeneous Dirichlet boundary conditions. The standard convergence proof needs the power-boundedness of the propagation matrix. This is already a non-trivial task and has been considered in [13]. Convergence results in the maximum norm for one-stage AMF-W methods can be found in [10] and [16]. For a one-stage method we have $s = 1$, $b_1 = 1$, $c_1 = 0$, and θ is a free parameter.

Theorem 3. *Consider the 1-stage AMF-W method* (14) *applied to* (9) *in space dimension $m \ge 2$ with time-independent Dirichlet boundary conditions. Under the assumptions made in [16] we have*

- *the method is PDE-convergent of order $p = 1$ for $\theta \ge 1/2$,*
- *the method is PDE-convergent of order $p = 2$ for $\theta = 1/2$.*

Remark 2. All the convergence results in the previous theorems also hold in dimension $m = 1$, which is a simpler case. This has been known for a long time, as it can be seen for Rosenbrock methods in arbitrary ℓ_p-norms in [21].

6.2 Interpolation preservation of AMF-W methods with expanded correction

This section is devoted to an interesting preservation property for AMF-W methods combined with expanded correction for the boundary. This will be an essential ingredient for extending convergence results for problems with homogeneous boundary conditions to problems with general time-dependent Dirichlet boundary conditions.

Lemma 3. *Consider an AMF-W method, where the boundary $\partial\Omega$ is treated by the expanded correction of Section 4.1. If $\widehat{U}_0$ and $\widehat{C}(t)$ are interpolated grid functions, then also $\widehat{K}_k^{(j)}$ ($k = 1, \ldots, s$, $j = 0, \ldots, m$) and $\widehat{U}_n$ ($n = 1, 2, \ldots, N = T/\tau$) are interpolated grid functions.*

Proof. For the "expanded correction" the border of Ω is treated in exactly the same way as its interior, so that Lemma 2 applies. The proof is by induction on n.

For $n = 0$ the initial value $\widehat{U}_0$ is an interpolated grid function by assumption. Assume now that $\widehat{U}_n$ is an interpolated grid function. The step to $n+1$ is by induction on the stages k. The first statement of Lemma 2 shows that $\widehat{K}_k^{(0)}$ is an interpolated grid function, and the second statement proves that also $\widehat{K}_k^{(1)}, \ldots, \widehat{K}_k^{(m)}, \widehat{K}_k$ are interpolated grid functions. Since the set of interpolated grid functions is a linear space, $\widehat{U}_{n+1}$ is an interpolated grid function. □

Note that Lemma 3 does not hold for the "explicit correction" of Remark 1, where the boundary is not discretized in the same way as the interior of Ω.

If we consider an AMF-W method with expanded correction of the boundary conditions and with projection to the exact boundary values after every time step (i.e., we put $\widehat{U}_{n+1,i_1,\ldots,i_m} = \widehat{U}_{i_1,\ldots,i_m}(t_{n+1})$ for $(i_1,\ldots,i_m) \in \partial\Omega$), we also destroy the interpolation property so that $\widehat{U}_{n+1}$ is no longer an interpolated grid function.

6.3 Bounds of interpolated grid functions

In this section we give bounds for interpolated grid functions in terms of their values on the border of Ω. For this we use the notation $\mathcal{I}_\sigma = \{\alpha = (\alpha_1,\ldots,\alpha_m)\,|\,s(\alpha) = m-\sigma\}$, $\sigma = 0,\ldots,m$, i.e., the set of all α having σ vanishing components.

Its connection to Ω is as follows: to a grid point $(x_1^{i_1},\ldots,x_m^{i_m})$ we associate $\alpha(i_1,\ldots,i_m) = (\alpha_1,\ldots,\alpha_m)$, where $\alpha_j = -1$ for $i_j = 0$, $\alpha_j = 1$ for $i_j = N_j+1$, and $\alpha_j = 0$ for $1 \le i_j \le N_j$, and we define

$$\partial_\sigma\Omega = \{(x_1^{i_1},\ldots,x_m^{i_m})\,;\,|\alpha(i_1,\ldots,i_m) \in \mathcal{I}_\sigma\},$$

such that $\partial\Omega = \cup_{\sigma=0}^{m-1}\partial_\sigma\Omega$. Observe that $\partial_\sigma\Omega$ consists of all σ-dimensional faces in $\partial\Omega$ of the m-hypercube. In particular, $\partial_0\Omega$ corresponds to corners of Ω, $\partial_1\Omega$ corresponds to all the interior points of each edge, $\partial_2\Omega$ corresponds to all the interior points of each side of the border and so on. We continue to use the notation $(i_1,\ldots,i_m) \in \partial_\sigma\Omega$ for $(x_1^{i_1},\ldots,x_m^{i_m}) \in \partial_\sigma\Omega$. The next two lemmas give bounds for interpolated grid functions.

Lemma 4. *Let $U_{i_1,\ldots,i_m}$ be an interpolated grid function (26) in dimension m. We then have for the maximum norm*

$$\|U\|_\infty = \max_{(i_1,\ldots,i_m)\in\Omega}|U_{i_1,\ldots,i_m}| \;\le\; \sum_{\sigma=0}^{m-1}\binom{m}{\sigma}\max_{(i_1,\ldots,i_m)\in\partial_\sigma\Omega}|U_{i_1,\ldots,i_m}| \;\le\; (2^m-1)\max_{(i_1,\ldots,i_m)\in\partial\Omega}|U_{i_1,\ldots,i_m}|.$$

Proof. The second inequality is a consequence of the identity $\sum_{\sigma=0}^{m-1}\binom{m}{\sigma} = 2^m - 1$. The first inequality follows from the fact that

$$\sum_{\alpha\in\mathcal{I}_\sigma}\prod_{\substack{j=1\\ \alpha_j\neq 0}}^{m}\left(\frac{1+\alpha_j x_j}{2}\right) = \binom{m}{\sigma} \tag{36}$$

for all $x_j \in [-1,1]$. This identity can be proved by induction on the dimension m. As a consequence of linear interpolation, the statement is obvious in dimension $m = 1$, since in this case $\mathcal{I}_0 = \{-1,1\}$ and

$$\sum_{\alpha\in\mathcal{I}_0}\prod_{\substack{j=1\\ \alpha_j\neq 0}}^{1}\left(\frac{1+\alpha_j x_j}{2}\right) = \frac{1-x_j}{2} + \frac{1+x_j}{2} = 1 = \binom{1}{0}.$$

Let now $m \ge 2$. We denote the left-hand expression of (36) by C_σ^m. Since α_m can take the values -1, $+1$, and 0, we have

$$C_\sigma^m = \left(\frac{1-x_m}{2}\right)C_\sigma^{m-1} + \left(\frac{1+x_m}{2}\right)C_\sigma^{m-1} + C_{\sigma-1}^{m-1} = C_\sigma^{m-1} + C_{\sigma-1}^{m-1},$$

which is the defining recursion for the binomial coefficients. This proves (36) and the statement of the lemma. □

The estimate of the preceding lemma considers the worst case, but for the interpolated grid function corresponding to $U_{i_1,\ldots,i_m} = (-1)^\sigma M$ if $(i_1,\ldots,i_m) \in \partial_\sigma\Omega$, it is optimal. For "smooth" grid functions, much smaller constants can be observed in the estimates. Note that the bound only depends on the dimension m of the problem, and not on the number of grid points.

We intend to extend the previous lemma to the Euclidean norm. Following (35) we define the Euclidean norm over the faces of the cube Ω by

$$\|U\|^2_{2,\partial_\sigma\Omega} = \sum_{\alpha\in\mathcal{I}_\sigma} \prod_{\substack{j=1\\ \alpha_j=0}}^{m} \left(\Delta x_j \sum_{i_j=1}^{N_j}\right) \left|U_{i_1^\alpha,\ldots,i_m^\alpha}\right|^2. \tag{37}$$

In this definition the first sum is over all σ-dimensional faces of the cube Ω, and the product (recall that $\Delta x_j = 2/(N_j+1)$) is over indices j satisfying $\alpha_j = 0$. Note that for $\sigma = m$, the zero vector is the only element of $\mathcal{I}_\sigma$, so that (37) becomes (35) with the exception that the m-tuple sum is only over grid points that are in the interior of Ω. For $\sigma = 0$, the product in (37) is empty, so that the right-hand side of (37) is $\sum_{\alpha\in\mathcal{I}_0} |U_{i_1^\alpha,\ldots,i_m^\alpha}|^2$, where $i_j^\alpha = 0$ for $\alpha_j = -1$ and $i_j^\alpha = N_j+1$ for $\alpha_j = +1$. Consequently, for $\sigma = 0$, (37) becomes just the sum over the corners of Ω.

Lemma 5. *Let $U_{i_1,\ldots,i_m}$ be an interpolated grid function (26) in dimension m. We then have for the Euclidean norm*

$$\|U\|^2_{2,\partial_m\Omega} \le m \sum_{\sigma=0}^{m-1} \binom{m}{\sigma} \|U\|^2_{2,\partial_\sigma\Omega}.$$

Proof. In view of the proof of Lemma 4 we write the interpolation formula (26) as

$$U_{i_1,\ldots,i_m} = \sum_{\sigma=0}^{m-1} (-1)^{m-\sigma+1}\, V^\sigma_{i_1,\ldots,i_m}, \quad V^\sigma_{i_1,\ldots,i_m} = \sum_{\alpha\in\mathcal{I}_\sigma} c_\alpha\, U_{i_1^\alpha,\ldots,i_m^\alpha}, \quad c_\alpha = \prod_{\substack{j=1\\ \alpha_j\neq 0}}^{m} \left(\frac{1+\alpha_j x_j^{i_j}}{2}\right).$$

Using several times the estimate $2ab \le a^2 + b^2$ we obtain

$$\left|U_{i_1,\ldots,i_m}\right|^2 \le m \sum_{\sigma=0}^{m-1} \left|V^\sigma_{i_1,\ldots,i_m}\right|^2. \tag{38}$$

Similarly, using $2\left|U_{i_1^\alpha,\ldots,i_m^\alpha} U_{i_1^\kappa,\ldots,i_m^\kappa}\right| \le \left|U_{i_1^\alpha,\ldots,i_m^\alpha}\right|^2 + \left|U_{i_1^\kappa,\ldots,i_m^\kappa}\right|^2$ and the fact that $c_\alpha > 0$, we get with the help of (36)

$$\left|V^\sigma_{i_1,\ldots,i_m}\right|^2 \le \sum_{\alpha\in\mathcal{I}_\sigma} c_\alpha \left(\sum_{\beta\in\mathcal{I}_\sigma} c_\beta\right) \left|U_{i_1^\alpha,\ldots,i_m^\alpha}\right|^2 = \binom{m}{\sigma} \sum_{\alpha\in\mathcal{I}_\sigma} c_\alpha \left|U_{i_1^\alpha,\ldots,i_m^\alpha}\right|^2.$$

We note that, for a fixed index vector α, c_α only depends on i_j with $\alpha_j \neq 0$, and $U_{i_1^\alpha,\dots,i_m^\alpha}$ only depends on those i_j for which $\alpha_j = 0$. Separating the sums we thus get

$$\begin{aligned}\left\|V^\sigma\right\|_{2,\partial_m\Omega}^2 &= \Delta x_1 \cdots \Delta x_m \sum_{i_1=1}^{N_1} \cdots \sum_{i_m=1}^{N_m} \left|V^\sigma_{i_1,\dots,i_m}\right|^2 \\ &\le \binom{m}{\sigma} \sum_{\alpha\in\mathcal{I}_\sigma} \left(\prod_{\substack{j=1\\ \alpha_j\neq 0}}^{m} \Delta x_j \sum_{i_j=1}^{N_j} \left(\frac{1+\alpha_j x_j^{i_j}}{2}\right)\right)\left(\prod_{\substack{j=1\\ \alpha_j=0}}^{m}\left(\Delta x_j \sum_{i_j=1}^{N_j}\right)\left|U_{i_1^\alpha,\dots,i_m^\alpha}\right|^2\right).\end{aligned} \tag{39}$$

Since $x_j^{i_j} = -1 + i_j\Delta x_j$ with $\Delta x_j = 2/(N_j+1)$, we have

$$\Delta x_j \sum_{i_j=1}^{N_j}\left(\frac{1\pm x_j^{i_j}}{2}\right) = \frac{\Delta x_j}{2}\left(N_j \pm \left(-N_j + \Delta x_j \frac{N_j(N_j+1)}{2}\right)\right) = \frac{N_j}{N_j+1} \le 1.$$

Consequently, in (39) the first expression in big brackets is bounded by 1, and we get

$$\left\|V^\sigma\right\|_{2,\partial_m\Omega}^2 \le \binom{m}{\sigma}\left\|U\right\|_{2,\partial_\sigma\Omega}^2.$$

Combined with (38) this completes the proof of the lemma. □

6.4 PDE-convergence for general boundary conditions

In this section we show how the interpolation preservation permits us to extend convergence results for homogeneous Dirichlet boundary conditions to general time-dependent Dirichlet boundary conditions. The statement holds in any norm for which interpolated grid functions can be bounded by the corresponding norm on the faces of Ω. This is true for the maximum norm (Lemma 4) and for the ℓ_2 norm (Lemma 5).

Theorem 4. *Consider an AMF-W method, where the boundary $\partial\Omega$ is treated by the expanded correction of Section 4.1. Assume that the method is PDE-convergent of order p for homogeneous Dirichlet boundary conditions up to dimension m. Then, the method is PDE-convergent of order p for general time-dependent Dirichlet boundary conditions in dimension m.*

Proof. We proceed by induction on the dimension m of the problem. For $m = 1$ we use the splitting (see (33))

$$U_n - U(t_n) = \left(\widetilde{U}_n - \widetilde{U}(t_n)\right) + \left(\widehat{U}_n - \widehat{U}(t_n)\right), \tag{40}$$

where the error $\widetilde{U}_n - \widetilde{U}(t_n)$, corresponding to homogeneous boundary conditions, is bounded by $\mathcal{O}(\tau^p)$ as indicated in Remark 2. Moreover, $\widehat{U}_n$ and $\widehat{U}(t_n)$ are interpolated grid functions (Lemma 3) and are completely determined by their values on the boundary. Observe that the corresponding differential equation for $\widehat{U}(t)$ reduces to a quadrature, see (24), and consequently any Rosenbrock method preserves its classical order which is greater or equal to p.

To prove the induction step from dimension $m-1$ to m, we recall that the global errors of the homogeneous boundary conditions part $\big(\widetilde{U}_n - \widetilde{U}(t_n)\big)$ are of order p independently of m, as indicated in the theorems of Section 6.1. On the other hand, for the error global errors $\widehat{U}_n - \widehat{U}(t_n)$ of the interpolated grid values we make the important observation that the use of expanded correction implies that the numerical approximations of the AMF-W method on the border of the m-hypercube is the same numerical solution given by the method when it is applied to the $(m-1)$-hypercubes forming the boundary of the m-hypercube. This order is p, since the dimension is $m-1$. Then, by virtue of that $\widehat{U}_n$ and $\widehat{U}(t_n)$ are interpolated grid functions in the m-hypercube, it follows from the estimates of Section 6.3 that the order p is preserved on the whole m-hypercube. □

7 Numerical experiments

This section is devoted to numerically illustrate the observed orders of PDE-convergence provided by AMF W-methods (14)-(15) along with expanded correction (22) as indicated in the Theorem 4 on the ODE (9) stemming from the central second order discretization of the linear diffusion PDE (8), with meshwidths $\Delta x_i = N^{-1}$, for each $i = 1, \ldots, m$. For two alternative PDE solutions given in (42) and (43), such numerical results for the expanded correction are collected below in Tables 1 and 2. Considering the storage limitations in our computers, we take $N = 2^j$, with $j = 2, \ldots, 8$ for spatial dimension $m = 3$. In (8) we consider initial and Dirichlet boundary conditions corresponding to a given exact PDE solution. For the semidiscrete ODE (9) the inhomogeneity C is computed from a given PDE solution u at each grid point as

$$C(t,x_1,x_2,x_3) = u_t(t,x_1,x_2,x_3) - \sum_{j=1}^{3}\Big(u_{x_j,x_j}(t,x_1,x_2,x_3) + \frac{\Delta x_j^2}{12}\, u_{x_j,x_j,x_j,x_j}(t,x_1,x_2,x_3)\Big). \tag{41}$$

To this aim, we consider two alternative PDE solutions. Firstly, a polynomial solution of degree two for each spatial variable

$$u(t,x_1,x_2,x_3) = \mathrm{e}^t \sum_{j=1}^{3}\Big(x_j + \frac{1}{j+2}\Big)^2 \tag{42}$$

for which the second order central spatial discretization is exact, i.e., (42) also fulfils the ODE (9). Secondly, we consider a non-polynomial exact PDE solution given by

$$u(t,x_1,x_2,x_3) = (1+e^r)^{-1}, \quad r = \frac{x_1 + 2x_2 + 3x_3 - t}{2}, \tag{43}$$

which, considering the associated function C in (41), fulfils the ODE (9) with an error of size $\sum_{j=1}^{3} \mathcal{O}(\Delta x_j^4)$.

We then consider the following time integrators endowed with AMF in $m = 3$ spatial dimensions along with the expanded boundary correction of (22). In all cases below we take $\eta = 0$ in (14).

- **W1**: is the 1-stage W-method (A, L, b, θ) with coefficients $A = L = 0$, $b = 1$ and $\theta = \frac{1}{2}$. This method has non-stiff order 2 whenever $W - J = \mathcal{O}(\tau)$ (where J is the exact ODE Jacobian at the current step point), which is the case of the AMF approach in the current manuscript.
- **W2**: is the 2-stage W-method (A, L, b, θ) with coefficients taken from the book by Hundsdorfer & Verwer [20, p. 400]

$$A = \begin{pmatrix} 0 & 0 \\ 2/3 & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 \\ -4/3 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 5/4 \\ 3/4 \end{pmatrix}, \quad \theta = (3 + \sqrt{3})/6.$$

  The method has non-stiff order 3 when $W - J = \mathcal{O}(\tau)$.
- **W4**: is the 4-stage W-method based in the Kutta's 3/8-rule method with coefficients given in [18, p. 153-154, (35), (37) and (38)]:

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 4/3 & 0 & 1 & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -4/3 & 0 & 0 & 0 \\ -5/3 & -1 & 0 & 0 \\ -3 & -3 & -6 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 13/8 \\ 9/8 \\ 9/8 \\ 1/8 \end{pmatrix}, \quad \theta = \frac{1}{2}.$$

  The method has non-stiff order 4 when $W - J = \mathcal{O}(\tau)$.

For different values of $\tau = \Delta x_i$, $i = 1, \ldots, m$, Tables 1 and 2 below collect, for spatial dimension $m = 3$, the observed errors and orders (computed in the corresponding norm at all grid points, including the ones in the boundary of the domain) in the Euclidean and maximum norms for the above-mentioned AMF W-methods with the expanded boundary correction. Here we are also interested in showing the effect on the order of convergence when projecting to the boundary the advancing solution using the corresponding Dirichlet boundary condition at each time integration step (in this case we compute the corresponding error norms at grid points in the interior of the domain).

For each case (42) and (43), it is observed that the expanded correction (without projection) recovers the order of convergence, in both norms, of the underlying AMF-W method as if homogeneous boundary conditions would have been imposed. This is in agreement with the statement of Theorem 4.

It is also observed that incorporating projection to the boundary at each integration step does not provide a full recovery, at least in the maximum norm, of the convergence order as in the homogeneous case.

Similar numerical experiments as above for the case of spatial dimension $m = 2$ and expanded boundary correction reveal that the use of projection to the boundary does not deteriorate the orders of convergence. In such dimension $m = 2$, using or not projection to the boundary produces very similar errors and orders of convergence.

W1	without projection				with projection			
$\tau = \Delta x_i$	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order
1/4	0.3223e-01	—	0.8026e-01	—	0.1606e-01	—	0.2366e-01	—
1/8	0.7583e-02	2.088	0.2072e-01	1.953	0.3004e-02	2.419	0.4323e-02	2.452
1/16	0.1831e-02	2.050	0.5264e-02	1.977	0.5322e-03	2.497	0.1209e-02	1.839
1/32	0.4493e-03	2.027	0.1326e-02	1.989	0.1035e-03	2.363	0.4263e-03	1.503
1/64	0.1113e-03	2.014	0.3329e-03	1.994	0.2231e-04	2.214	0.1370e-03	1.638
1/128	0.2768e-04	2.007	0.8339e-04	1.997	0.5155e-05	2.113	0.4166e-04	1.717
1/256	0.6903e-05	2.004	0.2087e-04	1.999	0.1238e-05	2.058	0.1216e-04	1.777
W2	without projection				with projection			
$\tau = \Delta x_i$	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order
1/4	0.7477e-02	—	0.1351e-01	—	0.1808e-01	—	0.1868e-01	—
1/8	0.1729e-02	2.113	0.2733e-02	2.306	0.2160e-02	3.066	0.2464e-02	2.923
1/16	0.3275e-03	2.400	0.4781e-03	2.515	0.2361e-03	3.194	0.3979e-03	2.630
1/32	0.5350e-04	2.614	0.7315e-04	2.708	0.2681e-04	3.138	0.7256e-04	2.455
1/64	0.7890e-05	2.762	0.1009e-04	2.859	0.3212e-05	3.061	0.1370e-04	2.405
1/128	0.1092e-05	2.853	0.1305e-05	2.951	0.3996e-06	3.007	0.2705e-05	2.341
1/256	0.1457e-06	2.906	0.1647e-06	2.986	0.5076e-07	2.977	0.6044e-06	2.162
W4	without projection				with projection			
$\tau = \Delta x_i$	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order
1/4	0.1498e-02	—	0.2567e-02	—	0.1661e-02	—	0.1922e-02	—
1/8	0.2358e-03	2.667	0.3348e-03	2.939	0.1840e-03	3.174	0.2467e-03	2.962
1/16	0.2789e-04	3.080	0.3405e-04	3.298	0.1668e-04	3.464	0.2569e-04	3.263
1/32	0.2775e-05	3.329	0.3771e-05	3.175	0.1452e-05	3.522	0.4844e-05	2.407
1/64	0.2628e-06	3.400	0.4622e-06	3.028	0.1449e-06	3.325	0.9630e-06	2.330
1/128	0.2522e-07	3.381	0.5799e-07	2.994	0.1547e-07	3.227	0.1918e-06	2.328
1/256	0.2455e-08	3.361	0.7268e-08	2.996	0.1664e-08	3.217	0.3765e-07	2.349

Table 1 Errors and orders of PDE-convergence for the AMF-W-methods with expanded correction on the semidiscrete linear diffusion PDE (8)-(9)-(41)-(42) in spatial dimension $m = 3$. A projection procedure of the advancing solution to the boundary at each integration step is considered on the right part of the table.

8 Conclusions

The interpolation property introduced in Section 5 establishes a sufficient condition to prove that the expanded correction of Section 4 preserves the order of PDE-convergence of AMF-W methods as for the situation of homogeneous Dirichlet boundary conditions. This is confirmed through numerical experiments in Section 7. For this boundary correction, the interpolation property is lost when adding to the advancing numerical solution a projection procedure to the Dirichlet boundary conditions. It is also observed in Section 7 that adding projection to the boundary does not necessarily improve the error behaviour.

The explicit correction of Remark 1 does not fulfil the property of interpolation preservation. Numerical experiments in two and three space dimensions show that it nevertheless avoids an order reduction for time-dependent boundary conditions.

Although the theoretical analysis in the paper for the interpolation preservation focuses on the standard second order central discretization, this approach is also applicable to other spatial discretization as long as they treat the boundary points similarly as to the interior points of the spatial domain. This is, e.g., the case of the mixed fourth/second order discretization recently proposed in [15, Section 2.1] for which the

W1	without projection				with projection			
$\tau = \Delta x_i$	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order
1/4	0.6579e-04	—	0.1564e-03	—	0.1404e-03	—	0.2604e-03	—
1/8	0.1602e-04	2.038	0.3917e-04	1.997	0.2547e-04	2.463	0.5921e-04	2.137
1/16	0.3985e-05	2.007	0.9792e-05	2.000	0.4474e-05	2.509	0.1080e-04	2.455
1/32	0.9958e-06	2.001	0.2449e-05	2.000	0.8666e-06	2.368	0.2354e-05	2.198
1/64	0.2490e-06	2.000	0.6122e-06	2.000	0.1866e-06	2.216	0.5496e-06	2.099
1/128	0.6226e-07	2.000	0.1531e-06	2.000	0.4313e-07	2.113	0.1329e-06	2.048
1/256	0.1557e-07	2.000	0.3826e-07	2.000	0.1037e-07	2.057	0.3265e-07	2.025
W2	without projection				with projection			
$\tau = \Delta x_i$	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order
1/4	0.4422e-04	—	0.1408e-03	—	0.1060e-03	—	0.2513e-03	—
1/8	0.1187e-04	1.897	0.3594e-04	1.969	0.2006e-04	2.402	0.5794e-04	2.117
1/16	0.2493e-05	2.251	0.7165e-05	2.327	0.2849e-05	2.816	0.7653e-05	2.920
1/32	0.4511e-06	2.467	0.1264e-05	2.503	0.4033e-06	2.820	0.1064e-05	2.847
1/64	0.7355e-07	2.617	0.2011e-06	2.652	0.5836e-07	2.789	0.2021e-06	2.395
1/128	0.1107e-07	2.733	0.2934e-07	2.777	0.8346e-08	2.806	0.4365e-07	2.211
1/256	0.1568e-08	2.819	0.3995e-08	2.877	0.1160e-08	2.847	0.9974e-08	2.130
W4	without projection				with projection			
$\tau = \Delta x_i$	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order	ℓ_2−error	ℓ_2−order	ℓ_∞−error	ℓ_∞−order
1/4	0.9338e-05	—	0.2190e-04	—	0.1127e-04	—	0.2090e-04	—
1/8	0.1604e-05	2.542	0.3681e-05	2.573	0.1469e-05	2.940	0.2886e-05	2.856
1/16	0.2215e-06	2.856	0.5386e-06	2.773	0.1795e-06	3.032	0.4327e-06	2.737
1/32	0.3039e-07	2.865	0.7752e-07	2.797	0.2528e-07	2.828	0.6580e-07	2.717
1/64	0.3865e-08	2.975	0.9787e-08	2.986	0.3251e-08	2.959	0.1036e-07	2.667
1/128	0.4266e-09	3.180	0.1158e-08	3.080	0.3604e-09	3.173	0.2123e-08	2.287
1/256	0.4353e-10	3.293	0.1420e-09	3.027	0.3750e-10	3.264	0.4669e-09	2.185

Table 2 Errors and orders of PDE-convergence for the AMF-W-methods with expanded correction on the semidiscrete linear diffusion PDE (8)-(9)-(41)-(43) in spatial dimension $m = 3$. A projection procedure of the advancing solution to the boundary at each integration step is considered on the right part of the table.

expanded correction also avoids the order reduction due to time-dependent Dirichlet boundary conditions.

Declarations

- **Data availability statement:** The data that supports the findings of this study are available within the article. A Fortran code for the numerical tests in Section 7 can be found at http://www.unige.ch/~hairer/preprints.html.
- **Ethical approval:** Not applicable.
- **Competing interests:** The author declares no competing interests.
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