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Abstract. The Peaceman–Rachford alternating direction implicit (ADI) method is considered for the time-integration of a class of wavetype equations for linear, isotropic materials on a tensorial domain, e.g., a cuboid in 3D or a rectangle in 2D. This method is known to be unconditionally stable and of classical order two. So far, it has been applied to specific problems and is mostly combined with finite differences in space, where it can be implemented at the cost of an explicit method.

In this paper, we consider the ADI method for a discontinuous Galerkin (dG) space discretization. We characterize a large class of first-order differential equations for which we show that on tensorial meshes, the method can be implemented with optimal (linear) complexity.

1 Introduction

In this paper, we investigate the efficiency of the Peaceman–Rachford scheme applied to a directional splitting for a central fluxes dG space discretization of the split operators. We characterize a class of wave-type problems for which we show that one timestep of the fully discrete scheme can be performed in linear complexity w.r.t. the total number of spatial degrees of freedom.

We start by providing definitions and results used to describe the aforementioned class of problems, which is then introduced in Section 2. In Section 3, we review the methods used for discretization and Section 4 is devoted to the efficiency of this discretization. Section 5 then provides some numerical tests to confirm the theoretical results.

Throughout the paper, we denote the ith canonical unit vector by e_i and the ith component of a vector v by v_i. By $(\cdot, \cdot)_S$, we denote the standard L^2 inner product over a set S and by δ_{ij} the Kronecker delta. Further, if S is a countable set, we denote the number of its elements by $|S|$.

1.1 Operators with decoupled partial derivatives

In order to characterize problems enabling splitting for which the Peaceman–Rachford method can be performed in linear complexity we start with some definitions.

Definition 1. Let $M_1, \ldots, M_d \in \mathbb{R}^{m \times m}$ be symmetric matrices and denote by $\mathcal{I}_i = \{j \in \{1, \ldots, m\} \mid M_i e_j \neq 0\}$ the set of indices of non-zero columns

(or rows) in M_i, $i = 1, \ldots, d$. Then we call $M_1, \ldots, M_d \in \mathbb{R}^{m \times m}$ *decoupled block-diagonal* if $\mathcal{I}_i \cap \mathcal{I}_j = \emptyset$ for all $i \neq j$.

Hence, d symmetric and decoupled block-diagonal matrices have pairwise disjoint non-zero rows and columns. The name decoupled block-diagonal is motivated by the following property.

Theorem 2. *Let $M_1, \ldots, M_d \in \mathbb{R}^{m \times m}$ be symmetric and decoupled block-diagonal. Then there is a permutation matrix $P \in \mathbb{R}^{m \times m}$ s.t. for all $i = 1, \ldots, d$, the matrix $P^T M_i P$ is block diagonal with at most one non-zero diagonal block which vanishes in all other matrices $P^T M_j P$, $j \neq i$.*

Proof. The assertion follows from the symmetry of the matrices M_i if we reorder the rows and columns by the indices in $\mathcal{I}_1$, then $\mathcal{I}_2, \ldots, \mathcal{I}_d$, and last the indices of those columns which vanish in all matrices. $\qquad\square$

Using this notion, we characterize first order differential operators, whose partial derivatives completely decouple.

Definition 3. Let $M = \sum_{i=1}^{d} M_i \partial_i$ be a first order differential operator with symmetric matrics $M_i \in \mathbb{R}^{m \times m}$, $i = 1, \ldots, d$. We say that M *has decoupled partial derivatives* if $M_1, \ldots, M_d$ are decoupled block-diagonal.

2   Framework

Let $\Omega \subset \mathbb{R}^d$ be a bounded paraxial tensorial domain with boundary $\partial\Omega$ and let n be the outer unit normal on $\partial\Omega$. Further, let $L = \sum_{i=1}^{d} L_i \partial_i$, $A = \sum_{i=1}^{d} A_i \partial_i$, $B = \sum_{i=1}^{d} B_i \partial_i$, with symmetric matrices $L_i, A_i, B_i \in \mathbb{R}^{m \times m}$. We consider homogeneous first order wave-type equations of the form

$$\partial_t u(t) = Lu(t) = (A + B)u(t), \qquad t \in [0, T], \qquad u(0) = u^0, \qquad (1)$$

where A and B have decoupled partial derivatives.

This class of problems includes, e.g., advection and wave equations in 2D and Maxwell's equations in 3D. These examples are given as follows.

2D advection equation Here, we have $m = 1$, $L_i = \alpha_i$ for $i = 1, 2$ with the advection velocity vector α. We consider homogeneous inflow boundary conditions, i.e., $u(t) = 0$ on the inflow boundary $\partial\Omega^- = \{\, x \in \partial\Omega \mid \alpha \cdot n < 0 \,\}$. The split operators are given by $A_1 = \alpha_1$, $A_2 = 0$ and $B_1 = 0$, $B_2 = \alpha_2$ and the boundary conditions are given by $n_1 u(t) = 0$ on $\partial\Omega^-$ for A and $n_2 u(t) = 0$ on $\partial\Omega^-$ for B, respectively

2D wave equation Here, we have $m = 3$ and

$$u = \begin{pmatrix} p \\ q_1 \\ q_2 \end{pmatrix}, \quad L_1 = e_1 e_2^T + e_2 e_1^T.$$

We consider homogeneous Dirichlet boundary conditions, i.e., $p(t) = 0$ on $\partial\Omega$. The split operators are given by $A_1 = L_1$, $A_2 = 0$ and $B_1 = 0$, $B_2 = L_2$ with boundary conditions given by $n_1 p(t) = 0$ on $\partial\Omega$ for A and $n_2 p(t) = 0$ on $\partial\Omega$ for B, respectively.

3D Maxwell's equations Here, we have $m = 6$ and

$$u = \begin{pmatrix} E \\ H \end{pmatrix}, \quad L_i = \begin{pmatrix} 0 & \tilde{L}_i^T \\ \tilde{L}_i & 0 \end{pmatrix},$$

where $\tilde{L}_1 = e_2 e_3^T - e_3 e_2^T$, $\tilde{L}_2 = e_3 e_1^T - e_1 e_3^T$ and $\tilde{L}_3 = e_1 e_2^T - e_2 e_1^T$. We consider perfectly conducting boundary conditions, i.e., $\sum_{i=1}^{3} \tilde{L}_i n_i E = 0$ on $\partial\Omega$. The split operators are given by (cf. [5,7])

$$A_i = \begin{pmatrix} 0 & \tilde{A}_i^T \\ \tilde{A}_i & 0 \end{pmatrix}, \quad B_i = \begin{pmatrix} 0 & \tilde{B}_i^T \\ \tilde{B}_i & 0 \end{pmatrix}$$

with $\tilde{A}_1 = -\tilde{B}_1^T = e_2 e_3^T$ $\tilde{A}_2 = -\tilde{B}_2^T = e_3 e_1^T$ $\tilde{A}_3 = -\tilde{B}_3^T = e_1 e_2^T$ and we subject A to $\sum_{i=1}^{3} \tilde{A}_i n_i E = 0$ and B to $\sum_{i=1}^{3} \tilde{B}_i n_i E = 0$ on $\partial\Omega$.

Remark 4. For ease of presentation, we omit material parameters in this paper. However, in the case of isotropic materials, all statements apply with only minor changes: the operator $D^{-1}L$ with $D = \text{diag}(\delta_1, \ldots, \delta_m)$, $\delta_1, \ldots, \delta_m \in L^\infty(\Omega)$, takes over the role of L (and analogously for A and B) and the average in the dG-discretization (see below) is replaced by a weighted average, taking possible jumps in the material parameters into account. Because of the diagonal structure of D, no further coupling is introduced, and the efficiency analysis can be performed completely analogously.

3 Discretization

In this section, we review the Peaceman–Rachford scheme for the temporal discretization [6] and the central flux discontinuous Galerkin (dG) scheme [2,3] used for the spatial discretization.

3.1 Temporal discretization

The Peaceman–Rachford scheme [6] applied to (1) reads

$$(I - \tfrac{\tau}{2} A) u^{n+1/2} = (I + \tfrac{\tau}{2} B) u^n,$$
$$(I - \tfrac{\tau}{2} B) u^{n+1} = (I + \tfrac{\tau}{2} A) u^{n+1/2}.$$

This scheme is of (classical) order two and unconditionally stable if A and B are dissipative operators (see e.g., [4]). It requires the solution of two linear systems whose coefficient matrices are given by the spatially discrete counterparts of $I - \frac{\tau}{2}A$ or $I - \frac{\tau}{2}B$. However, if the operators A and B have decoupled partial derivatives (cf. Definition 3), we will show that this can be achieved in optimal (linear) complexity w.r.t. the total number of degrees of freedom.

3.2   Spatial discretization

We use a central flux dG method to discretize the split differential operators in space [2,3]. For this, we equip Ω with a mesh $\mathcal{T} = \{K\}$ consisting of paraxial tensor-structured elements. We gather the faces of $\mathcal{T}$ in the set $\mathcal{F} = \{F\}$, which is further decomposed into the set of interior faces $\mathcal{F}^{\text{int}}$ and the set of boundary faces $\mathcal{F}^{\text{bnd}}$.

Due to the tensorial structure of the mesh, normal vectors to the faces in $\mathcal{F}$ are $\pm e_j$ for some $j \in \{1, \dots, d\}$. For $F \in \mathcal{F}$ we denote the unit normal vector to F in positive coordinate direction by n^F. Hence, we have

$$\mathcal{F}^\alpha = \dot{\bigcup}_{i=1}^d \mathcal{F}^{\alpha,i}, \qquad \mathcal{F}^{\alpha,i} = \{\, F \in \mathcal{F}^\alpha \mid n^F = e_i \,\}, \qquad \alpha \in \{\, \text{int}, \text{ext} \,\}, \quad (2)$$

where $\mathcal{F}^{\alpha,i}$ are the sets of faces with normals pointing in the ith direction. For each interior face $F \in \mathcal{F}^{\text{int}}$, we additionally denote the two elements containing F as K_1^F and K_2^F, where the numbering is done s.t. n^F is the outer normal to K_1^F.

To approximate functions in space, we use the broken polynomial space

$$V_h = \{\, v \in L^2(\Omega) \mid v|_K \in \mathbb{P}_k \text{ for all } K \in \mathcal{T} \,\}, \qquad (3)$$

where $\mathbb{P}_k$ denotes the set of polynomials of degree at most k in each variable. We could also allow the polynomial degree k to depend on K, but for the sake of presentation we do not pursue this further in this paper. For the efficiency analysis, we consider the basis

$$\mathcal{V}_h = \bigcup_{K \in \mathcal{T}} \{\, \phi_1^K, \dots, \phi_{N_k}^K \,\}$$

of V_h, where $\text{supp}(\phi_i^K) \subset K$ for $i = 1, \dots, N_k$, e.g., a standard discontinuous Lagrange basis. Since functions in the space V_h may be discontinuous across the faces of the mesh, we define the average and the jump of a (possibly vector-valued) function v over an interior face $F \in \mathcal{F}^{\text{int}}$ as

$$\{\!\{v\}\!\}_F = \frac{(v|_{K_1^F})|_F + (v|_{K_2^F})|_F}{2}, \qquad [\![v]\!]_F = (v|_{K_1^F})|_F - (v|_{K_2^F})|_F.$$

Note that the only change for isotropic materials is to replace the average by a weighted one, taking the material parameters into account.

Let $u_h, \varphi_h \in V_h$. We define the central flux dG-discretization $\partial_{i,h}$ of ∂_i as

$$
\begin{aligned}
(\partial_{i,h} u_h, \varphi_h)_\Omega &= \sum_{K \in \mathcal{T}} (\partial_i u_h, \varphi_h)_K - \sum_{F \in \mathcal{F}^{\mathrm{int}}} (n_i^F [\![u_h]\!]_F, \{\!\{ \varphi_h \}\!\}_F)_F \\
&= \sum_{K \in \mathcal{T}} (\partial_i u_h, \varphi_h)_K - \sum_{F \in \mathcal{F}^{\mathrm{int},i}} ([\![u_h]\!]_F, \{\!\{ \varphi_h \}\!\}_F)_F,
\end{aligned}
\tag{4}
$$

where the second equality follows by the definition of $\mathcal{F}^{\mathrm{int},i}$ in (2). With this, we define the dG-discretization of the split operators for $u_h, \varphi_h \in V_h^m$ as

$$
\begin{aligned}
(A_h u_h, \varphi_h)_\Omega &= \sum_{i=1}^{d} (A_i \partial_{i,h} u_h, \varphi_h)_\Omega - b_A(u_h, \varphi_h), \\
(B_h u_h, \varphi_h)_\Omega &= \sum_{i=1}^{d} (B_i \partial_{i,h} u_h, \varphi_h)_\Omega - b_B(u_h, \varphi_h),
\end{aligned}
\tag{5}
$$

where $\partial_{i,h}$ is meant to act componentwise and b_A, b_B model the boundary conditions of the corresponding operators, respectively. The concrete boundary terms for the examples in Section 2 are as follows.

2D advection equation (homogeneous inflow boundary conditions) For $u_h, \varphi_h \in V_h$, we have

$$
b_A(u_h, \varphi_h) = \sum_{F \in \mathcal{F}_-^{\mathrm{bnd},1}} (\alpha_1 u_h, \varphi_h)_F, \qquad b_B(u_h, \varphi_h) = \sum_{F \in \mathcal{F}_-^{\mathrm{bnd},2}} (\alpha_2 u_h, \varphi_h)_F,
$$

where $F \in \mathcal{F}_-^{\mathrm{bnd},i} = \{ F \in \mathcal{F}^{\mathrm{bnd},i} \mid F \cap \partial\Omega^- \neq \emptyset \}$.

2D wave equation (homogeneous Dirichlet boundary conditions) For $u_h = (p_h, q_{1,h}, q_{2,h})^T, \varphi_h = (\phi_h, \psi_{1,h}, \psi_{2,h})^T \in V_h^3$, we have

$$
b_A(u_h, \varphi_h) = \sum_{F \in \mathcal{F}^{\mathrm{bnd},1}} (p_h, \psi_{1,h})_F, \qquad b_B(u_h, \varphi_h) = \sum_{F \in \mathcal{F}^{\mathrm{bnd},2}} (p_h, \psi_{2,h})_F.
$$

3D Maxwell's equations (perfectly conducting boundary conditions) For $u_h = (E_h^T, H_h^T)^T, \varphi_h = (\Phi_h^T, \Psi_h^T)^T \in V_h^6$, we have

$$
b_A(u_h, \varphi_h) = \sum_{i=1}^{3} \sum_{F \in \mathcal{F}^{\mathrm{bnd},i}} (\tilde{A}_i E_h, \Psi_h)_F,
$$

$$
b_B(u_h, \varphi_h) = \sum_{i=1}^{3} \sum_{F \in \mathcal{F}^{\mathrm{bnd},i}} (\tilde{B}_i E_h, \Psi_h)_F.
$$

4   Efficiency

In this section, we investigate the efficiency of the Peaceman–Rachford dG scheme, which is mainly determined by the cost to solve linear systems involving the discrete counterparts of $I - \frac{\tau}{2} A$ and $I - \frac{\tau}{2} B$, respectively. We show that, using a suitable ordering of the degrees of freedom, the corresponding matrices have block-tridiagonal structure, where the block-sizes only depends on the polynomial degree k and the number of indices in the corresponding set $\mathcal{I}_i$, but is independent of the total number of degrees of freedom. Hence, the corresponding systems can be solved in linear time.

The mass matrix resulting from the discretization of I is block-diagonal if the degrees of freedom are ordered elementwise, which is well-known for dG-methods. Hence, it suffices to investigate the non-zero patterns of the matrices corrsponding to A_h and B_h, respectively. As these are defined in terms of the discrete partial derivatives $\partial_{i,h}$, $i = 1, \ldots, d$, we begin by investigating them.

4.1   Structure of $\partial_{i,h}$

To investigate the non-zero pattern of the discrete partial derivatives, we insert the basis functions in $\mathcal{V}_h$ into the bilinear form (4). For $K_1 \neq K_2$, we have

$$\sum_{K \in \mathcal{T}} (\partial_i \phi_j^{K_1}, \phi_\ell^{K_2})_K = 0, \quad j, \ell = 1, \ldots, N_k,$$

since $\mathrm{supp}(\phi_i^K) \subset K$. Hence, if we order the basis functions elementwise, these terms only contribute to the blockdiagonal with block-width N_k.

For the sum over the interfaces, we obtain contributions outside of the blockdiagonal. However, for $F \not\subset \partial K$, we have

$$\{\!\!\{ \phi_j^K \}\!\!\}_F = 0, \quad [\![\phi_j^K]\!]_F = 0.$$

Hence, for K_1 and K_2 with $K_1 \cap K_2 \notin \mathcal{F}^{\mathrm{int},i}$, i.e., K_1 and K_2 not sharing a common face with normal in the ith direction, it holds

$$\sum_{F \in \mathcal{F}^{\mathrm{int},i}} ([\![\phi_j^{K_1}]\!]_F, \{\!\!\{ \phi_\ell^{K_2} \}\!\!\}_F)_F = 0, \quad j, \ell = 1, \ldots, N_k.$$

Thus, these terms only contribute to off-blockdiagonal entries if the corresponding basis functions are non-zero on elements sharing such a face. If we, in addition to ordering the degrees of freedom elementwise, order the elements of the mesh along these normal vectors, the only additional entries appear in the first sub- and super-blockdiagonals. Altogether, with this ordering of the degrees of freedom, the discretized partial derivative $\partial_{i,h}$ is represented by a block-tridiagonal matrix.

Remark 5. Note that the tensorial structure of the mesh is indispensable. Otherwise, the normal vectors have multiple non-zero entries, resulting in coupling between neighbouring elements w.r.t. more than one face.

If, in addition, we use a product basis for the space V_h and if the material parameters have product structure as well, the resulting matrices even have a Kronecker-product structure. This can be exploited to further speed up the solution of the linear systems in each step.

4.2   Structure of the discrete split operators

To investigate the non-zero pattern of the discrete split operators, we insert the basis functions in $\mathcal{V}_h^m$ into the bilinear forms (5). We only consider A_h, since for B_h one can proceed completely analogously.

According to the ordering from Definition 1 corresponding to A, we decompose the basis $\mathcal{V}_h^m$ into $\mathcal{V}_h^m = \dot{\bigcup}_{i=1}^d \mathcal{V}_{h,i}^m$, where

$$\mathcal{V}_{h,i}^m = \dot{\bigcup}_{j \in \mathcal{I}_i} \{\, \phi\, e_j \mid \phi \in \mathcal{V}_h \,\}.$$

For $\psi_i \in \mathcal{V}_{h,i}^m$ and $\psi_j \in \mathcal{V}_{h,j}^m$, there exist $\ell_1 \in \mathcal{I}_i, \ell_2 \in \mathcal{I}_j$ and $\phi_1, \phi_2 \in \mathcal{V}_h$ s.t. $\psi_i = \phi_1 e_{\ell_1}$, $\psi_j = \phi_2 e_{\ell_2}$. This implies

$$\sum_{r=1}^d (A_r \partial_{r,h} \psi_i, \psi_j)_\Omega = \sum_{r=1}^d e_{\ell_2}^T A_r e_{\ell_1} (\partial_{r,h} \phi_1, \phi_2)_\Omega = \delta_{ij} e_{\ell_2}^T A_i e_{\ell_1} (\partial_{i,h} \phi_1, \phi_2)_\Omega,$$

where the last equality follows as a consequence of Theorem 2, since $A_1, \dots, A_d$ are symmetric and decoupled block diagonal. Hence, basis functions belonging to different $\mathcal{V}_{h,i}^m$, $i = 1, \dots, d$ completely decouple. By ordering the basis functions according to these sets, we thus obtain (up to) d diagonal blocks. The structure of these blocks is determined by the structure of $(\partial_{i,h} \phi_1, \phi_2)$, which was analyzed in Section 4.1. Therefore, by ordering the elements, and thus the basis functions in $\mathcal{V}_{h,i}^m$ belonging to them, according to the applied partial derivative, we obtain a block-tridiagonal structure for each $i = 1, \dots, d$ and thus globally, since these blocks decouple. However, in contrast to Section 4.1 the block-size is $|\mathcal{I}_i| N_k$, $i = 1, \dots, d$, since per element we have N_k basis functions for each index in $\mathcal{I}_i$ which are coupled through A_i.

For the boundary conditions used in the examples above, no further coupling is introduced by the boundary terms b_A and b_B, respectively. This can be seen with a similar argument as for the interfaces. Hence, these terms do not change the block-tridiagonal structure.

5   Numerical Results

We implemented the method in `deal.ii` [1] for Maxwell's equations to verify the theoretical results. Upon request, the code to perform these experiments will be provided.

Fig. 1. Runtimes of the ADI and the Verlet method (including assembling of the matrices). Computations are carried out on 14 uniform grids ranging from 6 to 32 elements per unit length with polynomial degree $k = 1$ on the grid elements. Time stepsize is $\tau = 0.01$ and 200 steps are performed.
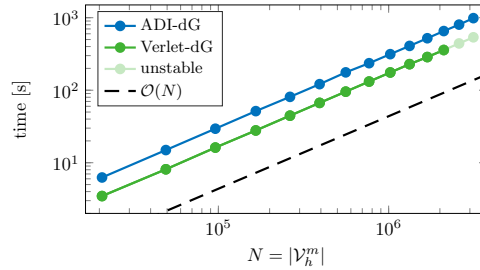
The computational domain is $\Omega = [0,2] \times [0,1]^2$ with material parameters chosen to be constant. For the solution of the linear systems in each timestep, a standard UMFPACK solver is used. For comparison, runtimes of the explicit Verlet or leap-frog method with the same configurations are shown.

The runtimes illustrated in Fig. 1 clearly show that the method takes only about 1.8 times longer than the explicit Verlet method, which is unstable on the two finest meshes. A rigorous error analysis showing temporal order two independent of the spatial mesh will be presented in a separate paper.

Acknowledgments

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