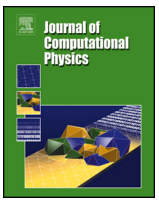
Journal of Computational Physics 524 (2025) 113689

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp



Projection based summation-by-parts methods, embeddings and the pseudoinverse

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ARTICLE INFO

Keywords:
Finite difference methods
High-order accuracy
Stability
Boundary treatment
Projection method

ABSTRACT

In the present work, we demonstrate how the pseudoinverse concept from linear algebra can be used to represent and analyze the boundary conditions of linear systems of partial differential equations. This approach has theoretical and practical implications; the theory applies even if the boundary operator is rank deficient, or near rank deficient. If desired, the pseudoinverse can be implemented directly using standard tools like Matlab. We also introduce a new and simplified version of the semidiscrete approximation of the linear PDE system, which completely avoids taking the time derivative of the boundary data, cf. [1]. The 2D stability results of the projection method in [2] are extended to nondiagonal summation-by-parts norms, which introduce boundary terms that require special attention in case of the projection method (equivalence of diagonal and nondiagonal boundary norms), see [3] for details. Another key result is the extension of summation-by-parts operators to multidomains by means of carefully crafted embedding operators. No extra numerical boundary conditions are required at the grid interfaces. The pseudoinverse allows for a compact representation of these multiblock operators, which preserves all relevant properties of the single-block operators. The embedding operators can be constructed for multiple space dimensions. Numerical results for the two-dimensional Maxwell's equations are presented, and they show very good agreement with theory.

1. Overview and introductory example

In the present study we will be concerned with finite difference methods for the model problem

$$\begin{aligned} u_t(x,t) + Qu(x,t) &= 0, \quad t > 0,\ x \in \Omega \\ Lu(x,t) &= g(t), \quad t \geq 0,\ x \in \Gamma \\ u(x,0) &= f(x). \end{aligned} \tag{1}$$

We will restrict ourselves to the case where Ω is a subset in $\mathbb{R}$ or $\mathbb{R}^2$; Γ refers to the boundary of Ω. The differential operator $Q = Q(\partial)$ is assumed to be semibounded, cf. [4], leading to a well-posed problem in the sense that any solution of (1) must satisfy an energy estimate

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https://doi.org/10.1016/j.jcp.2024.113689
Received 23 January 2024; Received in revised form 14 November 2024; Accepted 16 December 2024

Available online 20 December 2024

$$\|u(\cdot,t)\|^2 \le K e^{ct}\left(\|f\|^2 + \int_0^t \|g(\cdot,\tau)\|_\Gamma^2 d\tau\right),$$

where $\|\cdot\|$ and $\|\cdot\|_\Gamma$ are the L^2-norms on Ω and Γ. This kind of estimate typically follows from an integration-by-parts procedure (divergence theorem in multiple space dimensions) and a properly designed boundary condition operator L.

In this study we have adopted an operator centric approach for analyzing summation-by-parts difference methods and the implementation of boundary conditions, which are implemented by means of projections. This technique is also used to define multiblock difference operators. The analysis is based on two key concepts: *pseudoinverses* and *embedding* operators. The latter is used to define multiblock difference operators that satisfy summation by parts (SBP) given the existence of SBP operators for the individual blocks. There is no need to construct "extra" boundary conditions at the grid interfaces; the embedding operators will handle this automatically.

Rather than considering the state spaces as some space $\mathbb{R}^N$ equipped with a special scalar product $(\cdot,\cdot)_H$, we will regard the pair $[\mathbb{R}^N,(\cdot,\cdot)_H]$ as an inner product space V in its own right; the scalar product $(\cdot,\cdot)\equiv(\cdot,\cdot)_H$ will *define* V. In this context, difference operators, boundary operators, projections and embeddings will be regarded as mappings between inner products spaces with well-defined adjoints and pseudoinverses. This will lead to a systematic and concise notation for multiblock operators. Since the theory relies on well-defined concepts like adjoints and pseudoinversers, the resulting discretizations can be implemented directly using matrix algebra, e.g. MATLAB or similar packages.

In Section 2 we set the scene by defining the inner product spaces that will be used throughout the presentation. We also provide some basic background on summation-by-parts operators and how they relate to the inner product spaces. To prepare for multiblock theory, we introduce the concept of *augmented* state spaces and embedding operators. The concept of a *multiset* turns out to be very helpful in this context. After a brief overview of adjoint operators, we turn our interest to the derivation of multiblock operators and their corresponding inner product spaces.

Section 3 presents the Moore-Penrose conditions [5] for characterizing the pseudoinverse. We will use them in a shape that is particularly useful in an operator context [6]. They will play a fundamental role in the subsequent stability theory.

Eriksson and Wang [7] have used the pseudoinverse to solve the resulting SBP-SAT approximation for the one-dimensional Poisson equation. In Section 4 we present a framework how to construct the pseudoinverse of general linear boundary operators - not the total difference operator - for the semidiscrete version of the model problem (1). Once the pseudoinverse of the boundary operator L has been established, it is a simple task to compute the boundary projection following the approach in [2,1]. We also establish a simplified form of the semidiscrete model problem (29), which significantly reduces the implementation complexity of the corresponding method found in [2].

Sections 5 and 6 are devoted to the extension of the previous results to two space dimensions. The results presented in the one-dimensional case carry over to the two-dimensional case more or less verbatim. The technique used in two space dimensions can be generalized to higher-dimensional spaces. We also obtain a generalization of the main stability result in [2].

Finally, in Section 7 we tie all loose ends together by applying the theory to the two-dimensional Maxwell's equations on a curvilinear four-block domain. Numerical results confirming the expected convergence rate are presented.

The presentation that follows is a condensed version of an unpublished report [3], which provides the details that are omitted in the subsequent sections. Readers who want the full background are encouraged to read this report.

1.1. Introductory example

To illustrate the methodology, we consider the simplest possible model problem (1) with $Qu(x,t)\equiv u_x(x,t)$, $0<x<1, t>0$. The boundary operator is defined as $Lu(0,t)\equiv u(0,t)=0, t\ge 0$, and the initial condition is $u(x,0)=f(x), 0\le x\le 1$. By necessity, $f(0)=0$. Next, we divide the unit interval $\Omega=[0,1]$ into $\Omega=\Omega_1\cup\Omega_2$, where $\Omega_1=[0,0.5]$ and $\Omega_2=[0.5,1]$. The model problem is discretized using the standard second-order accurate difference stencil in the interior of the subintervals Ω_i with mesh sizes $h^{(i)}=1/(2N^{(i)})$; at the boundaries we use one-sided first-order accurate stencils. Two questions arise naturally: How does one ensure that the solution is single-valued at $x=0.5$, and how does one enforce the internal boundary condition at $x=0.5$? The necessity of a boundary at $x=0.5$ is an artefact of our decision to split the original domain Ω into two halves; it is not present in the original formulation. The embedding operator E defined in Section 2.5 will address both questions.

Step 1: Given the state vectors $v^{(i)}\in V_i$ on the subintervals Ω_i, define difference operators $D^{(i)}$ and norms $H^{(i)}$:

$$D^{(i)}\equiv\frac{1}{h^{(i)}}\begin{pmatrix} -1 & 1 & & & & \\ -0.5 & 0 & 0.5 & & & \\ & \ddots & \ddots & \ddots & & \\ & & & -0.5 & 0 & 0.5 \\ & & & & -1 & 1 \end{pmatrix}\quad H^{(i)}\equiv h^{(i)}\begin{pmatrix} 0.5 & & & & & \\ & 1 & & & & \\ & & \ddots & & & \\ & & & & 1 & \\ & & & & & 0.5 \end{pmatrix},$$

where V_i denotes the inner product space consisting of the state vectors $v^{(i)}\in\mathbb{R}^{N^{(i)}+1}$ subject to the scalar products $(u,v)_i\equiv u^T H^{(i)} v$. Obviously, $D^{(i)}$ satisfies summation by parts with respect to $H^{(i)}$.

Step 2: Construct a norm $H^{(+)}$ of the auxiliary state space V_+ using the norms $H^{(i)}$ of the existing state spaces V_+:

$$H^{(+)} \equiv \begin{pmatrix} H^{(1)} & \\ & H^{(2)} \end{pmatrix}.$$

State vectors in V_+ are defined as

$$u^{(+)} \equiv \begin{pmatrix} u^{(1)} \\ u^{(2)} \end{pmatrix} \in \mathbb{R}^{N+2}, \quad N = N^{(1)} + N^{(2)}.$$

It should be noted that $u^{(+)}$ is multiple-valued at $x = 0.5$ since $u^{(1)}_{N^{(1)}}$ and $u^{(2)}_0$ both correspond $x = 0.5$ (indexing starts at 0 for all state vectors), see Fig. 1.

Step 3: Let $u \in \mathbb{R}^{N+1}$ be a single-valued grid vector on all of $\Omega = \Omega_1 \cup \Omega_2$. Thus, $u_{N^{(1)}}$ represents the unique value at $x = 0.5$, $u_{N^{(1)}+1}$ represents $x = 0.5 + h^{(2)}$, etc. We will regard u as a member of an inner product space V whose scalar product H is yet to be defined. Begin by defining the embedding operator $E : V \to V_+$:

$$E \equiv \begin{pmatrix} I^{(1)} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & I^{(2)} \end{pmatrix}, \quad I^{(i)} \in \mathbb{R}^{N^{(i)} \times N^{(i)}}, \quad i = 1, 2,$$

see also (18). By construction, any vector of the form $u^{(e)} = Eu \in V_+$ satisfies $u^{(e)}_{N^{(1)}+1} = u^{(e)}_{N^{(1)}} = u_{N^{(1)}}$.

Next, define a norm H on V by

$$H \equiv E^T H^{(+)} E = \begin{pmatrix} \frac{h^{(1)}}{2} & & & & & & \\ & h^{(1)} & & & & & \\ & & \ddots & & & & \\ & & & \frac{h^{(1)}+h^{(2)}}{2} & & & \\ & & & & \ddots & & \\ & & & & & h^{(2)} & \\ & & & & & & \frac{h^{(2)}}{2} \end{pmatrix}.$$

Step 4: Define the extended difference operator $D^{(+)} : V_+ \to V_+$:

$$D^{(+)} \equiv \begin{pmatrix} D^{(1)} & \\ & D^{(2)} \end{pmatrix}.$$

Step 5: We are now ready to construct the aggregate difference operator $D : V \to V$ as

$$D \equiv E^+ D^{(+)} E = E^* H^{(+)} E = \left[H^{-1} E^T H^{(+)} \right] D^{(+)} E.$$

The first equality follows from the Moore-Penrose conditions (Theorem 25) and the second equality is the direct consequence of the definition of an adjoint operator (Definition 15). Hence, cf. (27),

$$E^+ = E^* = \begin{pmatrix} I^{(1)} & 0 & 0 & 0 \\ 0 & \chi & 1-\chi & 0 \\ 0 & 0 & 0 & I^{(2)} \end{pmatrix}, \quad \chi \equiv \frac{h^{(1)}}{h^{(1)} + h^{(2)}},$$

and thus

$$D = \begin{pmatrix} \frac{-1}{h^{(1)}} & \frac{1}{h^{(1)}} & & & & & & \\ \frac{-1}{2h^{(1)}} & 0 & \frac{1}{2h^{(1)}} & & & & & \\ & \ddots & \ddots & \ddots & & & & \\ & & \frac{-1}{h^{(1)}+h^{(2)}} & 0 & \frac{1}{h^{(1)}+h^{(2)}} & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & & \frac{-1}{2h^{(2)}} & 0 & \frac{1}{2h^{(2)}} & \\ & & & & & \frac{-1}{h^{(2)}} & \frac{1}{h^{(2)}} \end{pmatrix}.$$

As seen from the above expression, D can be constructed without matrix operations: Simply take the weighted average of the two first-order accurate difference stencils at the interface point $x = 0.5$:

$$\chi \frac{u_{N^{(1)}} - u_{N^{(1)}-1}}{h^{(1)}} + (1-\chi) \frac{u_{N^{(1)}+1} - u_{N^{(1)}}}{h^{(2)}} = \frac{u_{N^{(1)}+1} - u_{N^{(1)}-1}}{h^{(1)} + h^{(2)}}.$$

All other stencils of D are identical to those of $D^{(1)}$ and $D^{(2)}$. Summation by parts (7) follows immediately from the above definition of D.

Step 6: In the final step, we construct the projection operator P representing the analytical boundary condition $u(0,t)=0$:

$$P = I - L^+ L$$

where L^+ is the pseudoinverse of the boundary operator $L : V \to V_\Gamma$:

$$L = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \end{pmatrix} \in \mathbb{R}^{2\times(N+1)}.$$

The boundary state space V_Γ consists of vectors $u = \begin{pmatrix} u_0 & u_N \end{pmatrix}^T$ subject to the scalar product $\langle u, v\rangle \equiv u_0 v_0 + u_N v_N$. This is a natural choice for V_Γ given that D satisfies summation by parts with respect to H:

$$(u, Dv) = u_N v_N - u_0 v_0 - (Du, v).$$

Thus,

$$H_\Gamma = \begin{pmatrix} 1 & \\ & 1 \end{pmatrix}.$$

By the definition of the adjoint L^*:

$$L^* = H^{-1} L^T H_\Gamma = \frac{2}{h^{(1)}} L^T,$$

whence,

$$L^+ = L^* \left(LL^*\right)^+ = L^T \left(LL^T\right)^+ = L^T \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}^+ = L^T \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = L^T.$$

The first equality is true for any pseudoinverse [8,3]. In other words,

$$P = I - L^T L = \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix}.$$

We have thus arrived at the following semidiscrete formulation of (1):

$$v_t + PDPv = 0, t > 0$$
$$v(0) = f, f_0 = 0.$$

But D satisfies summation by parts, and so

$$\frac{d}{dt}\|v\|^2 = w_0^2 - w_N^2, \quad w \equiv Pv,$$

where we also used the fact that P is self-adjoint with respect to $(\cdot,\cdot)$, that is, $P^* = P \iff HP = P^T H \iff HL^+L = \left[L^+L\right]^T H$. But

$$Lw = LPv = Lv - LL^+Lv = 0$$

The last equality is a consequence of $LL^+L = L$, which is the first Moore-Penrose condition (Theorem 27), i.e., w satisfies the boundary condition $w_0 = 0$. This implies an energy estimate for $t > 0$ regardless of whether initial data f fulfills the boundary condition $Lf = 0$.

Premultiplying the semidiscrete system with L results in

$$[Lv]_t = 0, \quad t > 0,$$

and since $Lf = 0$ it follows immediately that $Lv = 0, v \geq 0$. Hence, $Lf = 0$ is a consistency requirement, not a stability requirement.

The subsequent sections will provide the general theory for the previous six steps. The example presented in this section is the simplest possible, but all results carry over to general to first-order systems of PDEs in multiblock domains in several space dimensions. The scalar product and the difference operator can always be expressed as

$$H = E^T H^{(+)} E, \quad D = E^+ D^{(+)} E$$

regardless of the number of blocks Ω_i. These expressions are valid for full and implicit norms as long as the embedding $E : V \to V_+$ is properly constructed.

From the example it is clear that the inner products H and the difference operators D of the compound domain $\Omega = \cup\Omega_i$ can be computed simply by "snapping" together the elements/stencils of the operators that share a common interface; for inner products one computes the sum of the diagonal elements, and in case of difference operators one calculates a *weighted* sum of the two one-sided stencils that share a common domain interface. This applies not only to diagonal norms, but also to restricted full norms. Two-dimensional examples will be presented in Section 6. How these operators are actually implemented in code (series of matrix multiplications or directly as in this example) is purely an implementation detail.

We conclude this introductory example by observing that stability and consistency follow from two of the four Moore-Penrose conditions: $LL^+L = L$ ("consistency") and $HL^+L = \left[L^+L\right]^T H$ ("stability"). The remaining ones ($L^+LL^+ = L^+$ and $H_\Gamma LL^+ = \left[LL^+\right]^T H_\Gamma$) are not used. This gives us some leeway when we want to simplify the construction of the boundary projection P in two space dimensions, where the inner products at the boundaries are non-trivial.

Table A.2 of the appendix summarizes the notation used most frequently in the subsequent presentation.

2. Inner product spaces and operators

Let $\Omega = [0, 1]$ be the computational domain in one space dimension. Define grid functions (grid vectors) u, v

$$u \equiv \begin{pmatrix} u_0 \\ \vdots \\ u_N \end{pmatrix}, \quad v \equiv \begin{pmatrix} v_0 \\ \vdots \\ v_N \end{pmatrix} \in \mathbb{R}^{N+1}, \tag{2}$$

corresponding to the grid $\{x_j\}$:

$$x_j \equiv jh, \quad j = 0, \dots, N, \quad h \equiv \frac{1}{N}.$$

2.1. Summation-by-parts operators D

It is well understood how to construct finite difference operators D that satisfy a summation-by-parts rule

$$(u, Dv)_H \equiv u_N v_N - u_0 v_0 - (Du, v)_H \tag{3}$$

for some inner product

$$(u, v)_H \equiv u^T H v, \quad H = H^T > 0. \tag{4}$$

Existence of such operators D and scalar products $(\cdot, \cdot)_H$ was first established in [9,10], where it is also shown that one cannot choose $H = I$.

We begin by recalling some terminology [11] regarding the matrix structure of the norm $H \in \mathbb{R}^{(N+1)\times(N+1)}$ (limiting ourselves to the upper left corner of H for brevity; the lower right is completely analogous):

$$H = h \overset{\texttt{full norm}}{\begin{pmatrix} \tilde{H} & \\ & I \end{pmatrix}}, \qquad H = h \overset{\texttt{restricted full norm}}{\begin{pmatrix} \mu & & \\ & \tilde{H} & \\ & & I \end{pmatrix}},$$

where $\tilde{H} \in \mathbb{R}^{r\times r}$ for some *fixed* number r independent of N. Implicit norms correspond to $\tilde{H} \in \mathbb{R}^{(N+1)\times(N+1)}$; restricted implicit norms are given by

$$H = h \begin{pmatrix} \mu & & \\ & \tilde{H} & \\ & & \mu \end{pmatrix}, \quad \tilde{H} \in \mathbb{R}^{(N-1)\times(N-1)}.$$

A common structure for explicit norms H is

$$H = h \begin{pmatrix} H_L & & \\ & I & \\ & & H_R \end{pmatrix}, \quad H_L, H_R \in \mathbb{R}^{r\times r}, \tag{5}$$

where

$$H_R = H_L^\tau \equiv J_r H_L J_r, \quad J_r \equiv \begin{pmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{pmatrix} \in \mathbb{R}^{r\times r}.$$

Thus, H_L^τ is obtained by reversing the rows and columns of H_L.

Remark 1. Only uniform grids will be considered in this presentation, which means that $H = h\tilde{H}$ where $\tilde{H}$ has exactly the same structure as H. The factor h will often be omitted when discussing the internal structure of H. Hence, we will use the same symbol (H) to denote H as well as $\tilde{H}$, unless circumstances explicitly require different symbols. □

Remark 2. The idea of swapping rows and columns can be extended to rectangular matrices $A \in \mathbb{R}^{n\times m}$ as well, where the elements of $A^\tau = J_n A J_m$ are obtained as

$$A^\tau_{ij} = A_{n-i+1,m-j+1}, \quad 1 \le i \le n, \quad 1 \le j \le m.$$

Note that the transformation $A^\tau = J_n A J_m$ preserves the shape of A as opposed to the usual matrix transposition. An example of this is provided by the difference operator D that corresponds to (5):

$$D = \begin{pmatrix} D_L \\ D_I \\ D_R \end{pmatrix} \begin{matrix} r \\ N+1-2r \\ r \end{matrix} \quad \begin{matrix} \\ \\ \\ \end{matrix} \quad \begin{matrix} N+1 \\ \\ \\ \end{matrix},$$

where $D_R \equiv -J_r D_L J_{N+1} = -D_L^\tau$, that is, D_R is the "anti-reflected" version of D_L. This is a very common situation in practical computations. The permutation matrices J will be encountered in Section 5 when analyzing summation-by-parts operators in two dimensions. □

2.2. The solution state space V

In the beginning of this section we defined grid functions u, v as members of $\mathbb{R}^{N+1}$ where

$$(u, v) = \sum_j u_j v_j \tag{6}$$

is the usual Euclidean scalar product in $\mathbb{R}^{N+1}$. From this scalar product, a second scalar product $(\cdot,\cdot)_H$ was established in $\mathbb{R}^{N+1}$. We will now change perspective and regard the pair $[\mathbb{R}^{N+1}, (\cdot,\cdot)_H]$ as an inner product space in its own right:

Definition 3. Let the inner product space V be a real vector space with the inner product

$$(\cdot,\cdot) : V \times V \to \mathbb{R}$$

for all vectors $u, v \in V$ given by (2) and where

$$(u, v) \equiv (u, v)_H.$$

The inner product $(\cdot,\cdot)_H$ is defined in (4). □

Remark 4. The notation $(\cdot,\cdot)$ is context dependent. If u, v are state vectors in V, then $(u, v) = (u, v)_H$ where u and v are interpreted as grid vectors in $\mathbb{R}^{N+1}$ in the scalar product of the right member; (u, v) refers to the Euclidean scalar product (6) for $u, v \in \mathbb{R}^{N+1}$. The vector space V will be known as the *solution state* space, or *state* space for short. In the subsequent presentation, all inner products will be regarded as bilinear forms over the field of real numbers. It is possible, however, to consider complex scalar products as well. □

Interpreting u, v as state vectors in V, we conclude from (3) and Definition 3 that

$$(u, Dv) \equiv u_N v_N - u_0 v_0 - (Du, v). \tag{7}$$

Hence, we regard D as a linear mapping $D : V \to V$ of the inner product space V into itself.

2.3. The boundary state space V_Γ

To facilitate the analysis of the numerical implementation of the boundary conditions of (1), it is convenient to introduce the concept of a *boundary state*. To this end, define the grid vectors

$$u_\Gamma \equiv \begin{pmatrix} u_0 \\ u_N \end{pmatrix}, \quad v_\Gamma \equiv \begin{pmatrix} v_0 \\ v_N \end{pmatrix} \in \mathbb{R}^2, \tag{8}$$

corresponding to the boundary points $x_0 = 0$ and $x_N = 1$. This concept will be extended to two space dimensions in Section 5.

Similar to Definition 3, we introduce

Definition 5. Let the inner product space V_Γ be a real vector space where the inner product is given by

$$\langle\cdot,\cdot\rangle : V_\Gamma \times V_\Gamma \to \mathbb{R}$$

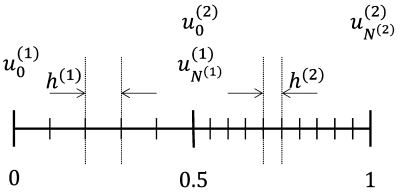

Fig. 1. Two uniform grids with states $u^{(1)}$ and $u^{(2)}$.

for all vectors $u_\Gamma, v_\Gamma \in V_\Gamma$ given by (8) and where

$$\langle u_\Gamma, v_\Gamma \rangle \equiv u_\Gamma^T v_\Gamma = u_0 v_0 + u_N v_N.$$

The space V_Γ equipped with the above inner product will be referred to as the boundary state space. □

Remark 6. When defining an abstract inner product space, the choice of inner product is arbitrary as long as the definition fulfills all the requirements of a scalar product. In our case, the choice is dictated by the summation-by-parts rule (7).

The notation $\langle \cdot, \cdot \rangle$ will be used exclusively for boundary state spaces. Thus, we will frequently drop the subscripts on u_Γ and v_Γ and simply write

$$\langle u, v \rangle = u_0 v_0 + u_N v_N.$$

Note that $\langle 1, 1 \rangle = 2$ is the "length" (number of boundary points) of Γ in one space dimension. Finally, it should be observed that $\langle \cdot, \cdot \rangle$ is identical with the Euclidean scalar product in $\mathbb{R}^2$, i.e., $V_\Gamma = \mathbb{R}^2$. This result is a special case in one space dimension and does not apply to higher dimensions, cf. Section 5. □

Next, we look at the discretization of the boundary operator L in (1). From an operator perspective, L maps the solution state $u(x,t)$ onto the boundary state $g(t)$, where $g(t)$ is a member of a suitable Hilbert space. This leads to the following

Definition 7. Let $u \in V$ and $g \in V_\Gamma$. The boundary operator $L : V \to V_\Gamma$ is defined as

$$Lu = g,$$

where L represents a consistent approximation of the analytic boundary conditions of (1). □

The reader is referred to [2] for more details on the structure of L, including examples of discrete boundary conditions for hyperbolic and parabolic systems in one and two dimensions.

2.4. The augmented state space V_+

Augmented state spaces will play an important role when developing multiblock stability theory for projection methods. It also comes in handy when analyzing boundary state spaces in higher dimensions.

Consider the 2-grid problem in one space dimension, cf. Fig. 1. The mesh sizes are defined as

$$h^{(1)} = \frac{1}{2N^{(1)}}, \qquad h^{(2)} = \frac{1}{2N^{(2)}}, \tag{9}$$

where we have adopted the convention that quantities related to Ω_i will be referred to via superscripts $^{(i)}$. Exceptions include the state spaces, which will be referenced by subscripts. Let

$$\begin{aligned} \Omega &\equiv \Omega_1 \cup \Omega_2 \\ \Omega_1 &\equiv [0, 1/2] \\ \Omega_2 &\equiv [1/2, 1] \end{aligned} \tag{10}$$

with the grid points x_j:

$$\begin{aligned} \Omega_1 &: \{x_j = j h^{(1)}\}, \quad j = 0, \dots, N^{(1)} \\ \Omega_2 &: \{x_j = 1/2 + j h^{(2)}\}, \quad j = 0, \dots, N^{(2)}. \end{aligned}$$

To set the stage for the discussion in subsequent sections, some additional terminology will be required. The notion of a *multiset* [12] is a useful concept in many situations. The canonical example is the representation of an integer in terms of its prime factors. Contrary to a regular set, in a multiset an element can occur more than once. Each element x in a multiset A is associated with a multiplicity $m(x)$. Set inclusion, union, intersection and sum are extended to multisets through the multiplicity function $m(x)$:

(i) Inclusion: $A \subset B$ if $m_A(x) \leq m_B(x)$
(ii) Union: $C = A \cup B$ where $m_C(x) = \max(m_A(x), m_B(x))$
(iii) Intersection: $C = A \cap B$ where $m_C(x) = \min(m_A(x), m_B(x))$
(iv) Sum: $C = A + B \equiv A \cup B$ where $m_C(x) = m_A(x) + m_B(x)$

Define the multiset

$$\Omega_+ \equiv \Omega_1 + \Omega_2.$$

This implies that the multiplicity of $x = 1/2$ is 2; all other grid points have multiplicity one. For future reference we also define

$$N \equiv N^{(1)} + N^{(2)}. \tag{11}$$

For each of the subintervals $\Omega_i, i = 1, 2$, there is an associated state space V_i in the sense of Definition 3 with the corresponding state vectors $u^{(i)}, v^{(i)}$ and inner products $(\cdot,\cdot)_i$.

Definition 8. Let the inner product space V_+ be a real vector space with the inner product

$$(\cdot,\cdot)_+ : V_+ \times V_+ \to \mathbb{R}$$

for all vectors $u^{(+)}, v^{(+)} \in V_+$ and where

$$(u^{(+)}, v^{(+)})_+ \equiv (u^{(1)}, v^{(1)})_1 + (u^{(2)}, v^{(2)})_2. \tag{12}$$

The space V_+ will be referred to as the augmented state space. □

Remark 9. From the definition of $(u^{(+)}, v^{(+)})_+$ it follows immediately that

$$(u^{(+)}, v^{(+)})_+ = \left[u^{(+)}\right]^T H^{(+)} v^{(+)},$$

where

$$H^{(+)} = \begin{pmatrix} H^{(1)} & \\ & H^{(2)} \end{pmatrix} \begin{matrix} N^{(1)}+1 \\ N^{(2)}+1 \end{matrix} \qquad \begin{matrix} N^{(1)}+1 & N^{(2)}+1 \end{matrix} \tag{13}$$

and where

$$u^{(+)} \equiv \begin{pmatrix} u^{(1)} \\ u^{(2)} \end{pmatrix}, \quad v^{(+)} \equiv \begin{pmatrix} v^{(1)} \\ v^{(2)} \end{pmatrix} \in \mathbb{R}^{N+2}.$$

It is clear that $u^{(+)}$ and $v^{(+)}$ are well-defined grid vectors on the multiset Ω_+, since $x = 1/2$ has multiplicity two corresponding to $u^{(1)}_{N^{(1)}}$ and $u^{(2)}_0$. Hence, the augmented state space V_+ is well defined. Augmented state spaces will be defined for higher dimensions in Section 5. □

2.5. The embedding operator E

Let $u, v \in \mathbb{R}^{N+1}$ be grid vectors on $\Omega = \Omega_1 \cup \Omega_2$ (10):

$$u \equiv \begin{pmatrix} u_0 \\ \vdots \\ u_N \end{pmatrix}, \quad v \equiv \begin{pmatrix} v_0 \\ \vdots \\ v_N \end{pmatrix} \in \mathbb{R}^{N+1}, \tag{14}$$

where $N = N^{(1)} + N^{(2)}$ (11). Note the formal similarity of this definition with (2). It should be pointed out that every point in Ω has multiplicity one.

Next, define a mapping $E : \mathbb{R}^{N+1} \to \mathbb{R}^{N+2}$:

$$E = \begin{pmatrix} E^{(1)} \\ E^{(2)} \end{pmatrix}, \tag{15}$$

where

$$E^{(1)} \equiv \left(\begin{array}{ccc|ccc} 1 & & & 0 & \dots & 0 \\ & \ddots & & \vdots & & \vdots \\ & & 1 & 0 & \dots & 0 \end{array}\right) \begin{matrix} 0 \\ \\ N^{(1)} \end{matrix} \qquad \begin{matrix} 0 & N^{(1)} & N^{(1)}+1 & N \end{matrix} \in \mathbb{R}^{(N^{(1)}+1)\times(N+1)} \tag{16}$$

$$E^{(2)} \equiv \left(\begin{array}{ccc|ccc} 0 & & & N^{(1)} & N^{(1)}+1 & N \\ 0 & \dots & 1 & 0 & & \\ 0 & \dots & 0 & 1 & & \\ \vdots & & \vdots & & \ddots & \\ 0 & \dots & 0 & & & 1 \end{array}\right) \begin{array}{c} 0 \\ 1 \\ \\ \\ N^{(2)} \end{array} \in \mathbb{R}^{(N^{(2)}+1)\times(N+1)}. \tag{17}$$

Partition $I^{(i)} \in \mathbb{R}^{(N^{(i)}+1)\times(N^{(i)}+1)}$:

$$I^{(1)} = \begin{pmatrix} \tilde{I}^{(1)} & \\ & 1 \end{pmatrix}, \quad I^{(2)} = \begin{pmatrix} 1 & \\ & \tilde{I}^{(2)} \end{pmatrix}, \quad \tilde{I}^{(i)} \in \mathbb{R}^{N^{(i)}\times N^{(i)}}, \quad i = 1,2.$$

The embedding E can then be alternatively written as:

$$E = \begin{pmatrix} \tilde{I}^{(1)} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \tilde{I}^{(2)} \end{pmatrix}, \quad \tilde{I}^{(i)} \in \mathbb{R}^{N^{(i)}\times N^{(i)}}, \quad i = 1,2. \tag{18}$$

This partitioning will be helpful when discussing the structure of the adjoint and pseudoinverse of the embedding operator E in later sections.

Define an inner product on $\mathbb{R}^{N+1} \times \mathbb{R}^{N+1}$, $N = N^{(1)} + N^{(2)}$, as follows:

$$(u,v)_H \equiv (Eu, Ev)_+ = (Eu)^T H^{(+)} Ev, \tag{19}$$

where we used (12).

Proposition 10. *The scalar product (19) is well defined.*

Proof: Bilinearity and symmetry are obvious. Positivity is also a straightforward consequence:

$$0 = (u,u)_H = (Eu)^T H^{(+)} Eu \iff Eu = 0 \iff u = 0.$$

The first equivalence follows from $H^{(+)} > 0$; the second equivalence holds since E is one-to-one. □

We are now ready to define the state space V for the grid vectors u, v (14) defined on $\Omega = \Omega_1 \cup \Omega_2$:

Definition 11. Let the inner product space V be a real vector space with the inner product

$$(\cdot,\cdot) : V \times V \to \mathbb{R}$$

for all vectors $u, v \in V$ given by (14) and where

$$(u,v) \equiv (u,v)_H.$$

The inner product $(\cdot,\cdot)_H$ is defined in (19). □

Remark 12. The single-domain Definition 3 is extended *verbatim* to the multidomain Definition 11. Only the inner products H differ as defined by (4) and (19). The inner product on V is obtained by restricting (12) to $\mathcal{R}(E) \subset \mathbb{R}^{N+2}$. The vectors

$$u^{(e)} = Eu, \quad v^{(e)} = Ev \in \mathbb{R}^{N+2},$$

are the embeddings of $u, v \in \mathbb{R}^{N+1}$ into $\mathbb{R}^{N+2}$. Completely analogous to interpreting D as a linear operator $D : V \to V$ we will from now on consider the *embedding* E as an operator $E : V \to V_+$. The embeddings $u^{(e)}, v^{(e)}$ satisfy $u^{(e)}_{N^{(1)}} = u^{(e)}_{N^{(1)}+1}$, $v^{(e)}_{N^{(1)}} = v^{(e)}_{N^{(1)}+1}$ by construction. □

Proposition 13. *The embedding operator $E : V \to V_+$ is an isometry.*

Proof: Follows immediately from Definition 11 and (19). □

Remark 14. The partitioning of $E^{(1)}$ and $E^{(2)}$ is arbitrary. Its purpose is to facilitate matrix manipulations involving E, cf. [3] for examples. An alternate partitioning is offered by

$$E^{(1)}_{\text{alt}} \equiv \left(\begin{array}{ccc|ccc} 0 & & & N^{(1)}-1 & N^{(1)} & N \\ 1 & & & 0 & \dots & 0 \\ & \ddots & & \vdots & & \vdots \\ & & 1 & 0 & \dots & 0 \\ & & 0 & 1 & \dots & 0 \end{array}\right) \begin{array}{c} 0 \\ \\ \\ N^{(1)}-1 \\ N^{(1)} \end{array} \in \mathbb{R}^{(N^{(1)}+1)\times(N+1)}$$

$$E^{(2)}_{\text{alt}} \equiv \left(\begin{array}{ccc|ccc} 0 & & N^{(1)}-1 & N^{(1)} & & N \\ 0 & \dots & 0 & 1 & & \\ \vdots & & \vdots & & \ddots & \\ 0 & \dots & 0 & & & 1 \end{array}\right) \begin{matrix} 0 \\ \\ \\ N^{(2)} \end{matrix} \in \mathbb{R}^{(N^{(2)}+1)\times(N+1)}.$$

Obviously, $E^{(i)}_{\text{alt}} = E^{(i)}, i = 1, 2$. The reason for introducing the alternate partitioning will become clear when discussing the structure of H (19) in Section 2.8.1. □

2.6. Adjoint operators

The adjoint of the embedding operator E and the boundary operator L will be needed when discussing operator structure in the subsequent sections. We begin by recalling the definition of the adjoint operator:

Definition 15. Given two inner product spaces V_1 and V_2, the adjoint T^* of a linear operator $T : V_1 \to V_2$ is defined as

$$(u, T^* w)_1 \equiv (Tu, w)_2, \quad u \in V_1, w \in V_2. \quad \square$$

Remark 16. The key observation is that it is not possible to speak of the adjoint without having defined the inner products in V_1 as well as in V_2. The usual transpose T^T is formally obtained by using the Euclidean scalar product in both vector spaces. □

In our case $V_1 = V$ always, where V is the state space discussed in the previous sections. On the other hand, V_2 will be one of V, V_+ or V_Γ depending on which of the operators D, E or L is considered.

Consider $E : V \to V_+$. Let $u \in V$ and $w \in V_+$. Thus, E^* is obtained as

$$(u, E^* w) = (Eu, w)_+ \quad \Longleftrightarrow \quad u^T H E^* w = u^T E^T H^{(+)} w,$$

i.e.,

$$E^* = H^{-1} E^T H^{(+)}. \tag{20}$$

Similarly, given $L : V \to V_\Gamma$:

$$L^* = H^{-1} L^T H_\Gamma, \tag{21}$$

where H_Γ is the matrix representation of the inner product of the boundary state space V_Γ. We know that $H_\Gamma = I \in \mathbb{R}^{2\times 2}$ in one dimension. But in higher dimensions the inner product of V_Γ will be non-trivial.

The expressions (20) and (21) follow directly from the definition of an adjoint operator. The adjoint of $D : V \to V$ satisfies a completely analogous expression, but in this case it is possible to take the analysis further. By definition:

$$(u, D^* v) = (Du, v), \quad u, v \in V,$$

and by (7)

$$(u, D^* v) = u_N v_N - u_0 v_0 - (u, Dv).$$

Next, we define the *outward normal* operator n_Γ:

Definition 17. Given the state space V and the boundary state space V_Γ, define the outward normal operator $n_\Gamma : V \to V_\Gamma$:

$$n_\Gamma \equiv \begin{pmatrix} -1 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix} \in \mathbb{R}^{2\times(N+1)}. \quad \square$$

Hence ($H_\Gamma = I$),

$$(u, D^* v) = \langle n_\Gamma u, v_\Gamma \rangle - (u, Dv) = (u, n_\Gamma^* v_\Gamma) - (u, Dv).$$

But $v_\Gamma = |n_\Gamma| v$. We have thus arrived at the following expression for the adjoint of D:

$$D^* = n_\Gamma^* |n_\Gamma| - D. \tag{22}$$

Remark 18. It is shown in [9,10] that

$$D = H^{-1} Q, \quad Q = \frac{1}{2} n_\Gamma^T |n_\Gamma| + Q_a.$$

The boundary operator $n_\Gamma^T|n_\Gamma|$ is zero everywhere, except for the first and last diagonal elements, which are -1 and 1; Q_a is antisymmetric. Hence,

$$D^* = H^{-1}D^T H = H^{-1}Q^T = H^{-1}\left[\frac{1}{2}|n_\Gamma|^T n_\Gamma - Q_a\right] = H^{-1}n_\Gamma^T|n_\Gamma| - H^{-1}Q$$

in complete accordance with (22) since $H_\Gamma = I$ and thus $n_\Gamma^* = H^{-1}n_\Gamma^T$ by the very definition of an adjoint operator. □

2.7. Multiblock difference operators D

Analogous to (13), define

$$D^{(+)} \equiv \begin{pmatrix} D^{(1)} & \\ & D^{(2)} \end{pmatrix} \begin{matrix} N^{(1)}+1 & N^{(2)}+1 \\ N^{(1)}+1 & \\ N^{(2)}+1 & \end{matrix}, \tag{23}$$

where $D^{(i)}$ satisfies the summation-by-parts rule (7) with respect to $(\cdot,\cdot)_i = (\cdot,\cdot)_{H^{(i)}}, i = 1,2$. It follows that $D^{(+)} : V_+ \to V_+$. Define the multiblock difference operator D:

Definition 19. Given the inner product space V as in Definition 11, the difference operator $D : V \to V$ is defined as

$$D \equiv H^{-1}E^T H^{(+)} D^{(+)} E. \quad \square \tag{24}$$

The main result can be formulated as

Proposition 20. *Let $D : V \to V$ be defined as in Definition 19. Then*

(i) *D satisfies summation by parts with respect to the inner product $(\cdot,\cdot)$ of Definition 11.*
(ii) *D is a consistent approximation of $\partial/\partial x$.*
(iii) *$D = E^* D^{(+)} E$.*

Proof: To prove the first statement, note that

$$\begin{aligned}(u, Dv) &= \left[u^{(1)}\right]^T H^{(1)} D^{(1)} v^{(1)} + \left[u^{(2)}\right]^T H^{(2)} D^{(2)} v^{(2)} \\ &= u^{(2)}_{N^{(2)}} v^{(2)}_{N^{(2)}} - u^{(1)}_0 v^{(1)}_0 - \left[D^{(1)}u^{(1)}\right]^T H^{(1)} v^{(1)} - \left[D^{(2)}u^{(2)}\right]^T H^{(2)} v^{(2)},\end{aligned}$$

since $u^{(2)}_0 = u^{(1)}_{N^{(1)}}$ with a similar constraint for v due to the embedding $Eu = u^{(e)} = \begin{pmatrix} u^{(1)} & u^{(2)} \end{pmatrix}^T$. Hence,

$$(u, Dv) = u_N v_N - u_0 v_0 - (Du, v), \quad N = N_1 + N_2,$$

which proves the first assertion.

To prove the second assertion, let $u(x)$ be a smooth function on $[0,1]$. Define

$$u \equiv \begin{pmatrix} u(x_0) \\ \vdots \\ u(x_N) \end{pmatrix}, \qquad x_0 = 0, x_N = 1.$$

Then,

$$\begin{aligned}D^{(+)}Eu = D^{(+)}u^{(e)} &= \begin{pmatrix} D^{(1)}u^{(1)} \\ D^{(2)}u^{(2)} \end{pmatrix} = \begin{pmatrix} u^{(1)}_x \\ u^{(2)}_x \end{pmatrix} + \mathcal{O}(h^p) \qquad \left[u^{(1)}_x[N^{(1)}] = u^{(2)}_x[0] + \mathcal{O}(h^p)\right] \\ &= u^{(e)}_x + \mathcal{O}(h^p) = Eu_x + \mathcal{O}(h^p).\end{aligned}$$

By Definition 19:

$$Du = H^{-1}E^T H^{(+)} D^{(+)} Eu = H^{-1}E^T H^{(+)} Eu_x + \mathcal{O}(h^p) = u_x + \mathcal{O}(h^p),$$

which finishes the proof of the second assertion.

The third statement, finally, follows immediately from (20). This concludes the proof. □

2.8. Structure of H, E^* and D

The matrix structure of H, E^* and D will play an important role for the actual implementation of multiblock difference operators. Under fairly mild assumptions on H, one can show that D has a particularly simple structure closely resembling the original difference operators $D^{(1)}$ and $D^{(2)}$. We will merely state the results. The reader is referred to [3] for details.

2.8.1. Structure of H

Straightforward but tedious computations show that

$$H = \left(\begin{array}{ccc|ccc} h^{(1)}_{00} & \cdots & h^{(1)}_{0N^{(1)}} & & & \\ \vdots & & \vdots & & & \\ h^{(1)}_{N^{(1)}0} & \cdots & \tilde{h}^{(1)}_{N^{(1)}N^{(1)}} & h^{(2)}_{01} & \cdots & h^{(2)}_{0N^{(2)}} \\ \hline & & h^{(2)}_{10} & h^{(2)}_{11} & \cdots & h^{(2)}_{1N^{(2)}} \\ & & \vdots & \vdots & & \vdots \\ & & h^{(2)}_{N^{(2)}0} & h^{(2)}_{N^{(2)}1} & \cdots & h^{(2)}_{N^{(2)}N^{(2)}} \end{array}\right), \tag{25}$$

where

$$\tilde{h}^{(1)}_{N^{(1)}N^{(1)}} = h^{(1)}_{N^{(1)}N^{(1)}} + h^{(2)}_{00}.$$

Remark 21. Pictorially, H is created by shifting $H^{(2)}$ one step towards NW along the main diagonal of $H^{(+)}$ and by adding the two overlapping elements. One can express (25) symbolically as

$$H = \begin{pmatrix} H^{(1)} & \\ & 0 \end{pmatrix}^{\begin{matrix} N^{(1)}+1 & N^{(2)} \end{matrix}}_{\begin{matrix} N^{(1)}+1 \\ N^{(2)} \end{matrix}} + \begin{pmatrix} 0 & \\ & H^{(2)} \end{pmatrix}^{\begin{matrix} N^{(1)} & N^{(2)}+1 \end{matrix}}_{\begin{matrix} N^{(1)} \\ N^{(2)}+1 \end{matrix}}. \tag{26}$$

Matrix addition is well defined at the element level, but not at the block level due to incompatible diagonal blocks. The expression serves as a useful mnemonic for how to implement H given $H^{(1)}$ and $H^{(2)}$, though. It should be emphasized that (25) and (26) are valid for *any* norms $H^{(1)}$ and $H^{(2)}$, including implicit ones. □

Using the alternate partitionings of Remark 14 yields the following equivalent expression for H:

$$H = \left(\begin{array}{ccc|ccc} h^{(1)}_{00} & \cdots & h^{(1)}_{0,N^{(1)}-1} & h^{(1)}_{0N^{(1)}} & & \\ \vdots & & \vdots & \vdots & & \\ h^{(1)}_{N^{(1)}-1,0} & \cdots & h^{(1)}_{N^{(1)}-1,N^{(1)}-1} & h^{(1)}_{N^{(1)}-1,N^{(1)}} & & \\ \hline h^{(1)}_{N^{(1)}0} & \cdots & h^{(1)}_{N^{(1)},N^{(1)}-1} & \tilde{h}^{(2)}_{00} & \cdots & h^{(2)}_{0N^{(2)}} \\ & & & \vdots & & \vdots \\ & & & h^{(2)}_{N^{(2)}0} & \cdots & h^{(2)}_{N^{(2)}N^{(2)}} \end{array}\right).$$

This time

$$\tilde{h}^{(2)}_{00} = h^{(1)}_{N^{(1)}N^{(1)}} + h^{(2)}_{00},$$

which can be interpreted as shifting $H^{(1)}$ towards SE along the main diagonal. We will use this expression when discussing the structure of H^{-1} in the next section. Note that (26) stays the same.

2.8.2. The inverse of H

To analyze the structure of E^*, the inverse of H is needed. If $H^{(1)}$ and $H^{(2)}$ are restricted full norms, then H and H^{-1} have a particularly simple structure:

Proposition 22. *Let H be as in Definition 11. Then H^{-1} is block diagonal iff $H^{(1)}$ and $H^{(2)}$ are restricted full norms. The resulting norm H becomes*

$$H = \begin{pmatrix} \tilde{H}^{(1)} & & \\ & h^{(1)}_{N^{(1)}N^{(1)}} + h^{(2)}_{00} & \\ & & \tilde{H}^{(2)} \end{pmatrix}, \quad \tilde{H}^{(i)} \in \mathbb{R}^{N^{(i)}\times N^{(i)}}, \quad i = 1, 2. \quad \square$$

Proof. See [3] for details. □

Remark 23. Restricted full norms are only required to prove block diagonal structure of H^{-1}. Proposition 20 is valid for any class of summation-by-parts norms, including implicit ones. Using restricted full forms will lead to *much* simpler implementation of multiblock difference operators D, which will be shown in Section 2.8.4. □

2.8.3. Structure of E^*

Since E^* involves H^{-1} it will be assumed that $H^{(1)}$ and $H^{(2)}$ are restricted full norms. By (18):

$$E^T H^{(+)} = \begin{pmatrix} \tilde{H}^{(1)} & 0 & 0 & 0 \\ 0 & h^{(1)}_{N^{(1)}N^{(1)}} & h^{(2)}_{00} & 0 \\ 0 & 0 & 0 & \tilde{H}^{(2)} \end{pmatrix}$$

and hence, by (20) and Proposition 22:

$$E^* = \begin{pmatrix} \tilde{I}^{(1)} & 0 & 0 & 0 \\ 0 & \chi & 1-\chi & 0 \\ 0 & 0 & 0 & \tilde{I}^{(2)} \end{pmatrix}, \quad \chi \equiv \frac{h^{(1)}_{N^{(1)}N^{(1)}}}{h^{(1)}_{N^{(1)}N^{(1)}} + h^{(2)}_{00}}. \tag{27}$$

Remark 24. Suppose that the restricted full norms $H^{(1)}$ and $H^{(2)}$ satisfy the structural requirements of (5), which is a very common situation in practical computations. Then

$$h^{(1)}_{N^{(1)}N^{(1)}} = \mu h^{(1)}, \quad h^{(2)}_{00} = \mu h^{(2)},$$

where $h^{(1)}$ and $h^{(2)}$ are the mesh sizes in the respective domains, whence

$$\chi = \frac{h^{(1)}}{h^{(1)} + h^{(2)}}. \quad \square$$

2.8.4. Structure of D

As before, $H^{(1)}$ and $H^{(2)}$ are assumed to be restricted full norms. Then D as defined in (24) can be written as

$$\begin{pmatrix} D^{(1)}_{00} & \cdots & D^{(1)}_{0N^{(1)}} & 0 & \cdots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ D^{(1)}_{N^{(1)}-1,0} & \cdots & D^{(1)}_{N^{(1)}-1,N^{(1)}} & 0 & \cdots & 0 \\ \chi D^{(1)}_{N^{(1)}0} & \cdots & \chi D^{(1)}_{N^{(1)}N^{(1)}} + (1-\chi)D^{(2)}_{00} & (1-\chi)D^{(2)}_{01} & \cdots & (1-\chi)D^{(2)}_{0N^{(2)}} \\ 0 & \cdots & D^{(2)}_{10} & D^{(2)}_{11} & \cdots & D^{(2)}_{1N^{(2)}} \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \cdots & D^{(2)}_{N^{(2)}0} & D^{(2)}_{N^{(2)}1} & \cdots & D^{(2)}_{N^{(2)}N^{(2)}} \end{pmatrix} \tag{28}$$

In practice, Du is computed by evaluating $D^{(i)}u^{(i)}$ in each subinterval followed by computing the weighted mean

$$\chi \left[D^{(1)}u^{(1)}\right]_{N^{(1)}} + (1-\chi)\left[D^{(2)}u^{(2)}\right]_0.$$

The arithmetic overhead is negligible compared to computing the difference stencils in each subinterval.

If the boundary stencils of $D^{(1)}$ and $D^{(2)}$ are the "anti-reflections" of one another, then

$$\chi D^{(1)}_{N^{(1)},N^{(1)}-j} = \frac{1}{h^{(1)}+h^{(2)}} d_{N^{(1)},N^{(1)}-j} = -\frac{1}{h^{(1)}+h^{(2)}} d_{0j} = -(1-\chi)D^{(2)}_{0j}.$$

In particular, for $j = 0$:

$$\chi D^{(1)}_{N^{(1)}N^{(1)}} + (1-\chi)D^{(2)}_{00} = 0.$$

For $j > s$, where s is some positive constant (independent of $N^{(1)}$ and $N^{(2)}$), the stencil coefficients d_{0j} are zero. Hence, the middle row of D represents an anti-symmetric difference stencil corresponding to different mesh sizes h_i to the left and right of the center point $x = 1/2$. For $h^{(1)} = h^{(2)} = h$ a centered anti-symmetric difference stencil is recovered.

3. Linear operators and the pseudoinverse

The theory of pseudoinverses harkens back to 1920, when they were introduced by Moore [13]. It was later picked up by Bjerhammar [14] and Penrose [5]. In the latter paper, the following theorem is proved:

Theorem 25. *Let $A \in \mathbb{R}^{n\times m}$ be given. The four equations*

$$AXA = A, \quad XAX = X, \quad (AX)^T = AX, \quad (XA)^T = XA$$

have a unique solution $X \in \mathbb{R}^{m\times n}$ denoted by

$$A^+ \equiv X. \quad \square$$

Remark 26. The four equations of Theorem 25 are collectively referred to as the Moore-Penrose conditions; A^+ is known as the pseudoinverse of A. The pseudoinverse A^+ shares many of its properties with the proper inverse A^{-1}, e.g.,

$$A^{++} = A, \quad \left[A^+\right]^T = \left[A^T\right]^+.$$

Also, if $A = (U\ V)$, then it is possible to derive an explicit expression for A^+ in terms the blocks U^+ and V^+ similar to what was done when discussing the block structure of H^{-1}. The reader is referred to [15], [16] and [8] for details. But the following relation is *not true* in general:

$$[AB]^+ = B^+ A^+.$$

It holds under certain circumstances, for instance if $A^T A = I$, $B^T B = I$, $B = A^T$ or $B = A^+$, cf. [17], [8]. □

In the derivation of Theorem 25, it is tacitly assumed that the matrix A represents a linear mapping $A : \mathbb{R}^n \to \mathbb{R}^m$ subject to the usual Euclidean scalar product. But we are interested in finding the pseudoinverse of the boundary mapping $L : V \to V_\Gamma$, which involves general inner product spaces:

$$Lu = g, \quad u \in V, \quad g \in V_\Gamma,$$

where L is the discrete operator representing the boundary conditions in (1). The Moore-Penrose conditions are therefore not directly applicable as expressed in Theorem 25. Instead, we follow the approach in Kreutz-Delgado [6], where the pseudoinverse is applied to operators between inner product spaces instead of the Euclidean spaces $\mathbb{R}^n$ and $\mathbb{R}^m$. We have the following

Theorem 27. *Let $T : V_1 \to V_2$ be a linear operator between two inner product spaces. Then $S : V_2 \to V_1$ is the pseudoinverse of T iff the four Moore-Penrose conditions*

$$TST = T, \quad STS = S, \quad (TS)^* = TS, \quad (ST)^* = ST$$

hold, in which case we write

$$T^+ \equiv S.$$

Proof. See [3] and [8] for details. □

Corollary 28. *Let $T : V_1 \to V_2$ and $S : V_2 \to V_1$ be two linear operators. The Moore-Penrose conditions can then be expressed as*

$$TST = T, \quad STS = S, \quad (TS)^T H_2 = H_2 TS, \quad (ST)^T H_1 = H_1 ST.$$

Proof. Since $ST : V_1 \to V_1$ and $TS : V_2 \to V_2$, the result follows immediately from Definition 15. □

3.1. Boundary operators

The boundary operator L is a mapping $L : V \to V_\Gamma$: $Lu = g$. By Corollary 28:

$$LL^+L = L, \quad L^+LL^+ = L^+, \quad \left[LL^+\right]^T = LL^+, \quad \left[L^+L\right]^T H = HL^+L,$$

where we used $H_1 = H$ and $H_2 = H_\Gamma = I$. If $LL^+ = I$, that is, if L^+ is the right inverse of L, then the Moore-Penrose conditions reduce to a single constraint:

$$\left[L^+L\right]^T H = HL^+L.$$

3.2. Embedding operators

The embedding operator E is a mapping $V \to V_+$, see Remark 12. By the definition of the adjoint operator:

$$E^* = H^{-1} E^T H^{(+)}.$$

Hence,

$$E^* E = H^{-1} \left[E^T H^{(+)} E\right] = I,$$

where we used the definition of H in the second equality. We are thus left with the single Moore-Penrose condition:

$$\left[EE^*\right]^* = EE^*,$$

which is trivially satisfied. It follows that

$$E^+ = E^*.$$

The next corollary is an immediate consequence of $E^+ = E^*$ and Proposition 20:

Corollary 29. *Let $D : V \to V$ be as in Definition 19. Then*

$$D = E^+ D^{(+)} E. \quad \square$$

4. Semidiscrete initial-boundary value problems

Following the approach in [2], [18], we discretize (1) as

$$v_t + PQ(D)[Pv + (I-P)\tilde{g}] = (I-P)\tilde{g}_t, \qquad t > 0 \tag{29}$$
$$v(0) = f,$$

where it is assumed that initial data satisfy the boundary conditions $Lf = g(0)$; $L : V \to V_\Gamma$ represents the discrete boundary operator, which is assumed to be (piecewise) constant in time. The precise structure of this operator is not important for the present discussion. Analogously, $Q(D)$ is a discretization of the semibounded analytic operator $Q(\partial)$, where $D : V \to V$ satisfies (3). Finally, $P : V \to V$ is the projection operator representing the analytic the boundary operator L in the sense of [2]:

$$P = I - H^{-1} L^T (L H^{-1} L^T)^{-1} L, \tag{30}$$

where it is temporarily assumed that L has full rank so that $P : V \to V$ is well defined. The data vector $\tilde{g}$ is defined implicitly through

$$L\tilde{g} \equiv g, \quad \tilde{g} \in V. \tag{31}$$

Any solution $v \in V$ of (29) will satisfy

$$(I-P)(v-\tilde{g}) = 0 \quad \Longleftrightarrow \quad L(v-\tilde{g}) = 0$$

as is shown in [2]. In other words, the boundary conditions are fulfilled for exactly those vectors $v - \tilde{g}$ that belong to $\mathcal{N}(L)$. As long as the rows of L are linearly independent, $\mathcal{N}(L)$ is invariant. We can therefore assume that the rows of L are orthogonal with respect to H^{-1}. Hence ($H_\Gamma = I$),

$$P = I - H^{-1} L^T L = I - L^* L = I - L^+ L.$$

We note that the last expression makes sense even if the rows of L are not orthogonal with respect to H^{-1}. In fact, the rows of L can be linearly dependent. Thus, from now on we drop the requirement that L have full rank [2].

Definition 30. Let $L : V \to V_\Gamma$ represent the discrete boundary operator of (1). The boundary projection $P : V \to V$ is defined as

$$P \equiv I - L^+ L,$$

where L^+ is the pseudoinverse of L. $\square$

Remark 31. Not requiring full rank makes it possible to treat all possible combinations of characteristic boundary conditions for hyperbolic systems in a uniform manner. It also simplifies the analysis in the presence of corners, since one can overspecify the boundary conditions at the corners as long as they make sense from a consistency point of view.

The boundary operator L can be interpreted as the restriction of the state space onto the boundary state space. Similarly, L^+ injects the boundary state space into the state space. $\square$

Proposition 32. *Let $v \in V$ be a solution of (29) and assume that $\tilde{g} \in V$ satisfies (31). Then*

$$(I-P)(v-\tilde{g}) = 0 \quad \Longleftrightarrow \quad Lv = g,$$

where $L : V \to V_\Gamma$ and $P : V \to V$ are is in Definition 30.

Proof. Assume that $(I-P)(v-\tilde{g}) = 0$. Then

$$L^+ L v = L^+ L \tilde{g}.$$

Multiplying by L from the left yields

$$L L^+ L v = L L^+ L \tilde{g},$$

which according to the Moore-Penrose conditions is the same as

$$Lv = L\tilde{g} = g,$$

where we used (31) in the last step. The opposite implication is obvious. □

4.1. The simplified semidiscrete form

The boundary operator P is independent of t given our assumptions on L. This situation is quite common in practice. Boundary data $g(t)$ may vary with t, however. Consider the *simplified* semidiscrete equations

$$\begin{aligned} w_t + PQ(D)(v) &= 0, \qquad t > 0 \\ w(0) &= Pf, \end{aligned} \tag{32}$$

where v is defined by

$$v \equiv Pw + L^+ g, \qquad t \geq 0. \tag{33}$$

Theorem 33. *If the initial data f satisfies the boundary condition $Lf = g(0)$, then the semidiscrete approximation (29) and the simplified semidiscrete approximation (32), (33) are equivalent.*

Proof. Equation (29) can be rewritten as

$$Pv_t + (I-P)v_t + PQ(Pv + (I-P)\tilde{g}) = (I-P)\tilde{g}_t,$$

which in turn can be expressed as

$$\begin{aligned} (I-P)(\tilde{g}_t - v_t) &= z \\ P\left[v_t + Q(Pv + (I-P)\tilde{g})\right] &= z. \end{aligned}$$

Thus, z is orthogonal to itself and so

$$\|z\|^2 = (z,z) = 0 \quad \Longleftrightarrow \quad z = 0.$$

This implies that eq. (29) decouples into two equations for $t > 0$:

$$\begin{aligned} (I-P)(v_t - \tilde{g}_t) &= 0 \\ P\left[v_t + Q(Pv + (I-P)\tilde{g})\right] &= 0. \end{aligned}$$

It should be noted that the decoupled system is equivalent to the original formulation (29).

Integrating the first equation of the decoupled system yields the necessary condition

$$(I-P)(v - \tilde{g}) = (I-P)(f - \tilde{g}(0)),$$

since P does not depend on t. Thus, v satisfies the boundary conditions for $t > 0$ iff initial data f fulfills the boundary conditions. The latter is true by assumption ($Lf = g(0)$). Consequently, there is no need to solve the first part, since the answer is known à priori ($Lv = g(t)$).

Let

$$w \equiv Pv \quad \Longrightarrow \quad w = Pw \quad \Longleftrightarrow \quad Lw = 0,$$

which is a consequence of the first Moore-Penrose condition. The second equation of the decoupled system may then be expressed as

$$w_t + PQ(Pw + L^+ g) = 0, \qquad t > 0,$$

where we used $Pv = w = Pw$. From the definition of w it follows immediately that $w(0) = Pf$. This shows that (29) implies (32).

Conversely, suppose that w solves (32), (33). Hence,

$$w = Pw, \quad t \geq 0.$$

Add $(I-P)\tilde{g}_t$ to both members of (32):

$$v_t + PQ(Pw + (I-P)\tilde{g}) = (I-P)\tilde{g}_t.$$

Thus, (29) has been recovered.

Verification of initial conditions of v:

$$v(0) = Pf + L^+ g(0) = f - L^+ Lf + L^+ g(0) = f,$$

since $Lf = g(0)$ by assumption. Analogously, for the boundary conditions of v one has

$$Lv = LPw + LL^+ g = LL^+ L\tilde{g} = L\tilde{g} = g$$

for $t > 0$. This shows that v fulfills the inhomogeneous boundary conditions of (29). □

Remark 34. The simplified form greatly reduces the implementation complexity of the semidiscrete system (29), since there is no need to compute the time derivative of the auxiliary vector $\tilde{g}$. This can be a challenge if the boundary data is obtained from measurements. □

4.2. The simplified projection P

By the formal definition of the boundary projection operator P:

$$P \equiv I - L^+ L = I - L^* \left[LL^*\right]^+ L = I - H^{-1} L^T H_\Gamma \left[\left(LH^{-1}L^T\right) H_\Gamma\right]^+ L.$$

If L has full rank, then

$$\left[\left(LH^{-1}L^T\right) H_\Gamma\right]^+ = \left[\left(LH^{-1}L^T\right) H_\Gamma\right]^{-1} = H_\Gamma^{-1} \left[LH^{-1}L^T\right]^{-1}$$

in complete agreement with (30), in which case P is independent of H_Γ. Since

$$[AB]^+ \neq B^+ A^+$$

for general operators A, B, we cannot deduce the same conclusion for rank-deficient boundary operators L. But as the following argument will show, we can nevertheless choose $H_\Gamma = I$.

To prove stability, one must have

$$Pv = v, \quad HP = P^T H, \tag{34}$$

where v is a solution of (29). The first requirement ensures that the boundary conditions are fulfilled. The second constraint will be used when proving stability using the energy method. But $Pv = v$ and $P^T H = HP$ follow from the two Moore-Penrose conditions:

$$LL^+ L = L, \quad HL^+ L = \left[L^+ L\right]^T H.$$

Given the state space V, let $L_i : V \to V_{\Gamma_i}$, $i = 1, 2$, denote two boundary operators that implement the same analytic boundary condition. For example,

$$L_1 = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \end{pmatrix}, \quad L_2 = \begin{pmatrix} 1 & 0 & \dots & 0 \end{pmatrix}$$

both implement the analytic boundary condition $Lu = 0$, c.f. introductory example. The pseudoinverses L_1^+ and L_2^+ will by necessity obey the above Moore-Penrose conditions no matter how we choose the boundary scalar products H_{Γ_i}. Hence, the solution v of (29) must satisfy

$$P_i v = v \iff L_i L_i^+ L_i v = 0 \iff L_i v = 0,$$

i.e., the projections P_1 and P_2 enforce the same boundary conditions. Furthermore, by the second Moore-Penrose condition:

$$HP_i = P_i^T H.$$

As a result, P_1 as well as P_2 satisfy (34). From an implementation perspective it is thus irrelevant which V_Γ and H_Γ we choose; the resulting projection P will always lead to a consistent and stable implementation of the analytic boundary conditions. In particular, we can choose $H_\Gamma = I$ when computing P, which implies (30) also in the general case:

$$P = I - H^{-1} L^T \left[LH^{-1}L^T\right]^+ L. \tag{35}$$

Remark 35. Superficially, it looks like P is independent of H_Γ also when L is rank deficient. This is not true, however, since (35) depends on our choice $H_\Gamma = I$, as opposed to (30), which is true for *any* H_Γ. In the case of a rank-deficient L it makes sense to speak of *a* projection, not *the* projection. On the other hand, if L has full rank, all projections reduce to a single projection (30).

Next, suppose that L and H satisfy

$$LH = \bar{H} L$$

for some $\bar{H} > 0$. Thus,

$$L^T = H^{-1} L^T \bar{H}.$$

If we choose $H_\Gamma = \bar{H}$, then

$$L^T = H^{-1} L^T H_\Gamma = L^*,$$

whence

$$P = I - L^+ L = I - L^* \left[L L^* \right]^+ L = I - L^T \left[L L^T \right]^+ L. \tag{36}$$

Remark 36. Expression (36) is an example of a situation where the algebraic expression is simplified even further if we choose $H_\Gamma = \bar{H}$ as opposed to the default $H_\Gamma = I$. This conclusion extends the corresponding result in [2] to the case where L is rank deficient. In the next section we will examine a concrete example where this condition holds. □

4.3. Characteristic boundary conditions

Let

$$L = \begin{pmatrix} L_L \\ L_R \end{pmatrix} = \begin{pmatrix} L_0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & L_1 \end{pmatrix}, \quad L_0, L_1 \in \mathbb{R}^{d \times d}. \tag{37}$$

be the matrix representation of the characteristic boundary conditions for the model system (1), which is assumed to be hyperbolic. L_0 and L_1 are the analytic boundary operators.

Let H be a restricted full norm. Then

$$LH = \bar{H} L \quad \Longleftrightarrow \quad L^T = H^{-1} L^T \bar{H},$$

where

$$\bar{H} = \begin{pmatrix} h_{00} I & \\ & h_{NN} I \end{pmatrix} \in \mathbb{R}^{2d \times 2d}.$$

Define $H_\Gamma = \bar{H}$. Thus, by (36):

$$P = I - L^T \left[L L^T \right]^+ L.$$

We conclude this section with the following

Proposition 37. *Let $L_i : \mathbb{R}^d \to \mathbb{R}^d$, $i = 0, 1$ be the analytic boundary operators of (1) with pseudoinverses L_i^+, $i = 1, 2$. Define $L : V \to V_\Gamma$ as in (37). If H is a restricted full norm, then*

$$L^+ = \begin{pmatrix} L_L^+ & L_R^+ \end{pmatrix} \equiv \begin{pmatrix} L_0^+ & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ 0 & L_1^+ \end{pmatrix}$$

for any

$$H_\Gamma \equiv \begin{pmatrix} h_L I & \\ & h_R I \end{pmatrix} > 0, \quad I \in \mathbb{R}^{d \times d}. \tag{38}$$

Proof: The four Moore-Penrose conditions

$$L L^+ L = L, \quad L^+ L L^+ = L^+, \quad H \left[L^+ L \right] = \left[L^+ L \right]^T H, \quad H_\Gamma \left[L L^+ \right] = \left[L L^+ \right]^T H_\Gamma$$

follow immediately from the structure of L, L^+, H and H_Γ. The details are left as an exercise. □

Remark 38. According to Proposition 37, LL^+ is self-adjoint with respect to *any* norm H_Γ of the form (38). In particular, it is true for

$$H_\Gamma = \begin{pmatrix} I & \\ & I \end{pmatrix} \quad \text{and} \quad H_\Gamma \equiv \begin{pmatrix} h_{00} I & \\ & h_{NN} I \end{pmatrix}.$$

The former expression represents the choice of scalar product in Definition 5. Proposition 37 is a stronger result than (36), since L^+ is independent of H and H_Γ, yet it fulfills the Moore-Penrose conditions for any H_Γ (38) (and any $\tilde{H} > 0$), not just for $H_\Gamma = \bar{H}$. For restricted full norms, H and H_Γ are completely decoupled from one another as far as the Moore-Penrose conditions are concerned. □

5. Two space dimensions, single-block case

Consider the unit square $\Omega = [0,1] \times [0,1]$ with grid points

$$(x_i, y_j) \equiv (ih_1, jh_2), \quad h_1 = 1/N_1, \quad h_2 = 1/N_2.$$

For future reference we define the discrete boundaries corresponding to $y = 0$, $x = 1$, $y = 1$ and $x = 0$:

$$\Gamma_1 \equiv \{(ih_1, 0), i = 0, \dots, N_1\} \quad \Gamma_2 \equiv \{(1, jh_2), j = 0, \dots, N_2\} \tag{39}$$
$$\Gamma_3 \equiv \{(ih_1, 1), i = N_1, \dots, 0\} \quad \Gamma_4 \equiv \{(0, jh_2), j = N_2, \dots, 0\}.$$

The ordering of the boundary segments Γ_i corresponds to traversing the boundary Γ in the positive (counter-clockwise) direction:

$$\Gamma \equiv \cup_{i=1}^{4} \Gamma_i.$$

Internally, the boundary segments Γ_1 and Γ_2 are ordered according to increasing i and j; the ordering of Γ_3 and Γ_4 corresponds to decreasing i and j, cf. (39).

Each grid point (including the four corner points)

$$(0,0), \quad (1,0), \quad (1,1), \quad (0,1), \tag{40}$$

has multiplicity one. Analogous to the one-dimensional case we introduce

$$\Gamma_+ = \sum_{i=1}^{4} \Gamma_i.$$

Hence, the multiplicity of the four corner points (40) is two; all other points have multiplicity one. Just like the one-dimensional case, the increased multiplicity at the corner points is triggered by partial summation occurring twice at the same grid point. In the one-dimensional multidomain formulation, this situation occurred at the interface between the two computational domains. In the two-dimensional formulation, the boundary state representing the corner points is needed twice: once for partial summation in the x-direction and once in the y-direction.

5.1. The solution state space V

At each point (x_i, y_j) we define a state variable $u_{ij}(t)$. Analogous to the one-dimensional case, we arrange the state variables into a column vector:

$$u \equiv \begin{pmatrix} u_0 \\ \vdots \\ u_{N_2} \end{pmatrix}, \quad u_j \equiv \begin{pmatrix} u_{0j} \\ \vdots \\ u_{N_1 j} \end{pmatrix} \in \mathbb{R}^{N_1+1}, \quad 0 \le j \le N_2. \tag{41}$$

This block structure corresponds to ordering the state variables u_{ij} by grid row with i being the inner index and j the outer one.

Summation by parts is simplified if we also introduce an alternate representation of the grid function u corresponding to column ordering of u_{ij}, where j is the inner index:

$$u \equiv \begin{pmatrix} u^0 \\ \vdots \\ u^{N_1} \end{pmatrix}, \quad u^i \equiv \begin{pmatrix} u_{i0} \\ \vdots \\ u_{iN_2} \end{pmatrix} \in \mathbb{R}^{N_2+1}, \quad 0 \le i \le N_1, \tag{42}$$

where we have adopted the convention of using superscripts for column reference.

The two-dimensional norm is constructed as

$$H \equiv H_2 \otimes H_1 = H_y H_x = H_x H_y \in \mathbb{R}^{(N_1+1)(N_2+1) \times (N_1+1)(N_2+1)}, \tag{43}$$

where $H_i, i = 1, 2$, represent one-dimensional scalar products (4). Use H to define an inner product on $\mathbb{R}^{(N_1+1)(N_2+1) \times (N_1+1)(N_2+1)}$:

$$(u, v)_H \equiv u^T H v. \tag{44}$$

Definition 39. Let the inner product space V be a real vector space with the inner product

$$(\cdot, \cdot) : V \times V \to \mathbb{R}$$

for all vectors $u, v \in V$ given by (41) and where

$$(u, v) \equiv (u, v)_H.$$

The inner product $(\cdot, \cdot)_H$ is defined in (44). □

Remark 40. Definition 39 together with definitions (41) and (42) implies that

$$u_j \in V_1, \quad u^i \in V_2,$$

where V_1 and V_2 correspond to Definition 3 with scalar products $(u_j, v_j)_1 \equiv u_j^T H_1 v_j$ and $(u^i, v^i)_2 \equiv \left[u^i\right]^T H_2 v^i$. The vector space V of Definition 39 will be referred to as the two-dimensional solution state space. □

5.2. Summation-by-parts operators D_x and D_y

Define the two-dimensional difference operators $D_x, D_y : V \to V$

$$D_x \equiv I_2 \otimes D_1, \quad D_y \equiv D_2 \otimes I_1, \tag{45}$$

where

$$I_1, D_1 : V_1 \to V_1, \quad I_2, D_2 : V_2 \to V_2.$$

$D_i, i = 1, 2$, satisfies summation by parts with respect to $(\cdot,\cdot)_i$; $\otimes$ denotes the Kronecker product of two matrices. The following theorem is well known:

Theorem 41. *Let $D_x, D_y : V \to V$ be given by (45) and $(\cdot,\cdot)$ by Definition 39. Then*

$$(u, D_x v) = (u^{N_1}, v^{N_1})_2 - (u^0, v^0)_2 - (D_x u, v)$$
$$(u, D_y v) = (u_{N_2}, v_{N_2})_1 - (u_0, v_0)_1 - (D_y u, v).$$

Remark 42. Theorem 41 holds for any one-dimensional norms H_1 and H_2, i.e., any scalar products $(\cdot,\cdot)_1$ and $(\cdot,\cdot)_2$. This includes implicit norms as long as the summation-by-parts rule (3) holds. □

5.3. The boundary state V_Γ

For each boundary segment Γ_i, define the grid vectors u_{Γ_i}:

$$u_{\Gamma_1} \equiv u_0, \quad u_{\Gamma_2} \equiv u^{N_1}, \quad u_{\Gamma_3} \equiv J_1 u_{N_2}, \quad u_{\Gamma_4} \equiv J_2 u^0, \tag{46}$$

where $J_1 \in \mathbb{R}^{(N_1+1)\times(N_1+1)}$ and $J_2 \in \mathbb{R}^{(N_2+1)\times(N_2+1)}$ are anti-diagonal permutation matrices, cf. Remark 2. The reason for including the permutation matrices is to ensure that the definition of the boundary state corresponds to the positive orientation of the boundary Γ (39). Let

$$u_\Gamma^{(e)} \equiv \begin{pmatrix} u_{\Gamma_1} \\ u_{\Gamma_2} \\ u_{\Gamma_3} \\ u_{\Gamma_4} \end{pmatrix} \in \mathbb{R}^{2(N+2)}, \quad u_\Gamma \equiv \begin{pmatrix} u_{\Gamma_1}[:N_1] \\ u_{\Gamma_2}[:N_2] \\ u_{\Gamma_3}[:N_1] \\ u_{\Gamma_4}[:N_2] \end{pmatrix} \in \mathbb{R}^{2N} \tag{47}$$

represent the grid vectors on Γ_+ and Γ, $N = N_1 + N_2$; $u_{\Gamma_i}[:N_i]$ refers to the standard Python notation for extracting all but the last element of u_{Γ_i}. Since

$$u_{\Gamma_1}[N_1] = u_{\Gamma_2}[0] = u_{N_1 0}, \; u_{\Gamma_2}[N_2] = u_{\Gamma_3}[0] = u_{N_1 N_2}, \; u_{\Gamma_3}[N_1] = u_{\Gamma_4}[0] = u_{0 N_2}, \; u_{\Gamma_4}[N_2] = u_{\Gamma_1}[0] = u_{00}, \tag{48}$$

it follows that $u_\Gamma^{(e)}$ is indeed an embedding of u_Γ, and conversely, u_Γ is the restriction of $u_\Gamma^{(e)}$. Hence,

$$u_\Gamma^{(e)} = E u_\Gamma \tag{49}$$

in complete analogy with Remark 12. The reader is referred to [3] for the explicit matrix structure of $E \in \mathbb{R}^{2(N+2)\times 2N}$.

For arbitrary $2(N+2)$-dimensional grid vectors u_{Γ_+}, v_{Γ_+}, not necessarily subject to the constraints (48), we define the scalar product

$$\langle u, v \rangle_+ \equiv u_{\Gamma_+}^T H_\Gamma^{(+)} v_{\Gamma_+}^T,$$

where

$$H_\Gamma^{(+)} = \begin{pmatrix} H_1 & & & \\ & H_2 & & \\ & & J_1 H_1 J_1 & \\ & & & J_2 H_2 J_2 \end{pmatrix} \in \mathbb{R}^{2(N+2)\times 2(N+2)} \tag{50}$$

with H_i being one-dimensional norms and J_i anti-diagonal permutation matrices. Note that $H_\Gamma^{(+)}$ has the same structure as $H^{(+)}$ in (13). Following the same pattern as before, we define a scalar product on $\mathbb{R}^{2N} \times \mathbb{R}^{2N}$:

$$\langle u_\Gamma, v_\Gamma \rangle \equiv \left(u_\Gamma^{(e)}\right)^T H_\Gamma^{(+)} u_\Gamma^{(e)} = \left(Eu_\Gamma\right)^T H_\Gamma^{(+)} \left(Eu_\Gamma\right), \tag{51}$$

where we used (49). It follows immediately from the definition that $\langle \cdot, \cdot \rangle$ is a well-defined scalar product, cf. (19). In particular, for grid vectors given by (46) and (47):

$$\begin{aligned}\langle u_\Gamma, v_\Gamma \rangle &\equiv \langle u_{\Gamma_1}, v_{\Gamma_1} \rangle_1 + \langle u_{\Gamma_2}, v_{\Gamma_2} \rangle_2 + \langle u_{\Gamma_3}, v_{\Gamma_3} \rangle_3 + \langle u_{\Gamma_4}, v_{\Gamma_4} \rangle_4 \\ &= (u_0, v_0)_1 + (u^{N_1}, v^{N_1})_2 + (u_{N_2}, v_{N_2})_1 + (u^0, v^0)_2\end{aligned}$$

and thus $\langle 1, 1 \rangle = 4$ since $(1, 1)_i = 1$.

Definition 43. Let the inner product space V_Γ be a real vector space with the inner product

$$\langle \cdot, \cdot \rangle : V_\Gamma \times V_\Gamma \to \mathbb{R}$$

for all vectors $u_\Gamma, v_\Gamma \in V_\Gamma$ given by (47) and where $\langle \cdot, \cdot \rangle$ is defined in (51). □

Remark 44. Given Definition 43, Theorem 41 can be expressed as

$$\begin{aligned}(u, D_x v) &= \langle u, v \rangle_2 - \langle u, v \rangle_4 - (D_x u, v) \\ (u, D_y v) &= \langle u, v \rangle_3 - \langle u, v \rangle_1 - (D_y u, v),\end{aligned}$$

where we have dropped the subscripts of $u_{\Gamma_i}, v_{\Gamma_i}$ in the inner products $\langle \cdot, \cdot \rangle_i$ for each boundary segment Γ_i. The restriction of u and v to a particular boundary Γ_i is implied by the notation. □

5.4. Energy estimates

Consider the symmetric hyperbolic model equation in two space dimensions:

$$\begin{aligned}u_t + Au_x + Bu_y &= 0, \quad (x, y) \in \Omega, \quad t > 0 \\ u(x, y, 0) &= f(x, y)\end{aligned} \tag{52}$$

with characteristic boundary conditions

$$L_i u = \left(Q_I^{(i)} - S_i Q_{II}^{(i)}\right) u = 0, \quad (x, y) \in \Gamma_i, \quad t > 0. \tag{53}$$

The d by d matrices $Q^{(1)} = Q^{(3)}$ diagonalize $B^T = B$. Similarly, $Q^{(2)} = Q^{(4)}$ diagonalize $A^T = A$:

$$Q^{(2,4)} A \left[Q^{(2,4)}\right]^T = \Lambda_A, \quad Q^{(1,3)} B \left[Q^{(1,3)}\right]^T = \Lambda_B.$$

Q_I corresponds to the (locally) ingoing characteristics and Q_{II} to the outgoing ones.

The semidiscrete approximation of (52) is written as

$$\begin{aligned}v_t + P(AD_x + BD_y)Pv &= 0, \quad t > 0 \\ v(0) &= f, \quad f = Pf,\end{aligned} \tag{54}$$

where $A, B : V \to V$ are defined by

$$A \equiv \operatorname{diag}(A_{ij}), B \equiv \operatorname{diag}(B_{ij}) \in \mathbb{R}^{(N_1+1)(N_2+1)d \times (N_1+1)(N_2+1)d}$$

with $A_{ij} = A \in \mathbb{R}^{d \times d}$, $B_{ij} = B \in \mathbb{R}^{d \times d}$. We have deliberately used the same symbols for the coefficient matrices in the analytic and semidiscrete formulations. As usual,

$$P = I - L^+ L.$$

The boundary operator $L : V \to V_{\Gamma_+}$ is represented as a block matrix

$$L \equiv \begin{pmatrix} L_1 \\ L_2 \\ L_3 \\ L_4 \end{pmatrix}, \tag{55}$$

where L_i is the matrix representation of (53). As opposed to the traditional theory of boundary projections [2], it is not necessary to require that $L : V \to V_{\Gamma_+}$ have full rank thanks to the pseudoinverse formalism. Without proof we state the following

Proposition 45. *The semidiscrete system (54) - (55) is a strictly stable approximation of (52) - (53).*

Remark 46. Proposition 45 extends the results in [2] to general norms $H_i \in \mathbb{R}^{(N_i+1)\times(N_i+1)}$ in the presence of corners. Also, there is no need to require that L have full rank to prove strict stability. The reader is referred to [3] for a detailed proof. □

5.5. The simplified projection P revisited

Consider the semidiscrete approximation (54) of the two-dimensional hyperbolic system (52). The boundary conditions are expressed as

$$Lv = 0,$$

where L is defined by (55) and the matrix representation of (53). Let the scalar product in V be represented by

$$H = H_2 \otimes H_1;$$

H_1 and H_2 are restricted full norms. In [3] it is shown that

$$LH = \tilde{H} L,$$

where

$$\tilde{H} \equiv \begin{pmatrix} h_{00}^{(2)} H_1 & & & \\ & h_{N_1 N_1}^{(1)} H_2 & & \\ & & h_{N_2 N_2}^{(2)} H_1 & \\ & & & h_{00}^{(1)} H_2 \end{pmatrix}. \tag{56}$$

We then regard L as a mapping $L : V \to V_{\Gamma_+}$ with $H_\Gamma^{(+)}$ of (50) redefined so as to correspond to (56) Hence,

$$L^* = L^T$$

and thus

$$P = I - L^T \left[L L^T \right]^+ L,$$

completely analogous to the results of Section 4.3.

Remark 47. In Sections 5.4 and 5.5 it was assumed that L is a mapping $L : V \to V_{\Gamma_+}$ and not $L : V \to V_\Gamma$. The underlying Euclidean spaces of V_{Γ_+} and V_Γ are $\mathbb{R}^{2(N+2)d}$ and $\mathbb{R}^{2Nd}$. It is largely a matter of convenience which boundary state space to choose. Both lead to projection operators that satisfy

$$Pv = v, \quad HP = P^T H,$$

which is what the stability analysis requires. As a general rule, algebraic manipulation becomes easier if one chooses $L : V \to V_{\Gamma_+}$. In our case, all state vectors in V_{Γ_+} satisfy the constraints (48) by construction. The case $L : V \to V_\Gamma$ corresponds to redefining (55) to account for the corner points only once. □

6. Two space dimensions, multiblock case

The embedding operator $E : V \to V_+$ introduced in Section 2.5 played a crucial role when establishing difference operators $D : V \to V$ that satisfy summation by parts in a multiblock scenario. This was done by embedding a lower-dimensional vector space as a manifold in a higher-dimensional space. This technique will now be generalized to domains Ω in two space dimensions. We will restrict ourselves to the case where grid lines match at the subdomain interfaces. The proofs of the results in this section can be found in [3].

6.1. Two-block difference operators

Theorem 41 will be generalized to two-dimensional difference operators defined on $\Omega = \Omega_1 \cup \Omega_2$, $\Omega_1 = [0, 1/2] \times [0, 1]$, $\Omega_2 = [1/2, 1] \times [0, 1]$. The grid points are defined as

$$\Omega_1: \quad (x_i, y_j) = (ih_1^{(1)}, jh_2), \quad 0 \le i \le N_1^{(1)}, 0 \le j \le N_2$$
$$\Omega_2: \quad (x_i, y_j) = (0.5 + ih_1^{(2)}, jh_2), \quad 0 \le i \le N_1^{(2)}, 0 \le j \le N_2,$$

where the mesh sizes are defined as

$$h_1^{(i)} = \frac{1}{2N_1^{(i)}}, \ i = 1, 2, \quad h_2 = \frac{1}{N_2}.$$

It should be observed that the grid spacing in the y-dimension is assumed to be the same across the interface between Ω_1 and Ω_2. On each domain we define grid vectors (41), scalar products (43), (44) and difference operators (45):

$$\Omega_i: \quad u^{(i)}, v^{(i)}, \quad H^{(i)} = H_x^{(i)} H_y^{(i)}, \quad D_x^{(i)}, D_y^{(i)}.$$

Analogous to the one-dimensional case, cf. Remark 9, we define grid vectors on $\Omega_+ = \Omega_1 + \Omega_2$:

$$u^{(+)} \equiv \begin{pmatrix} u^{(1)} \\ u^{(2)} \end{pmatrix} \begin{matrix} r_1 \\ r_2 \end{matrix}, \quad v^{(+)} \equiv \begin{pmatrix} v^{(1)} \\ v^{(2)} \end{pmatrix} \begin{matrix} r_1 \\ r_2 \end{matrix}.$$

The augmented state space V_+ is defined exactly as in Definition 8, whence:

$$(u^{(+)}, v^{(+)})_+ = \left[u^{(+)}\right]^T H^{(+)} v^{(+)}, \quad H^{(+)} = \begin{pmatrix} \overset{c_1}{H^{(1)}} & \overset{c_2}{} \\ & H^{(2)} \end{pmatrix} \begin{matrix} r_1 \\ r_2 \end{matrix},$$

where

$$c_i = r_i = (N_1^{(i)} + 1)(N_2 + 1), \ i = 1, 2.$$

6.1.1. The embedding operator E_x

Let u, v be grid vectors on $\Omega = \Omega_1 \cup \Omega_2$ as defined in (41):

$$u, v \in \mathbb{R}^{(N_1+1)(N_2+1)}, \quad N_1 \equiv N_1^{(1)} + N_1^{(2)}.$$

Note that we traverse all of Ω horizontally and then vertically, that is

$$u_j, v_j \in \mathbb{R}^{N_1+1}, \quad j = 0, \dots, N_2.$$

As in Section 2.5, we define a mapping $E_x : \mathbb{R}^{(N_1+1)(N_2+1)} \to \mathbb{R}^{(N_1+2)(N_2+1)}$:

$$E_x = \begin{pmatrix} E_x^{(1)} \\ E_x^{(2)} \end{pmatrix}, \quad E_x^{(i)} \equiv I_2 \otimes E_1^{(i)}, \quad I_2 \in \mathbb{R}^{(N_2+1)\times(N_2+1)},$$

and where $E_1^{(1)}$ and $E_1^{(2)}$ are defined by (16), (17) replacing $N^{(1)} \to N_1^{(1)}$, $N^{(2)} \to N_1^{(2)}$ and $N \to N_1$, which reflects the fact that Ω_1 and Ω_2 are joined in the x-direction.

Define an inner product on $\mathbb{R}^{(N_1+1)(N_2+1)} \times \mathbb{R}^{(N_1+1)(N_2+1)}$:

$$(u, v)_H \equiv (E_x u)^T H^{(+)} E_x v \quad \Longleftrightarrow \quad H = E_x^T H^{(+)} E_x. \tag{57}$$

Definition 11 carries over with (19) replaced by (57). Hence, E_x is a mapping between two inner product spaces V and V_+, formally written as $E_x : V \to V_+$. The adjoint E_x^* is given by

$$E_x^* = H^{-1} E_x^T H^{(+)} \quad \Longrightarrow \quad E_x^* E_x = I.$$

The Moore-Penrose conditions thus imply that

$$E_x^+ = E_x^*$$

just like in the one-dimensional case.

6.1.2. Multiblock difference operators D_x and D_y

Similar to (23), define $D_x^{(+)}, D_y^{(+)} : V_+ \to V_+$:

$$D_x^{(+)} = \begin{pmatrix} \overset{c_1}{D_x^{(1)}} & \overset{c_2}{} \\ & D_x^{(2)} \end{pmatrix} \begin{matrix} r_1 \\ r_2 \end{matrix}, \quad D_y^{(+)} = \begin{pmatrix} \overset{c_1}{D_y^{(1)}} & \overset{c_2}{} \\ & D_y^{(2)} \end{pmatrix} \begin{matrix} r_1 \\ r_2 \end{matrix}.$$

Definition 48. Given the inner product space V with inner product (57), the difference operators $D_x, D_y : V \to V$ are defined as

$$D_x \equiv H^{-1} E_x^T H^{(+)} D_x^{(+)} E_x, \quad D_y \equiv H^{-1} E_x^T H^{(+)} D_y^{(+)} E_x. \quad \square$$

Without proof we state

Proposition 49. *Let $D_x, D_y : V \to V$ be as in Definition 48. Then*

(i) *D_x, D_y satisfy summation by parts with respect to the inner product (57):*

$$(u, D_x v) = \langle u, v\rangle_2 - \langle u, v\rangle_4 - (D_x u, v), \quad (u, D_y v) = \langle u, v\rangle_3 - \langle u, v\rangle_1 - (D_y u, v),$$

iff $H_2^{(1)} = H_2^{(2)} = H_2 \in \mathbb{R}^{(N_2+1)\times(N_2+1)}$, where the one-dimensional norm H_2 is that of (43); H_1 corresponds to (25).

(ii) *D_x, D_y are consistent approximations of $\partial/\partial x$ and $\partial/\partial y$.*

(iii) *$D_x = E_x^+ D_x^{(+)} E_x$ and $D_y = E_x^+ D_y^{(+)} E_x$.* $\square$

The reader is referred to [3] for details. See Remark 44 for notation.

6.1.3. Structure of H, D_x, D_y and E_x^*

We have gathered some results pertaining to the matrix representation of the operators H, D_x, D_y and E_x^*. The results are merely presented; no proof is given. Detailed derivations can be found in [3]

Proposition 50. *Let H be as in (57). If $H_2^{(1)} = H_2^{(2)} \equiv H_2$, then*

$$H = H_x H_y = H_y H_x, \quad H_x = I_2 \otimes H_1, \quad H_y = H_2 \otimes I_1,$$

where H_1 is the one-dimensional norm defined in (25). $\square$

Proposition 51. *Let D_x and D_y be as in Definition 48. If $D_2^{(1)} = D_2^{(2)} \equiv D_2$, then*

$$D_x = I_2 \otimes D_1, \quad D_y = D_2 \otimes I_1, \quad D_x H_y = H_y D_x, \quad D_y H_x = H_x D_y,$$

where D_1 is the one-dimensional difference operator defined in (24). $\square$

Proposition 52. *Let $E_x : V \to V_+$. Then*

$$E_x^+ = E_x^* = \left(I_2 \otimes \left[E_1^{(1)}\right]^* \; I_2 \otimes \left[E_1^{(2)}\right]^* \right). \quad \square$$

Remark 53. For restricted full norms $H_1^{(1)}$ and $H_1^{(2)}$ one has

$$\left[E_1^{(1)}\right]^* = \begin{pmatrix} \tilde{I}_1^{(1)} & 0 \\ 0 & \chi \\ 0 & 0 \end{pmatrix}, \quad \left[E_1^{(2)}\right]^* = \begin{pmatrix} 0 & 0 \\ 1-\chi & 0 \\ 0 & \tilde{I}_1^{(2)} \end{pmatrix},$$

in complete agreement with (27); $\tilde{I}_1^{(i)} \in \mathbb{R}^{N_1^{(i)} \times N_1^{(i)}}, i = 1, 2$. Hence, the adjoint of the embedding operator $E : V \to V_+$, can be viewed as an averaging operator. The one-dimensional expression (27) is formally recovered by setting $N_2 = 0$. But

$$\left[E_1^{(i)}\right]^* E_1^{(i)} \neq I_1^{(i)} \quad \Longrightarrow \quad \left[E_1^{(i)}\right]^+ \neq \left[E_1^{(i)}\right]^*.$$

As a final remark, it should be noted that D_1 is given by (28) if $H^{(i)}, i = 1, 2$, are restricted full norms. $\square$

We conclude the discussion on multiblocks by observing that partitioning Ω as $\Omega = \Omega_1 \cup \Omega_2$, $\Omega_1 = [0, 1] \times [0, 1/2]$, $\Omega_2 = [0, 1] \times [1/2, 1]$ will lead to completely analogous results. In the next section, we will present numerical results when splitting $\Omega = \cup_{ij} \Omega_{ij}$ horizontally and vertically into four subsquares. This example also involves curvilinear coordinates. The reader is referred to [3] for a detailed account.

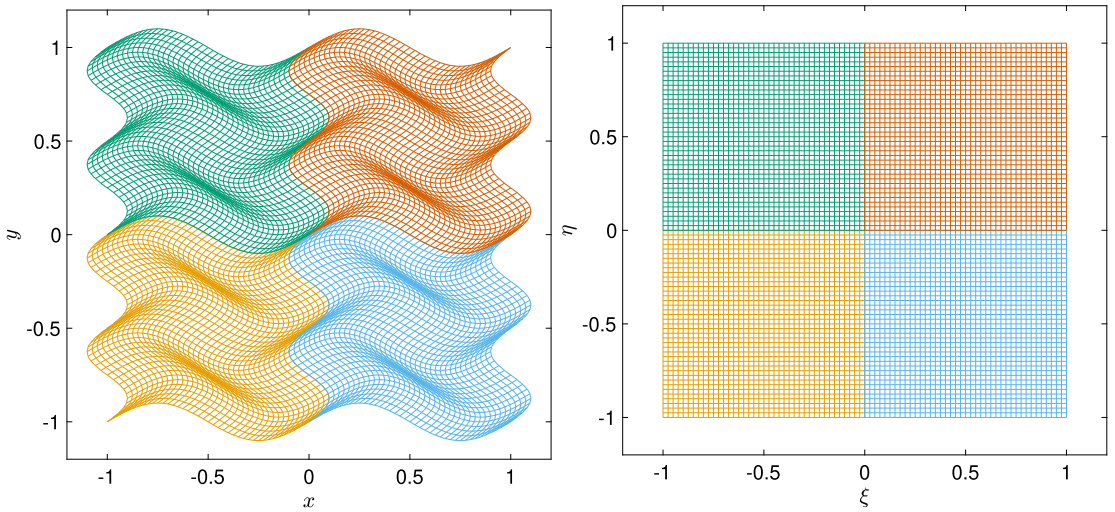

Fig. 2. Physical (left) and computational (right) domains.

7. Numerical results

We want to verify the embedding method by considering Maxwell's equations in two space dimensions:

$$\begin{aligned} Cu_t &= Au_x + Bu_y, \quad && x,y \in \Omega, \quad && t > 0 \\ H(x,y,t) &= g(x,y,t), && x,y \in \Gamma, && t \geq 0 \\ u(x,y,t) &= f(x,y), && x,y \in \Omega, && t = 0, \end{aligned}$$

where

$$u = \begin{pmatrix} E_x \\ H \\ E_y \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{and} \quad C = \begin{pmatrix} \epsilon & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & \epsilon \end{pmatrix}.$$

The solution vector u consists of the x and y components of the electric field $E_{x,y}$ (not to be confused with the embedding operators $E_{x,y}$) and the magnetic field H. The material parameters ϵ and μ will in general be space and time dependent functions but are considered constant in the following computations. As boundary conditions we specify the magnetic field at all boundaries. The spatial domain is $\Omega \subset \mathbb{R}^2$ and its boundary is denoted Γ.

To test the embedding method, we consider the multiblock curvilinear domain shown in Fig. 2. The physical domain is rectified using a reference domain $\Omega' = [-1,1] \times [-1,1]$, see Fig. 2, and a diffeomorphism $x = x(\xi,\eta)$ and $y = y(\xi,\eta)$, where $\xi, \eta \in \Omega'$. The state $u(x,y,t) \in \mathbb{R}^3$ is represented by

$$v(\xi,\eta,t) \equiv u(x(\xi,\eta), y(\xi,\eta), t)$$

Maxwell's equations are then cast into a form amenable to summation by parts for curvilinear domains, where we follow the approach in [1]:

$$\begin{aligned} Cu_t &= A\frac{1}{2}J^{-1}\left[(y_\eta u)_\xi + y_\eta u_\xi - (y_\xi u)_\eta - y_\xi u_\eta\right], \\ &\quad + B\frac{1}{2}J^{-1}\left[-(x_\eta u)_\xi - x_\eta u_\xi + (x_\xi u)_\eta + x_\xi u_\eta\right] && \xi,\eta \in \Omega', && t > 0 \\ H &= g(x(\xi,\eta), y(\xi,\eta), t), && \xi,\eta \in \Gamma', && t \geq 0 \\ u &= f(x(\xi,\eta), y(\xi,\eta)), && \xi,\eta \in \Omega', && t = 0. \end{aligned}$$

Note that $J = \xi_x\eta_y - \xi_y\eta_x$ in [1].

Define $D_{x,y} : V \to V$:

$$D_x \equiv \frac{1}{2}J^{-1}(Y_\eta D_\xi + D_\xi Y_\eta - Y_\xi D_\eta - D_\eta Y_\xi), \quad D_y \equiv \frac{1}{2}J^{-1}(X_\xi D_\eta + D_\eta X_\xi - X_\eta D_\xi - D_\xi X_\eta),$$

where X_ξ, X_η, Y_ξ, Y_η and J are diagonal matrices containing the metric coefficients; $D_{\xi,\eta}$ is shorthand for $D_{\xi,\eta} \otimes I$. They correspond to $D_{x,y}$ of Section 6.1.2 and share all structural results with $D_{x,y}$. Straightforward but somewhat tedious computations show that D_x and D_y satisfy summation by parts in the curvilinear domain $\Omega = \cup_{ij}\Omega_{ij}$ [3]. Let

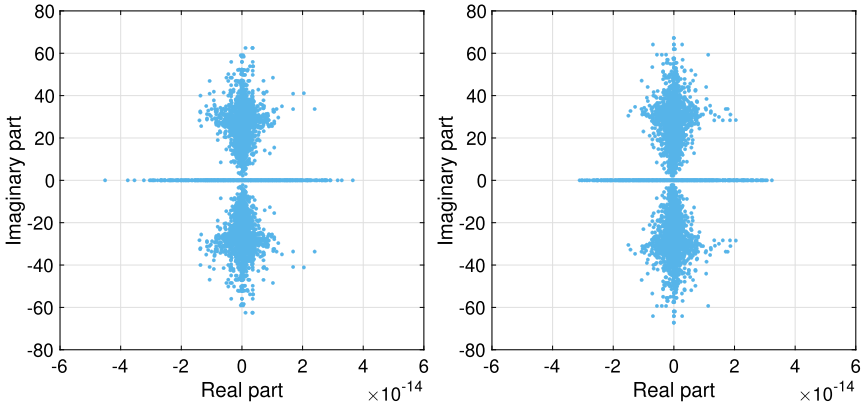

Fig. 3. Spectrum of Q for 4th (left) and 6th (right) order SBP operators.

$$A \equiv I \otimes \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \quad B \equiv I \otimes \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad C \equiv I \otimes \begin{pmatrix} \epsilon & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & \epsilon \end{pmatrix}, \quad I \in \mathbb{R}^{M \times M},$$

where $M = (N_1+1)^2, N_1 = 2N$ is the total number of grid points. The discrete boundary operator $L : V \to V_{\Gamma_+}$ is defined as in (55):

$$L \equiv \begin{pmatrix} L_1 \\ L_2 \\ L_3 \\ L_4 \end{pmatrix}, \qquad \begin{aligned} L_1 &= I_0 \otimes I \otimes L_0 \\ L_2 &= I \otimes I_{N_1} \otimes L_0 \\ L_3 &= I_{N_1} \otimes I \otimes L_0 \\ L_4 &= I \otimes I_0 \otimes L_0 \end{aligned}, \qquad L_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix};$$

I is the $(N_1+1)\times(N_1+1)$ identity matrix, I_{0,N_1} are the first and last and rows of I. The boundary conditions $Lv = g(t)$ are imposed using the simplified projection method (32). The resulting scheme is given by

$$\begin{aligned} w_t &= Qw + G(t), \quad t > 0, \\ w &= Pv_0, \qquad\quad t = 0, \end{aligned} \tag{58}$$

where

$$\begin{aligned} Q &= PC^{-1}\left(AD_x + BD_y\right)P, \\ G(t) &= PC^{-1}\left(AD_x + BD_y\right)L^+ g(t). \end{aligned}$$

The approximate solution v is obtained using (33):

$$v = w + L^+ g(t),$$

where we also used $Pw = w$. It is shown formally in [3] that (58) satisfies an energy estimate.

7.1. Numerical verification of stability and convergence

The stability of (58) can be verified numerically by studying the eigenvalues of Q. In Fig. 3 the real and imaginary eigenvalues are plotted with 41×41 points in each dimension, corresponding to a total of 5,043 degrees of freedom. Clearly, Q has only imaginary eigenvalues, which again indicates stability and energy conservation.

To evaluate the accuracy properties of the scheme, we use an analytical solution given by

$$E_x(x,y,t) = -\frac{4}{5}\cos(3x+4y-5t), \quad H(x,y,t) = \cos(3x+4y-5t), \quad E_y(x,y,t) = \frac{3}{5}\cos(3x+4y-5t), \tag{59}$$

which corresponds to choosing $\epsilon = 1/5$ and $\mu = 5$. The boundary and initial data are given by (59). The time stepping is done using the classical fourth order explicit Runge-Kutta method, with the time step given by $\Delta t = \frac{h_{\min}}{10}$ where $h_{\min}$ is the smallest spatial step size. This choice of time step ensures that the temporal error is negligible in relation to the spatial error. The error is measured in the discrete L^2-norm

$$e_{p,M} \equiv \|v - v_{\text{exact}}\| = \sqrt{(v - v_{\text{exact}})^T J H (v - v_{\text{exact}})}, \quad p = 2,4,6$$

at $t = 1$, and the convergence as

Table 1
Error (in base 10 logarithm) and convergence of Maxwell simulation with interface conditions imposed using the embedding method and 2nd, 4th, and 6th order SBP operators.

N	$\log_{10}(e_{2,M})$	q_2	$\log_{10}(e_{4,M})$	q_4	$\log_{10}(e_{6,M})$	q_6
40	-1.45	-	-2.15	-	-2.33	-
120	-2.39	1.99	-3.54	2.93	-4.15	3.85
200	-2.83	1.98	-4.20	2.97	-5.08	4.18
280	-3.11	1.98	-4.63	2.98	-5.69	4.16
360	-3.33	1.98	-4.96	2.98	-6.14	4.13
440	-3.50	1.98	-5.22	2.98	-6.49	4.10
520	-3.65	1.98	-5.43	2.98	-6.79	4.08
600	-3.77	1.98	-5.62	2.98	-7.04	4.06

$$q_p \equiv \frac{\log \frac{e_{p,M_1}}{e_{p,M_2}}}{\log \left(\frac{M_2}{M_1} \right)^{1/2}},$$

where the subscript p indicates the interior accuracy of the SBP operators.

In Table 1, the error and convergence for varying grid resolutions are presented for SBP operators of interior orders 2, 4, and 6. The boundary accuracies of the SBP operators are 1, 2, and 3. We see that for all operators the global convergence rate is one higher than the boundary accuracy, which is in accordance with the theoretical convergence analysis found in [19]. Python code to reproduce the results presented here can be found at https://github.com/guer7/sbp_embed.

8. Discussion and conclusion

In the present work, we have taken a vector space centric approach when discussing summation-by-parts operators and the implementation of analytic boundary conditions. The difference operators and boundary operators are regarded as mappings $D : V \to V$ and $L : V \to V_\Gamma$. The inner product of the state space V is given by the summation-by-parts norms H; the scalar product of the boundary state V_Γ is implicitly determined by H via summation by parts. With these definitions in place, it is possible to give a formal definition of the adjoint operators D^* and L^*, cf. (22).

We have also shown how the pseudoinverse of the boundary operator can be used to generalize the implementation of boundary conditions as a projection:

$$P = I - L^+ L.$$

The above expression is valid for *any* linear boundary operator L regardless of rank. This facilitates theoretical analysis in the presence of corners, which potentially may cause rank deficient, or near rank deficient, boundary operators. The projection P is not uniquely determined in general. We used this fact to our advantage to simplify the expression for L^+ as much as possible, see Section 4.2. It was shown that one can always choose $H_\Gamma = I$ when constructing the boundary projection. Under certain circumstances, the boundary projection is completely independent of H_Γ *and* H, cf. (36), thus extending the conclusions of [2] to the general, possibly rank deficient, case. The pseudoinverse provides a concise way of representing the boundary data $Lv = g$ as a state vector defined on Ω:

$$v = w + L^+ g,$$

where w solves the simplified semidiscrete equations (32).

The embedding operator E introduced in Section 2.5 provides a convenient mechanism for extending summation-by-parts operators defined in multiple domains to a single operator defined in the union of the individual domains. Given two difference operators $D^{(i)} : V_i \to V_i$, the resulting multidomain operator $D : V \to V$ can be expressed as

$$D = E^+ D^{(+)} E,$$

where the embedding $E : V \to V_+$ is defined in (15) - (17); E^+ is the pseudoinverse of E. The new operator D will inherit all properties of its constituent operators $D^{(1)}$ and $D^{(2)}$, most notably summation by parts and accuracy. We have also demonstrated how to construct embedding operators in two space dimensions. The results from the one-dimensional theory carry over verbatim. In summary, given $D^{(i)}, H^{(i)}, V_i$, the construction of the multidomain difference operator D follows the same pattern regardless of dimensionality:

1. Form the inner product $H^{(+)}$ in the extended state space V_+ using the inner products $H^{(i)}$ of the existing state spaces V_i.
2. Construct the embedding $E : V \to V_+$.
3. Define the scalar product in V as $H = E^T H^{(+)} E$.
4. Define the extended difference operator $D^{(+)} : V_+ \to V_+$.
5. Let $D : V \to V$ be defined as $D = E^+ D^{(+)} E$.

To illustrate the theory, we have implemented a test scenario involving the two-dimensional Maxwell's equations on four curvilinear domains, which are joined together using two-dimensional embedding operators E_x, E_y. The boundary conditions are implemented using a projection operator. The rate of convergence as measured for 2nd, 4th, and 6th-order accurate methods agrees very well with the theoretical convergence analysis.

The overarching goal of this work has been to lay the theoretical foundation for a "plug & play" methodology in which stability of the semidiscrete problem follows more or less directly from well-posedness of the analytic problem. As soon as the analytic boundary conditions are known, there is recipe for how to construct the corresponding projection, such that it leads to a stable approximation. Similarly, given the norms and difference operators $H^{(i)}, D^{(i)}$ that satisfy summation by parts on their respective domains Ω, we can construct

$$H = E^T H^{(+)} E, \quad D = E^+ D^{(+)} E,$$

such that D satisfies summation by parts on $\Omega = \cup_i \Omega_i$ with respect to H. In a future study we will extend this to more general domains and look deeper into algorithmic aspects, such as blocking and memory efficiency. The latter is important when solving large problems in a multithreaded environment.

CRediT authorship contribution statement

Pelle Olsson: Writing – review & editing, Writing – original draft, Methodology, Investigation, Formal analysis, Conceptualization. **Gustav Eriksson:** Writing – review & editing, Writing – original draft, Software, Methodology, Investigation, Formal analysis. **Ken Mattsson:** Writing – review & editing, Writing – original draft, Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors are indebted to Prof. Ken Kreutz-Delgado, Department of Electrical and Computer Engineering, UC San Diego, CA, for sharing his lecture notes for ECE 174, which offer the theoretical framework for implementing boundary conditions as pseudoinverses.

Gustav Eriksson was supported by the Swedish Research Council (grant 2021-05830 VR) and FORMAS (grant 2022-00843). Ken Mattsson was partially supported by the Swedish Research Council (grant 2021-05830 VR), and FORMAS (grant 2022-00843).

Appendix A. Notation

Table A.2
Notation.

Symbols	
Ω_i	1D or 2D Cartesian computational grid
Ω	$\cup_i \Omega_i$. Each point has multiplicity one
Ω_+	Multiset: $\sum_i \Omega_i$. Interface grid points have multiplicity two
Γ	Positively ordered boundary points. All grid points have multiplicity one
Γ_+	Multiset: Positively ordered boundary points. Corner points have multiplicity two
V_i	State space on Ω_i. Each grid point has single state. State vector: $u^{(i)}$
V	Solution state space on Ω. Each grid point has single state. State vector: u
V_+	Augmented state space on Ω_+. Interface points have two states. State vector $u^{(+)}$ obtained by stacking $u^{(i)}$ in a single vector
V_Γ	Boundary state space on Γ. All grid points have single state
V_{Γ_+}	Augmented boundary state space on Γ_+. Corner points have two states
E	One-to-one embedding $E : V \to V_+$: $u^{(e)} = Eu$. Element of u that corresponds to grid interface between two grids Ω_i will be mapped to two consecutive elements in $u^{(e)}$
$H^{(i)}, D^{(i)}$	Summation-by-parts pair (norm and difference operator) $H^{(i)}, D^{(i)} : V_i \to V_i$
$H^{(+)}, D^{(+)}$	Summation-by-parts pair: $H^{(+)}, D^{(+)} : V_+ \to V_+$ are obtained by stacking $H^{(i)}, D^{(i)}$ along the main diagonals
H	Resulting norm (inner product) in solution state space V: $H = E^T H^{(+)} E$
D	Resulting summation-by-parts operator $D : V \to V$: $D = E^+ D^{(+)} E$

Data availability

No data was used for the research described in the article.

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