

Efficient higher-order local time integration for Friedrichs' systems*

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In this paper, we construct an efficient higher-order local time integration scheme for spatially discretized linear Friedrichs' systems. In particular, our interest is in problems where only a few of the mesh elements are small while the majority of the elements is much larger. The special combination of two methods like the leapfrog method on the coarse part of the mesh and the Crank-Nicolson method on the fine part as was done in [33, 28] is not suitable for higher-order time integration. Therefore, we suggest to approximate the solution of the linear systems arising in each time step by a preconditioned Krylov subspace method, e.g., the quasi-minimal residual method by Freund and Nachtigal [19]. The techniques developed here for linear problems also carry over to nonlinear problems, where linear systems of the same type arise within a Newton-type iteration.

Motivated by the analysis of locally implicit methods by Hochbruck and Sturm [33], we show how to construct a preconditioner in such a way that the number of iterations required by the Krylov subspace method to achieve a certain accuracy is bounded independently of the diameter of the small mesh elements. We prove this behavior by using Faber polynomials and complex approximation theory.

The cost to apply the preconditioner consists of the solution of a small linear system, whose dimension corresponds to the degrees of freedom within the fine part of the mesh (and its next coarse neighbors). If this dimension is small compared to the size of the full mesh, the preconditioner is very efficient.

We conclude by verifying our theoretical results with numerical experiments for the fourth-order Gauß-Legendre Runge-Kutta method.

Key words. local time-integration, Friedrichs' system, higher-order method, discontinuous Galerkin method, Krylov subspace methods, error analysis

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1 Introduction

Friedrichs' systems play a crucial role in the modeling of various physical phenomena. Important examples are advection equations, acoustic wave equations, Maxwell's equations, and Dirac

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equations; see [13] for more details. Though finite difference time-domain methods [41] are still predominantly utilized to solve Maxwell’s equations, numerous other methods based on finite element or finite volume space discretizations have been introduced and are gaining more and more importance.

The numerical solution of time-dependent partial differential equations by a method of lines approach involves first discretizing in space and then integrating the semi-discrete system in time. For the space discretization, discontinuous Galerkin (dG) methods (see [11] and references therein) are popular due to their flexibility in treating complex geometries and discontinuous material parameters. Since dG methods lead to block-diagonal mass matrices, explicit time integration schemes can be implemented very efficiently. Unfortunately, explicit time integration methods are subject to the Courant–Friedrichs–Lewy (CFL) condition depending on the minimum diameter of all mesh elements, denoted by $h_{\min}$, that is, the time step τ needs to satisfy $\tau \lesssim h_{\min}$. Here, we are interested in locally refined meshes, where most of the mesh elements are coarse but a very small number of mesh elements are fine. The latter require very small time steps on all mesh elements, which makes the computation inefficient. An alternative is to use implicit time integrators which can eliminate the CFL condition completely but require solving a large linear system of equations in all degrees of freedom at each time step. Unfortunately, this is expensive and might not even be feasible for large 3D problems.

To tackle this problem, locally implicit (LI) methods [40, 9, 33, 7, 10, 34] and local time-stepping (LTS) methods [37, 12, 22, 21] or more general local time integrators (LTI) from our previous work [32] were introduced and studied. While there is a rigorous analysis of LTI methods of order two for linear problems, it is not clear how to prove the stability for higher-order LTI methods constructed via composition methods [24, Section II.4].

In this paper, we introduce a new strategy to develop a higher-order time integration method to solve the general class of linear Friedrichs’ systems possessing a two-field structure on a locally refined spatial grid in a computationally efficient way. For the time integration, we propose to use higher-order implicit Gauß collocation methods [25, Sec. IV.5]. It is well known that these methods are A-stable and symplectic, and have maximum order $2s$ for nonstiff problems. Moreover, for all s , rigorous error bounds are available for a class of problems which includes Friedrichs’ systems, cf. [31, Section 3.1]. This makes them the ideal candidates for our applications. Unfortunately, the analysis only holds for Runge-Kutta methods which are not only A-stable but also algebraically stable and coercive, properties which are not satisfied for general implicit methods such as the computationally attractive DIRK methods.

The drawback of implicit schemes is that one has to solve large linear systems of equations in each time step. For this, iterative solvers, especially (preconditioned) Krylov subspace methods, are popular choices; see [38] and references therein. For instance, block preconditioners for structure-preserving discretizations of Maxwell’s equations were proposed in [36, 1]. Other popular preconditioners include those based on multigrid [26, 4, 3] and Schwarz domain decomposition [5, 39]. However, these preconditioning techniques have not yet been adapted to locally refined meshes.

We show that the linear systems of equations which arise in the implementation of Gauß Runge-Kutta methods for linear Friedrichs’ systems can be transformed using techniques from [25, Sec. IV.5] in such a way that we obtain an equivalent linear system with a complex symmetric coefficient matrix. Thus, we use the quasi-minimal residual (QMR) method to solve it iteratively [16, 19, 20]. Our main contribution is to construct a suitable preconditioner for the QMR method and to prove that the number of iterations required to reach a certain accuracy is independent of the fine mesh. Roughly speaking, this preconditioner only acts on the fine mesh and is thus very efficient if the number of fine mesh elements is small compared to the total degrees of freedom. Hence, the overall algorithm is unconditionally stable, obeys rigorous error bounds which do not deteriorate under mesh refinement, and has linear complexity with a constant that only depends

on the coarse mesh.

The paper is organized as follows. In Section 2, we present our model problem and notation, and recall properties of the spatial discretization of Friedrichs' systems using discontinuous Galerkin methods with central fluxes. Section 3 is dedicated to higher-order implicit Runge-Kutta methods. In Section 4, we recall known results on Krylov subspace methods, in particular error bounds. Our main contribution is to prove that the field of values of the preconditioned matrix is independent of the fine mesh and to combine this with error bounds for Krylov subspace methods. Finally, in Section 5, we verify our theoretical findings with numerical experiments and compare the efficiency of the higher-order locally implicit method with other local time integration schemes [33, 32] and a low-storage Runge-Kutta method [35].

2 Problem setting

Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, be an open, polygonal domain. The linear Friedrichs' system in a two field formulation reads

$$\partial_t u = \mathcal{L}_v v + g_u, \quad \Omega \times \mathbb{R}_+, \quad (2.1a)$$

$$\partial_t v = \mathcal{L}_u u + g_v, \quad \Omega \times \mathbb{R}_+, \quad (2.1b)$$

$$u(0) = u^0, \quad v(0) = v^0, \quad \Omega, \quad (2.1c)$$

where ∂_t denotes the partial derivative with respect to time and $g_u: \mathbb{R}_+ \rightarrow L^2(\Omega)^{m_u}$, $g_v: \mathbb{R}_+ \rightarrow L^2(\Omega)^{m_v}$ are forcing terms. The Friedrichs' operators $\mathcal{L}_u$ and $\mathcal{L}_v$ are defined by

$$\mathcal{M}_v \mathcal{L}_u u = \sum_{i=1}^d L_i \partial_i u, \quad \mathcal{M}_u \mathcal{L}_v v = \sum_{i=1}^d L_i^T \partial_i v, \quad (2.2)$$

with coefficients $L_i \in \mathbb{R}^{m_v \times m_u}$ for $i = 0, \dots, d$. Here ∂_i denotes the partial derivative with respect to the i th spatial variable. The material tensors $\mathcal{M}_u \in L^\infty(\Omega)^{m_u \times m_u}$, $\mathcal{M}_v \in L^\infty(\Omega)^{m_v \times m_v}$ are assumed to be symmetric and uniformly positive definite, and by $m_u, m_v \in \mathbb{N}$ we count the components of u and v . To make the system (2.1) well-posed we have to prescribe boundary conditions. These are embodied into the domains $\mathcal{D}(\mathcal{L}_u)$ and $\mathcal{D}(\mathcal{L}_v)$, see [11, 13] for details. We assume that the boundary conditions do not introduce damping, cf. [13, Assump. 11.8], which leads to the adjointness property

$$(\mathcal{L}_u u, v)_\Omega = -(u, \mathcal{L}_v v)_\Omega \quad \text{for all } u \in \mathcal{D}(\mathcal{L}_u), v \in \mathcal{D}(\mathcal{L}_v), \quad (2.3)$$

in the weighted L^2 inner products defined via

$$(u, \tilde{u})_\Omega = (\mathcal{M}_u u, \tilde{u})_{L^2(\Omega)}, \quad u, \tilde{u} \in L^2(\Omega)^{m_u}. \quad (2.4)$$

The corresponding norm is denoted by $\|\cdot\|_\Omega$. The inner product weighted by $\mathcal{M}_v$ is defined analogously, and it is always clear from the inserted argument which inner product or norm is meant.

For a full discretization of (2.1), we first discretize in space using a dG method with central fluxes on a suitable mesh $\mathcal{T}_h$ [11], [27, Section 4]. On this mesh we define the spaces

$$\mathbb{V}_h^u = \{u \in L^2(\Omega) \mid u|_K \in \mathbb{P}_d^k(K) \text{ for all } K \in \mathcal{T}_h\}^{m_u}, \quad (2.5a)$$

$$\mathbb{V}_h^v = \{v \in L^2(\Omega) \mid v|_K \in \mathbb{P}_d^k(K) \text{ for all } K \in \mathcal{T}_h\}^{m_v}, \quad (2.5b)$$

consisting of functions in $L^2(\Omega)$ which are polynomials of total degree at most k on each mesh element. If it is clear by context which space we mean, we simply write $\mathbb{V}_h$. The dG method then yields

$$\partial_t u_h = \mathcal{L}_{v,h} v_h + g_{u,h}, \quad \mathbb{R}_+, \quad (2.6a)$$

$$\partial_t v_h = \mathcal{L}_{u,h} u_h + g_{v,h}, \quad \mathbb{R}_+, \quad (2.6b)$$

$$u_h(0) = u_h^0, \quad v_h(0) = v_h^0, \quad (2.6c)$$

where $\mathcal{L}_{u,h}$ and $\mathcal{L}_{v,h}$ are spatially discretized Friedrichs' operators, and u_h^0, v_h^0 , and $g_{u,h}, g_{v,h}$ are L^2 projections of u^0, v^0 and g_u, g_v respectively, onto $\mathbb{V}_h^u, \mathbb{V}_h^v$ with respect to the weighted inner products defined in (2.4). We refer to [11, 27] for details on the dG discretization.

For $w \in \{u, v\}$, let $\{\phi_1^w, \dots, \phi_{N_w}^w\}$ be a basis of $\mathbb{V}_h^w$. Then an element $x_h: (0, T) \rightarrow \mathbb{V}_h^w$ can be represented as

$$x_h(t) = \sum_{j=1}^N x_j(t) \phi_j^w,$$

with coefficient vector $\mathbf{x}(t) = (x_j(t))_{j=1}^{N_w}$. This results in mass and stiffness matrices given by

$$(\mathbf{M}_u)_{l,j} = (\phi_j^u, \phi_l^u)_\Omega, \quad (\tilde{\mathbf{L}}_u)_{l,j} = (\mathcal{L}_{u,h} \phi_j^u, \phi_l^u)_\Omega, \quad (2.7a)$$

$$(\mathbf{M}_v)_{l,j} = (\phi_j^v, \phi_l^v)_\Omega, \quad (\tilde{\mathbf{L}}_v)_{l,j} = (\mathcal{L}_{v,h} \phi_j^v, \phi_l^v)_\Omega. \quad (2.7b)$$

Then, (2.6) is equivalent to the following system of ordinary differential equations,

$$\begin{aligned} \partial_t \mathbf{u} &= \mathbf{L}_v \mathbf{v} + \mathbf{g}_u, & \mathbf{L}_v &= \mathbf{M}_u^{-1} \tilde{\mathbf{L}}_v, \\ \partial_t \mathbf{v} &= \mathbf{L}_u \mathbf{u} + \mathbf{g}_v, & \mathbf{L}_u &= \mathbf{M}_v^{-1} \tilde{\mathbf{L}}_u, \\ \mathbf{u}(0) &= \mathbf{u}^0, \quad \mathbf{v}(0) = \mathbf{v}^0. \end{aligned} \quad (2.8)$$

Here, $\mathbf{u}^0$ and $\mathbf{v}^0$ are the coefficient vectors of u_h^0 and v_h^0 respectively.

With an abuse of notation, given $x_h, y_h \in \mathbb{V}_h^w$, $w \in \{u, v\}$, with coefficient vectors $\mathbf{x}, \mathbf{y} \in \mathbb{C}^{N_w}$, we define

$$(\mathbf{x}, \mathbf{y})_\Omega := \mathbf{y}^* \mathbf{M}_w \mathbf{x} = (x_h, y_h)_\Omega, \quad (2.9)$$

and do so analogously for the induced norms in $\mathbb{C}^{N_w}$. Here, $*$ denotes the conjugate transpose. For the matrix norms, we also take these weights into account, since then these norms are equivalent to the operator norms of the discrete operators $\mathcal{L}_{u,h}$ and $\mathcal{L}_{v,h}$, i.e., we have

$$\|\mathbf{L}_u\|_{\mathbb{V}_h^u \leftarrow \mathbb{V}_h^u} = \sup_{\mathbf{x} \in \mathbb{C}^{N_u} \setminus \{0\}} \frac{\|\mathbf{L}_u \mathbf{x}\|_\Omega}{\|\mathbf{x}\|_\Omega} = \sup_{x_h \in \mathbb{V}_h^u \setminus \{0\}} \frac{\|\mathcal{L}_{u,h} x_h\|_\Omega}{\|x_h\|_\Omega} = \|\mathcal{L}_{u,h}\|_{\mathbb{V}_h^u \leftarrow \mathbb{V}_h^u}, \quad (2.10a)$$

$$\|\mathbf{L}_v\|_{\mathbb{V}_h^v \leftarrow \mathbb{V}_h^v} = \sup_{\mathbf{x} \in \mathbb{C}^{N_v} \setminus \{0\}} \frac{\|\mathbf{L}_v \mathbf{x}\|_\Omega}{\|\mathbf{x}\|_\Omega} = \sup_{x_h \in \mathbb{V}_h^v \setminus \{0\}} \frac{\|\mathcal{L}_{v,h} x_h\|_\Omega}{\|x_h\|_\Omega} = \|\mathcal{L}_{v,h}\|_{\mathbb{V}_h^v \leftarrow \mathbb{V}_h^v}. \quad (2.10b)$$

In this paper, we are interested in locally refined meshes. We refer to our earlier papers [33, 34, 32] for detailed explanations on these meshes, but to keep this paper self-contained, we introduce the necessary notation here. A locally refined mesh is a mesh in which most of the mesh elements are coarse and very few mesh elements are fine. Let $\mathcal{T}_{h,c}$ and $\mathcal{T}_{h,f}$ denote the collection of all coarse and fine mesh elements, respectively. We denote by h_f and h_c the size of smallest mesh elements in $\mathcal{T}_{h,f}$ and in $\mathcal{T}_{h,c}$, respectively. These two sets are related to each other via

$$h_f \ll h_c \quad \text{and} \quad \text{card}(\mathcal{T}_{h,f}) \ll \text{card}(\mathcal{T}_{h,c}).$$

Based on this decomposition of the mesh, the matrices defined in (2.8) can be split into

$$\mathbf{L}_u = \mathbf{L}_u^f + \mathbf{L}_u^c, \quad \mathbf{L}_v = \mathbf{L}_v^f + \mathbf{L}_v^c, \quad (2.11)$$

cf. [33, 32] for more details. The indices f and c indicate that the elements on which $\mathbf{L}_u^f, \mathbf{L}_v^f$ act belong to the fine submesh $\mathcal{T}_{h,f}$ and the ones on which $\mathbf{L}_u^c, \mathbf{L}_v^c$ act, belong to the coarse submesh $\mathcal{T}_{h,c}$. In fact, it was shown in [33] that not only the fine elements have to be considered but also their direct coarse neighbors.

Let us state some properties of these matrices which are inherited from their corresponding discrete operators, cf. [33]. First, $\mathbf{L}_u$ and $\mathbf{L}_v$ are adjoint to each other, i.e., for all $\mathbf{u} \in \mathbb{C}^{N_u}, \mathbf{v} \in \mathbb{C}^{N_v}$, it holds

$$(\mathbf{L}_u \mathbf{u}, \mathbf{v})_\Omega = -(\mathbf{u}, \mathbf{L}_v \mathbf{v})_\Omega. \quad (2.12)$$

It is easy to verify that these split matrices preserve the adjointness property of their respective full ones, i.e.,

$$(\mathbf{L}_u^c \mathbf{u}, \mathbf{v})_\Omega = -(\mathbf{u}, \mathbf{L}_v^c \mathbf{v})_\Omega, \quad (\mathbf{L}_u^f \mathbf{u}, \mathbf{v})_\Omega = -(\mathbf{u}, \mathbf{L}_v^f \mathbf{v})_\Omega. \quad (2.13)$$

In addition, they satisfy

$$\mathbf{L}_v^c \mathbf{L}_u^c = \mathbf{L}_v^c \mathbf{L}_u, \quad \mathbf{L}_v^f \mathbf{L}_u^f = \mathbf{L}_v^f \mathbf{L}_u. \quad (2.14)$$

Furthermore, combining the above properties, it holds

$$\|\mathbf{L}_u \mathbf{u}\|_\Omega^2 = \|\mathbf{L}_u^c \mathbf{u}\|_\Omega^2 + \|\mathbf{L}_u^f \mathbf{u}\|_\Omega^2. \quad (2.15)$$

One of the important results from [33] is that the explicit split matrices $\mathbf{L}_u^c$ and $\mathbf{L}_v^c$ can be bounded independently of the fine mesh, that is, using the weighted norms in (2.10), we have

$$\|\mathbf{L}_u^c\|_{\mathbb{V}_h^v \leftarrow \mathbb{V}_h^u} \leq ch_c^{-1}, \quad \|\mathbf{L}_v^c\|_{\mathbb{V}_h^u \leftarrow \mathbb{V}_h^v} \leq ch_c^{-1}, \quad (2.16)$$

with a constant c that is independent of h_f and h_c .

In [33, 34], these split matrices were constructed to develop local time integration methods. Here, we use these split matrices in a different way, namely to construct preconditioners which improve the performance of Krylov subspace methods.

3 Higher-order implicit Runge–Kutta methods

In this section, we consider the time integration of (2.8) by an s -stage implicit Runge–Kutta (RK) methods given by its matrix $\mathcal{Q} = (a_{ij})_{i,j=1}^s$, weights b_i and nodes c_i , $i = 1, \dots, s$, cf., [24, Section II.1].

The two-field linear Friedrichs' system (2.1) fits into the general framework considered in [31, Eq. (2.8)] since the Friedrichs' operator $\mathcal{L}$ is skew-adjoint on its domain $\mathcal{D}(\mathcal{L})$. Therefore, the time discretization error bound [31, Thm. 3.5] holds under certain regularity assumptions on the exact solution of (2.1). Regarding the full discretization error using a central fluxes discontinuous Galerkin discretization in space we refer to [31, Thm 5.4 and Rem 5.7] Even though these results are derived for linear Maxwell's equations, it is straightforward to extend them to two-field linear Friedrichs' systems discretized in space.

To simplify the presentation, we write (2.8) in the compact form

$$\begin{aligned} \partial_t \mathbf{x} &= \mathbf{L} \mathbf{x} + \mathbf{g}, & (0, T), \\ \mathbf{x}^0 &= \mathbf{x}(0), \end{aligned} \quad (3.1)$$

where

$$\mathbf{x} = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}, \quad \mathbf{g} = \begin{pmatrix} \mathbf{g}_u \\ \mathbf{g}_v \end{pmatrix} \in \mathbb{R}^N, \quad \text{and} \quad \mathbf{L} = \begin{pmatrix} \mathbf{0} & \mathbf{L}_v \\ \mathbf{L}_u & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{N \times N},$$

with $N := N_u + N_v$. Assume that we already computed an approximation $\mathbf{x}^n \approx \mathbf{x}(t_n)$ at time $t_n = n\tau$, where $\tau > 0$ denotes the step size. Then, the implicit Runge–Kutta method applied to (3.1) leads to the following coupled linear system of equations for the intermediate stages $\mathbf{X}_i \approx \mathbf{x}(t_n + c_i\tau)$

$$\mathbf{X}_i = \mathbf{x}^n + \tau \sum_{j=1}^s a_{ij}(\mathbf{L}\mathbf{X}_j + \mathbf{G}_j), \quad i = 1, \dots, s, \quad (3.2a)$$

where $\mathbf{G}_j = \mathbf{g}(t_n + c_j\tau)$. The new approximation $\mathbf{x}^{n+1} \approx \mathbf{x}(t_{n+1})$ is then given explicitly by

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \tau \sum_{i=1}^s b_i(\mathbf{L}\mathbf{X}_i + \mathbf{G}_i). \quad (3.2b)$$

3.1 Gauß collocation methods

We use Gauß collocation methods to construct higher-order implicit RK methods. It is well known that these methods are algebraically stable [25, Theorem IV.12.9] and the RK matrix $\mathcal{Q}$ is invertible [25, Section IV.14]. In addition, the error analysis for linear wave-type problems [31, Section 3.1] makes use of the existence of a diagonal positive definite matrix $\widehat{\mathbf{D}}$ and a positive scalar $\eta > 0$ such that

$$\mathbf{v}^\top \widehat{\mathbf{D}} \mathcal{Q}^{-1} \mathbf{v} \geq \eta \mathbf{v}^\top \widehat{\mathbf{D}} \mathbf{v}, \quad \text{for all } \mathbf{v} \in \mathbb{R}^s. \quad (3.3)$$

Here, $^\top$ denotes the transpose. For Gauß collocation methods, the coercitivity condition (3.3) is satisfied for $\widehat{\mathbf{D}} = \widehat{\mathbf{B}}(\widehat{\mathbf{C}}^{-1} - \mathbf{I}_s)$, where $\widehat{\mathbf{B}} := \text{diag}(b_1, \dots, b_s)$, $\widehat{\mathbf{C}} := \text{diag}(c_1, \dots, c_s)$, and $\mathbf{I}_s$ is the identity matrix of size s , cf. [25, Theorem IV.14.5].

To obtain an efficient implementation for solving (3.2a), we use Kronecker products [24, Section VIII.6] to rewrite it as

$$\mathbf{X} = \mathbb{1}_s \otimes \mathbf{x}^n + \tau((\mathcal{Q} \otimes \mathbf{L})\mathbf{X} + (\mathcal{Q} \otimes \mathbf{I}_N)\mathbf{G}), \quad (3.4)$$

where $\mathbf{X} = (\mathbf{X}_i)_{i=1}^s$, $\mathbf{G} = (\mathbf{G}_i)_{i=1}^s \in \mathbb{C}^{Ns}$, $\mathbf{I}_N$ is the identity matrix of size N , and the term $\mathbb{1}_s$ denotes the vector in $\mathbb{R}^s$ consisting of all ones. Diagonalization of $\mathcal{Q}$ yields a nonsingular matrix $\mathbf{T} \in \mathbb{C}^{s \times s}$ containing the eigenvectors and a diagonal matrix $\Lambda_{\mathcal{Q}} \in \mathbb{C}^{s \times s}$ containing eigenvalues λ_i , such that

$$\mathbf{T}^{-1} \mathcal{Q} \mathbf{T} = \Lambda_{\mathcal{Q}}, \quad \Lambda_{\mathcal{Q}} = \text{diag}(\lambda_1, \dots, \lambda_s). \quad (3.5)$$

Substituting $\mathcal{Q} = \mathbf{T} \Lambda_{\mathcal{Q}} \mathbf{T}^{-1}$ into (3.4) and performing some Kronecker product operations leads to s decoupled linear systems of the form

$$(\mathbf{I}_s \otimes \mathbf{I}_N - \tau(\Lambda_{\mathcal{Q}} \otimes \mathbf{L}))\mathbf{Z} = \mathbf{Z}^0 + \tau(\Lambda_{\mathcal{Q}} \otimes \mathbf{I}_N)\widetilde{\mathbf{G}}, \quad (3.6)$$

where,

$$\mathbf{Z} = (\mathbf{T}^{-1} \otimes \mathbf{I}_N)\mathbf{X}, \quad \mathbf{Z}^0 = (\mathbf{T}^{-1} \otimes \mathbf{I}_N)(\mathbb{1}_s \otimes \mathbf{x}^n), \quad \widetilde{\mathbf{G}} = (\mathbf{T}^{-1} \otimes \mathbf{I}_N)\mathbf{G}. \quad (3.7)$$

Note that $\mathcal{Q}$ might have complex conjugate pairs of eigenvalues. For such eigenvalues (say $\lambda_j = \overline{\lambda_i}$), the corresponding linear systems are

$$(\mathbf{I}_N - \tau \lambda_i \mathbf{L})\mathbf{Z}_i = \mathbf{Z}_i^0 + \tau \lambda_i \widetilde{\mathbf{G}}_i, \quad (3.8a)$$

$$(\mathbf{I}_N - \tau \overline{\lambda_i} \mathbf{L})\mathbf{Z}_j = \mathbf{Z}_j^0 + \tau \overline{\lambda_i} \widetilde{\mathbf{G}}_j. \quad (3.8b)$$

In the homogeneous case, i.e., $\mathbf{g} \equiv 0$ which leads to $\widetilde{\mathbf{G}} \equiv 0$, the first term on the right-hand sides of (3.8a) and (3.8b) are conjugate to each other and so are the solutions.

Lemma 3.1. *If $\mathbf{g} \equiv 0$ and $\lambda_j = \overline{\lambda_i}$, then the solutions of (3.8) satisfy $\mathbf{Z}_j = \overline{\mathbf{Z}_i}$.*

Proof. The RK matrix $\mathcal{Q}$ is real and thus complex eigenvalues and eigenvectors appear in complex conjugate pairs. Hence there exists a symmetric permutation matrix $\widehat{\mathbf{P}} \in \mathbb{R}^{s \times s}$ s.t.,

$$\overline{\mathbf{T}} = \mathbf{T}\widehat{\mathbf{P}}, \quad \overline{\Lambda_{\mathcal{Q}}} = \widehat{\mathbf{P}}\Lambda_{\mathcal{Q}}\widehat{\mathbf{P}}, \quad (3.9)$$

which implies $\mathbf{T}^{-1} = \widehat{\mathbf{P}}\overline{\mathbf{T}}^{-1}$. We choose an arbitrary index $i \in \{0, \dots, s\}$ corresponding to a complex eigenvalue $\lambda_i \notin \mathbb{R}$ and define the index j such that $\mathbf{e}_j = \widehat{\mathbf{P}}\mathbf{e}_i$. By (3.7) and $\mathbf{x}^n \in \mathbb{R}^N$ we have

$$\overline{\mathbf{Z}}_i^0 = (\mathbf{e}_i^\top \otimes \mathbf{I}_N)\overline{\mathbf{Z}}^0 = (\mathbf{e}_i^\top \overline{\mathbf{T}}^{-1} \mathbb{1}_s \otimes \mathbf{x}^n) = ((\widehat{\mathbf{P}}\mathbf{e}_i)^\top \mathbf{T}^{-1} \mathbb{1}_s) \otimes \mathbf{x}^n = \mathbf{Z}_j^0. \quad (3.10)$$

Conjugating (3.8a) proves that $\overline{\mathbf{Z}}_i$ solves (3.8b). $\square$

In addition to this, $\mathbf{Z}_i$ and $\tilde{\mathbf{G}}_i$ in (3.8a) can be further decomposed into

$$\mathbf{Z}_i = \begin{pmatrix} \mathbf{Z}_{u,i} \\ \mathbf{Z}_{v,i} \end{pmatrix}, \quad \tilde{\mathbf{G}}_i = \begin{pmatrix} \tilde{\mathbf{G}}_{u,i} \\ \tilde{\mathbf{G}}_{v,i} \end{pmatrix},$$

where $\mathbf{Z}_{u,i}, \mathbf{Z}_{v,i}$ denote unknowns corresponding to the transformed intermediate stages of $\mathbf{u}$ and $\mathbf{v}$ respectively. Taking the Schur complement, the linear systems in (3.8a) can be reduced to

$$(\mathbf{I}_{N_u} - \alpha_i \mathbf{L}_v \mathbf{L}_u) \mathbf{Z}_{u,i} = \mathbf{Z}_{u,i}^0 + \tau \lambda_i (\mathbf{L}_v \mathbf{Z}_{v,i}^0 + \tilde{\mathbf{G}}_{u,i}) + \alpha_i \mathbf{L}_v \tilde{\mathbf{G}}_{v,i}, \quad \alpha_i := \tau^2 \lambda_i^2 \in \mathbb{C}, \quad (3.11)$$

to compute the u -component of $\mathbf{Z}_i$. After solving this linear system of dimension N_u , the v -component of $\mathbf{Z}_i$ can be calculated explicitly via

$$\mathbf{Z}_{v,i} = \mathbf{Z}_{v,i}^0 + \tau \lambda_i (\mathbf{L}_u \mathbf{Z}_{u,i} + \tilde{\mathbf{G}}_{v,i}). \quad (3.12)$$

An efficient implementation of an s -stage implicit Runge-Kutta method using Gauß collocation points thus requires solving a linear system of the form

$$\mathbf{A}\mathbf{x} = \mathbf{b} \quad \text{where} \quad \mathbf{A} := \mathbf{I}_{N_u} - \alpha \mathbf{L}_v \mathbf{L}_u, \quad (3.13)$$

with a possibly complex parameter α , in each time step. Therefore, the size of the linear system to be solved is reduced from $s(N_u + N_v)$ in (3.4) to N_u in (3.13). The adjointness property (2.12) implies that $\mathbf{L}_v \mathbf{L}_u$ is symmetric with respect to the discrete inner product $(\cdot, \cdot)_\Omega$ defined in (2.9). Hence, $\mathbf{A}$ is complex symmetric, that is,

$$(\mathbf{A}\mathbf{x}, \mathbf{x})_\Omega = (\mathbf{x}, \overline{\mathbf{A}}\mathbf{x})_\Omega, \quad \mathbf{x} \in \mathbb{C}^{N_u}.$$

and also normal. If $\alpha \in \mathbb{R}$, then $\mathbf{A} \in \mathbb{R}^{N \times N}$ is symmetric. However, for $\alpha \notin \mathbb{R}$ it follows immediately that $\mathbf{A} \neq \mathbf{A}^*$ with respect to $(\cdot, \cdot)_\Omega$. Moreover, for

$$\alpha \in \mathbb{C} \setminus \{z \in \mathbb{R} : z < 0\}, \quad (3.14)$$

the matrix $\mathbf{A}$ is invertible. For Gauß collocation methods, the coercivity condition (3.3) guarantees that the eigenvalues of $\mathcal{Q}$ are not purely imaginary, and hence (3.14) is satisfied.

4 Preconditioned Krylov subspace methods

In this section, we aim at designing a tailored preconditioner for solving the sparse linear system (3.13) by a preconditioned Krylov subspace method. We will prove that the number of Krylov iterations to achieve a certain tolerance is independent of the fine mesh. The overall method can be considered as a locally implicit scheme, because it only requires the solution of a small linear system as it is required for the second-order method in [33].

We remark that in Section 4.1, we consider the Euclidean inner product and norm in $\mathbb{C}^N$, but using weighted inner products would be possible as well.

4.1 Krylov subspace methods for complex symmetric matrices

For a nonsingular, complex symmetric matrix $\mathbf{K} = \mathbf{K}^\top \in \mathbb{C}^{N \times N}$ and a given vector $\mathbf{f} \in \mathbb{C}^N$, we consider the linear system

$$\mathbf{K}\mathbf{x} = \mathbf{f}. \quad (4.1)$$

Given an initial guess $\mathbf{x}_0 \in \mathbb{C}^N$ and its initial residual vector $\mathbf{r}_0 = \mathbf{f} - \mathbf{K}\mathbf{x}_0$, a Krylov subspace method yields an approximation of the form

$$\mathbf{x}_m = \mathbf{x}_0 + \mathbf{W}_m \mathbf{y}_m, \quad m = 1, 2, \dots, \quad (4.2)$$

where $\mathbf{W}_m \in \mathbb{C}^{N \times m}$ is a basis of the m th Krylov subspace

$$\mathcal{K}_m(\mathbf{K}, \mathbf{r}_0) := \text{span}(\mathbf{r}_0, \mathbf{K}\mathbf{r}_0, \dots, \mathbf{K}^{m-1}\mathbf{r}_0),$$

and $\mathbf{y}_m \in \mathbb{C}^m$ is a suitable coefficient vector. The choices of $\mathbf{W}_m$ and $\mathbf{y}_m$ characterize the Krylov subspace method, cf. [17, 23, 38] for more details.

To exploit the complex symmetric structure of $\mathbf{K}$, we suggest to use the quasi-minimal residual (QMR) algorithm for complex symmetric matrices [16, Section 3], which is based on the complex symmetric Lanczos process. Here, $\mathbf{W}_m$ satisfies

$$\mathbf{K}\mathbf{W}_m = \mathbf{W}_{m+1} \tilde{\mathbf{H}}_m, \quad \mathbf{D}_{m+1} \tilde{\mathbf{H}}_m = \mathbf{W}_{m+1}^\top \mathbf{K} \mathbf{W}_m, \quad (4.3)$$

with a diagonal matrix $\mathbf{D}_{m+1} = \mathbf{W}_{m+1}^\top \mathbf{W}_{m+1} \in \mathbb{C}^{(m+1) \times (m+1)}$. The complex symmetry of $\mathbf{K}$ implies that $\tilde{\mathbf{H}}_m \in \mathbb{C}^{(m+1) \times m}$ is tridiagonal and the upper $m \times m$ submatrix of $\mathbf{D}_{m+1} \tilde{\mathbf{H}}_m$ is again complex symmetric. $\tilde{\mathbf{H}}_m$ has full column rank m until $\mathcal{K}_m(\mathbf{K}, \mathbf{r}_0)$ becomes a $\mathbf{K}$ -invariant subspace.

With $\beta = \|\mathbf{r}_0\|$, the QMR approximation is defined as

$$\mathbf{x}_m = \mathbf{x}_0 + \mathbf{W}_m \mathbf{y}_m, \quad \mathbf{y}_m = \beta \tilde{\mathbf{H}}_m^+ \mathbf{e}_1, \quad \tilde{\mathbf{H}}_m^+ = (\tilde{\mathbf{H}}_m^* \tilde{\mathbf{H}}_m)^{-1} \tilde{\mathbf{H}}_m^*, \quad (4.4)$$

where $\mathbf{e}_1$ denotes the first canonical unit vector. The corresponding residual can be written as

$$\mathbf{r}_m = \mathbf{f} - \mathbf{K}\mathbf{x}_m = \mathbf{W}_{m+1}(\beta \mathbf{e}_1 - \tilde{\mathbf{H}}_m \mathbf{y}_m).$$

Since $\tilde{\mathbf{H}}_m$ has full column rank, $\mathbf{y}_m$ is equivalently characterized as the unique solution of the least-squares problem

$$\mathbf{y}_m = \underset{\mathbf{y} \in \mathbb{C}^m}{\text{argmin}} \|\beta \mathbf{e}_1 - \tilde{\mathbf{H}}_m \mathbf{y}\|.$$

The advantage of this algorithm compared to methods based on the Arnoldi process (e.g., GMRES) is that it uses three-term recurrences for the computation of the basis as well as for the approximation. It can be combined with look-ahead strategies [18] to prevent breakdowns of the Lanczos process, which might appear because it constructs a basis which is orthogonal w.r.t. the indefinite bilinear form $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^\top \mathbf{y}$, instead of the Euclidean inner product $(\mathbf{x}, \mathbf{y}) = \mathbf{x}^* \mathbf{y}$, see [16, Section 4]. For the sake of presentation, we assume that breakdowns do not appear until a sufficiently accurate solution is computed, but we note that with minor modifications, our analysis also holds for the (complex symmetric) look-ahead Lanczos method [18]. This assumption ensures that

$$\|\mathbf{D}_{m+1}^{-1}\| \leq \delta, \quad (4.5)$$

for a given (small) tolerance $\delta > 0$, because otherwise, one would switch to the look-ahead version of the Lanczos process.

In the following, $\mathbb{P}_m$ denotes the set of all polynomials over $\mathbb{C}$ of degree at most m .

Theorem 4.1. Let $\mathbf{K}$ be a nonsingular, complex symmetric matrix, and $\mathbf{x}_m$ be the QMR approximation (4.4) after m steps. Then the error of the QMR method satisfies

$$\|\mathbf{K}^{-1}\mathbf{f} - \mathbf{x}_m\| \leq \|\mathbf{K}^{-1}\mathbf{P}_m\| \min_{\substack{p_m \in \mathcal{P}_m \\ p_m(0)=1}} \|p_m(\mathbf{K})\mathbf{r}_0\| \quad (4.6)$$

with a projection matrix $\mathbf{P}_m$ given by

$$\mathbf{P}_m = \mathbf{I}_{N_u} - \mathbf{W}_{m+1} \tilde{\mathbf{H}}_m \tilde{\mathbf{H}}_m^+ \mathbf{D}_{m+1}^{-1} \mathbf{W}_{m+1}^\top.$$

Moreover, if $\|\mathbf{W}_{m+1}\mathbf{e}_j\| = 1$, $j = 1, \dots, m+1$, and (4.5) holds, we have

$$\|\mathbf{P}_m\| \leq 1 + (m+1)\delta. \quad (4.7)$$

Proof. Analogously to the proof of [30, Theorem 2] it can be seen from (4.3) that $\mathbf{P}_m \mathbf{K} \mathbf{W}_m = 0$. Using (4.4) this implies

$$\mathbf{K}^{-1}\mathbf{f} - \mathbf{x}_m = \mathbf{K}^{-1}\mathbf{P}_m \mathbf{r}_0 = \mathbf{K}^{-1}\mathbf{P}_m p_m(\mathbf{K})\mathbf{r}_0$$

for all $p_m \in \mathcal{P}_m$ with $p_m(0) = 1$.

The bound on $\|\mathbf{P}_m\|$ follows from (4.5) and $\|\mathbf{W}_m\| \leq m^{1/2}$. $\square$

Since $\|p_m(\mathbf{K})\mathbf{r}_0\| \leq \|p_m(\mathbf{K})\| \|\mathbf{r}_0\|$, it remains to bound

$$\min_{\substack{p_m \in \mathcal{P}_m \\ p_m(0)=1}} \|p_m(\mathbf{K})\|.$$

This can be done by means of Faber polynomials and complex approximation theory, cf. [15], based on a superset $\mathcal{S}$ of the field of values of $\mathbf{K}$ defined as

$$\mathcal{F}(\mathbf{K}) := \{\rho_{\mathbf{K}}(\mathbf{u}), \mathbf{u} \in \mathbb{C}^{N_u}, \mathbf{u} \neq \mathbf{0}\}, \quad \rho_{\mathbf{K}}(\mathbf{u}) := \frac{(\mathbf{u}, \mathbf{K}\mathbf{u})}{(\mathbf{u}, \mathbf{u})}.$$

Theorem 4.2. Let $\mathcal{S} \subset \mathbb{C}$ be a convex and bounded superset of $\mathcal{F}(\mathbf{K})$ with $0 \notin \mathcal{S}$ and let ϕ be the conformal map which maps the exterior of $\mathcal{S}$ onto the exterior of the unit disc with $\phi(\infty) = \infty$. Then

$$\min_{\substack{p_m \in \mathcal{P}_m \\ p_m(0)=1}} \|p_m(\mathbf{K})\| \leq (1 + 2^{1/2}) \min \left\{ \frac{3}{|\phi(0)|^m}, \frac{2}{|\phi(0)|^m - 1} \right\}. \quad (4.8)$$

Proof. It was shown in [8] that

$$\|p_m(\mathbf{K})\| \leq (1 + 2^{1/2}) \max_{z \in \mathcal{S}} |p_m(z)|.$$

The statement then follows from [29, Eq. (2.14)] and [15, Theorem 2]. $\square$

The conformal map ϕ can be determined numerically by using the Schwarz-Christoffel toolbox [14].

4.2 Preconditioning for locally refined grids

Our aim and the content of this section is the construction of a preconditioner such that the field of values of the preconditioned matrix with respect to the discrete weighted inner product $(\cdot, \cdot)_\Omega$ defined in (2.9) is independent of the fine mesh elements. Then by Theorem 4.2, the same holds for the error of the preconditioned Krylov method in this weighted inner product.

Motivated by locally implicit methods for Maxwell's equations in [33, 40], we suggest to precondition $\mathbf{A}$ from (3.13) with its dominant part,

$$\mathbf{A} \approx \mathbf{B} := \mathbf{I}_{N_u} - \gamma \mathbf{L}_v^f \mathbf{L}_u^f, \quad (4.9)$$

where $\gamma > 0$ is a suitably chosen parameter. Note that this basically boils down to replacing the Friedrichs' matrices $\mathbf{L}_u, \mathbf{L}_v$ in (3.13) defined on the full mesh by the split matrices acting on the implicitly treated mesh elements, cf. Section 2 and by replacing the possibly complex factor α by $\gamma > 0$. By (2.13) and $\gamma > 0$, the preconditioner $\mathbf{B}$ is symmetric and positive definite with respect to $(\cdot, \cdot)_\Omega$, and thus it has a symmetric and positive definite square root $\mathbf{B}^{1/2}$. This allows us to define an equivalent preconditioned linear system

$$\tilde{\mathbf{A}} \tilde{\mathbf{x}} = \tilde{\mathbf{b}}, \quad (4.10a)$$

where

$$\tilde{\mathbf{A}} := \mathbf{B}^{-1/2} \mathbf{A} \mathbf{B}^{-1/2}, \quad \tilde{\mathbf{x}} := \mathbf{B}^{1/2} \mathbf{x} \quad \text{and} \quad \tilde{\mathbf{b}} := \mathbf{B}^{-1/2} \mathbf{b}. \quad (4.10b)$$

Since $\mathbf{A}$ is complex symmetric and $\mathbf{B}$ is real symmetric, the preconditioned matrix $\tilde{\mathbf{A}}$ is again complex symmetric (with respect to $(\cdot, \cdot)_\Omega$).

We now apply the QMR method for complex symmetric matrices to the preconditioned linear system (4.10) and refer to this method as the preconditioned QMR (pQMR) method, cf. [20, Alg. 8.1.]. Since the computation of $\mathbf{B}^{1/2}$ is usually very expensive, it is essential that it is not required for the implementation. In fact, one only has to solve linear systems with $\mathbf{B}$ but neither compute $\mathbf{B}^{1/2}$ nor $\mathbf{B}^{-1/2}$. Solving linear systems with $\mathbf{B}$ does not lead to too much overhead costs because $\mathbf{L}_v^f \mathbf{L}_u^f$ only acts on the fine elements and their direct neighbors and thus is of small dimension compared to $\mathbf{A}$. Moreover, systems with $\mathbf{B}$ can also be solved iteratively, e.g., using standard preconditioning techniques for symmetric positive definite matrices.

It remains to show that the error of pQMR can indeed be bounded independently of the fine mesh. Note that Theorems 4.1 and 4.2. also hold for $\|\cdot\| = \|\cdot\|_\Omega$, if the Lanczos process and the field of values are defined w.r.t. $(\cdot, \cdot) = (\cdot, \cdot)_\Omega$. Using these theorems, it is sufficient to show that the field of values $\mathcal{F}(\tilde{\mathbf{A}})$ can be bounded independent of the fine mesh.

We split the factor α in (3.13) into its real and imaginary part,

$$\alpha := \alpha_R + i \alpha_I, \quad \alpha_R, \alpha_I \in \mathbb{R}, \quad (4.11)$$

and define

$$\Gamma_\zeta^e = 1 + \zeta \|\mathbf{L}_u^e\|_{\mathbb{V}_h^v \leftarrow \mathbb{V}_h^u}^2, \quad \Gamma_\zeta^i = 1 + \zeta \|\mathbf{L}_u^f\|_{\mathbb{V}_h^v \leftarrow \mathbb{V}_h^u}^2, \quad \text{for } \zeta \in \mathbb{C}. \quad (4.12)$$

Defining quadrilaterals

$$Q = \text{conv}\{1, \Gamma_\alpha^e, \frac{\alpha}{\gamma}, \frac{\alpha}{\gamma} \Gamma_\gamma^e\}, \quad (4.13a)$$

$$R = \text{conv}\{1, \Gamma_\gamma^e, 1 + (\frac{\alpha}{\gamma} - 1)(\Gamma_\gamma^e - \frac{1}{\Gamma_\gamma^i}), \Gamma_\gamma^e + (\frac{\alpha}{\gamma} - 1)(\Gamma_\gamma^e - \frac{1}{\Gamma_\gamma^i})\}, \quad (4.13b)$$

allows us to construct a superset $\mathcal{S}$ of $\mathcal{F}(\tilde{\mathbf{A}})$ which is independent of the fine mesh.

Theorem 4.3. Let $\alpha \neq 0$ satisfy (3.14) and let $\tilde{\mathbf{A}}$ be defined in (4.10b) where the preconditioner $\mathbf{B}$ is given in (4.9) for some parameter $\gamma > 0$. Then we have $\mathcal{F}(\tilde{\mathbf{A}}) \subset \mathcal{S}$, where

$$\mathcal{S} = \begin{cases} Q \cap R, & \alpha_I \neq 0, \\ [\frac{\alpha}{\gamma}, \Gamma_\alpha^e], & \alpha_I = 0, \quad 0 < \alpha_R = \alpha \leq \gamma, \\ [1, \frac{\alpha}{\gamma} \Gamma_\gamma^e], & \alpha_I = 0, \quad 0 < \gamma \leq \alpha_R = \alpha, \end{cases}$$

is independent of the fine mesh and $0 \notin \mathcal{S}$.

Proof. Let $\mathbf{u} \in \mathbb{C}^{N_u}$, $\mathbf{u} \neq \mathbf{0}$ and $\tilde{\mathbf{u}} := \mathbf{B}^{1/2} \mathbf{u}$. Then, by the symmetry of $\mathbf{B}$ (and thus of $\mathbf{B}^{1/2}$), the adjointness and split properties eqs. (2.12), (2.13), and (2.15), we have

$$(\tilde{\mathbf{u}}, \tilde{\mathbf{A}} \tilde{\mathbf{u}})_\Omega = (\mathbf{u}, \mathbf{A} \mathbf{u})_\Omega = \|\mathbf{u}\|_\Omega^2 + (\alpha_R + i\alpha_I)(\|\mathbf{L}_u^c \mathbf{u}\|_\Omega^2 + \|\mathbf{L}_u^f \mathbf{u}\|_\Omega^2), \quad (4.14a)$$

$$(\tilde{\mathbf{u}}, \tilde{\mathbf{u}})_\Omega = (\mathbf{u}, \mathbf{B} \mathbf{u})_\Omega = \|\mathbf{u}\|_\Omega^2 + \gamma \|\mathbf{L}_u^f \mathbf{u}\|_\Omega^2. \quad (4.14b)$$

We now distinguish the two cases of α being real or complex.

(a) For $\alpha_I \neq 0$, it is easy to see that

$$1 \leq \operatorname{Re}(\rho_{\tilde{\mathbf{A}}}(\tilde{\mathbf{u}})) + \frac{\gamma - \alpha_R}{\alpha_I} \operatorname{Im} \rho_{\tilde{\mathbf{A}}}(\tilde{\mathbf{u}}) = 1 + \frac{\gamma \|\mathbf{L}_u^c \mathbf{u}\|_\Omega^2}{\|\mathbf{u}\|_\Omega^2 + \gamma \|\mathbf{L}_u^f \mathbf{u}\|_\Omega^2} \leq \Gamma_\gamma^e. \quad (4.15a)$$

The first inequality is obvious and the second follows from the definition of the weighted matrix norm in (2.10) and $\gamma > 0$. In addition, we have

$$0 \leq \operatorname{Re}(\rho_{\tilde{\mathbf{A}}}(\tilde{\mathbf{u}})) - \frac{\alpha_R}{\alpha_I} \operatorname{Im} \rho_{\tilde{\mathbf{A}}}(\tilde{\mathbf{u}}) = \frac{\|\mathbf{u}\|_\Omega^2}{\|\mathbf{u}\|_\Omega^2 + \gamma \|\mathbf{L}_u^f \mathbf{u}\|_\Omega^2} \leq 1. \quad (4.15b)$$

A simple calculation shows that the inequalities (4.15) are satisfied if and only if $\rho_{\tilde{\mathbf{A}}} \in Q$ with Q defined in (4.13a).

Next we consider only the imaginary part. Using (4.14), and (4.12) we obtain

$$0 \leq \frac{\gamma}{\alpha_I} \operatorname{Im} \rho_{\tilde{\mathbf{A}}}(\tilde{\mathbf{u}}) = 1 + \frac{\gamma \|\mathbf{L}_u^c \mathbf{u}\|_\Omega^2}{\|\mathbf{u}\|_\Omega^2 + \gamma \|\mathbf{L}_u^f \mathbf{u}\|_\Omega^2} - \frac{\|\mathbf{u}\|_\Omega^2}{\|\mathbf{u}\|_\Omega^2 + \gamma \|\mathbf{L}_u^f \mathbf{u}\|_\Omega^2} \leq \Gamma_\gamma^e - \frac{1}{\Gamma_\gamma^i}. \quad (4.16)$$

The bounds (4.15a) and (4.16) are satisfied if and only if $\rho_{\tilde{\mathbf{A}}} \in R$ with R defined in (4.13b). Hence we proved $\mathcal{F}(\tilde{\mathbf{A}}) \subset Q \cap R$.

(b) For $\alpha_I = 0$, the matrix $\tilde{\mathbf{A}} \in \mathbb{R}^{N_u \times N_u}$ is symmetric and thus $\rho_{\tilde{\mathbf{A}}}(\tilde{\mathbf{u}}) \in \mathbb{R}$ for all $\tilde{\mathbf{u}} \in \mathbb{C}^{N_u}$. Since $\alpha = \alpha_R$ we have

$$\rho_{\tilde{\mathbf{A}}}(\tilde{\mathbf{u}}) = \frac{\alpha}{\gamma} + \frac{(1 - \frac{\alpha}{\gamma})\|\mathbf{u}\|_\Omega^2 + \alpha \|\mathbf{L}_u^c \mathbf{u}\|_\Omega^2}{\|\mathbf{u}\|_\Omega^2 + \gamma \|\mathbf{L}_u^f \mathbf{u}\|_\Omega^2}. \quad (4.17)$$

If $\alpha \geq \gamma$, (4.17) can be bounded by

$$1 = \frac{\alpha}{\gamma} + \frac{(1 - \frac{\alpha}{\gamma})\|\mathbf{u}\|_\Omega^2}{\|\mathbf{u}\|_\Omega^2} \leq \rho_{\tilde{\mathbf{A}}}(\tilde{\mathbf{u}}) \leq \frac{\alpha}{\gamma} + \frac{\alpha \|\mathbf{L}_u^c \mathbf{u}\|_\Omega^2}{\|\mathbf{u}\|_\Omega^2} \leq \frac{\alpha}{\gamma} \Gamma_\gamma^e,$$

Similarly, for $0 < \alpha \leq \gamma$, it is straightforward to see

$$\frac{\alpha}{\gamma} \leq \rho_{\tilde{\mathbf{A}}}(\tilde{\mathbf{u}}) \leq \frac{\alpha}{\gamma} + \frac{(1 - \frac{\alpha}{\gamma})\|\mathbf{u}\|_\Omega^2 + \alpha \|\mathbf{L}_u^c \mathbf{u}\|_\Omega^2}{\|\mathbf{u}\|_\Omega^2} \leq \Gamma_\alpha^e.$$

Furthermore, since

$$0 \leq \Gamma_\gamma^e - \frac{1}{\Gamma_\gamma^i} \leq \Gamma_\gamma^e, \quad \gamma > 0,$$

all quantities defining the superset $\mathcal{S}$ are bounded independently of the implicitly treated mesh elements and thus, $\mathcal{S}$ is independent of h_f . Finally, in all cases we have $0 \notin \mathcal{S}$. $\square$

Further, we point out that $\gamma > 0$ can be chosen freely and thus used to improve the convergence factor. For example, a natural choice would be

$$\gamma = |\alpha_R| \text{ if } \alpha_R \neq 0 \quad \text{or} \quad \gamma = |\alpha| \text{ else.} \quad (4.18)$$

In any case, one should choose $\gamma \sim \tau^2$ so that the dominating part of $\mathbf{A}$ is well approximated by the preconditioner $\mathbf{B}$.

As a special case of Theorem 4.3, we obtain an inclusion set for the field of values of $\mathbf{A}$ itself. Hence, we can state an error bound for the complex symmetric QMR method without preconditioning.

Corollary 4.4. *For the matrix $\mathbf{A}$ defined in (3.13), Theorem 4.3 holds by substituting $\mathbf{L}_u^c = \mathbf{L}_u$ and $\mathbf{L}_u^f = 0$ in (4.13).*

Recall that by an inverse estimate [11, Lemma 1.44] there is a constant c independent of the mesh width such that $\|\mathbf{L}_u\|_{\mathbb{V}_h^v \leftarrow \mathbb{V}_h^u} \leq ch_{\min}^{-1}$. Hence, without preconditioning, the superset will scale with $h_{\min}^{-1}$. Applying Theorems 4.1 and 4.2 to the preconditioned system (4.10a) provides the following error bound:

Theorem 4.5. *Let $\mathbf{x}_m$ be the QMR approximation to the solution of the preconditioned linear system (4.10). If (4.5) is satisfied, then there is a constant $\phi_0 > 1$ independent of the fine mesh such that the error of the m th pQMR iterate satisfies*

$$\|\tilde{\mathbf{A}}^{-1}\tilde{\mathbf{b}} - \mathbf{x}_m\|_\Omega \leq c_{\tilde{\mathbf{A}}} (1 + \sqrt{2})(1 + (m+1)\delta) \min \left\{ \frac{3}{\phi_0^m}, \frac{2}{\phi_0^m - 1} \right\}, \quad (4.19)$$

where

$$\begin{cases} c_{\tilde{\mathbf{A}}} = 1, & \text{if } 0 < \gamma \leq \alpha_R, \alpha_I = 0 \quad \text{or} \quad \alpha_I \neq 0, \\ c_{\tilde{\mathbf{A}}} = \frac{\gamma}{\alpha_R}, & \text{if } 0 < \alpha_R \leq \gamma, \alpha_I = 0. \end{cases} \quad (4.20)$$

Proof. Since $\tilde{\mathbf{A}}$ is complex symmetric, we apply Theorem 4.1 for $\mathbf{K} = \tilde{\mathbf{A}}$ with $\|\cdot\| = \|\cdot\|_\Omega$. By Theorem 4.3, $\mathcal{F}(\tilde{\mathbf{A}}) \subset \mathcal{S}$ is independent of the fine mesh and the same holds for the conformal map ϕ used in Theorem 4.2, in particular for $|\phi(0)| =: \phi_0$. Thus, the bound (4.19) follows from (4.6), (4.7), and (4.8), if we can show

$$\|\tilde{\mathbf{A}}^{-1}\mathbf{w}\|_\Omega \leq c_{\tilde{\mathbf{A}}} \|\mathbf{w}\|_\Omega \quad \text{for all } \mathbf{w} \in \mathbb{C}^{N_u}. \quad (4.21)$$

We choose an arbitrary $\mathbf{w} \in \mathbb{C}^{N_u}$, $\mathbf{w} \neq \mathbf{0}$ and define $\mathbf{u} = \tilde{\mathbf{A}}^{-1}\mathbf{w}$. Then, Theorem 4.3 with $c_{\tilde{\mathbf{A}}}$ defined in (4.20) and the Cauchy-Schwarz inequality yield

$$\frac{1}{c_{\tilde{\mathbf{A}}}} \leq \operatorname{Re}(\rho_{\tilde{\mathbf{A}}}(\mathbf{u})) = \operatorname{Re} \frac{(\mathbf{w}, \tilde{\mathbf{A}}^{-1}\mathbf{w})_\Omega}{\|\tilde{\mathbf{A}}^{-1}\mathbf{w}\|_\Omega^2} \leq \frac{\|\mathbf{w}\|_\Omega \|\tilde{\mathbf{A}}^{-1}\mathbf{w}\|_\Omega}{\|\tilde{\mathbf{A}}^{-1}\mathbf{w}\|_\Omega^2} = \frac{\|\mathbf{w}\|_\Omega}{\|\tilde{\mathbf{A}}^{-1}\mathbf{w}\|_\Omega}. \quad (4.22)$$

This proves (4.21). $\square$

As an immediate consequence of Theorem 4.5 we see that the error of the pQMR method is bounded independently of the fine mesh, since $\mathcal{S}$ only depends on the coarse mesh. In particular, the number of iterations is uniformly bounded with respect to further refinement of the fine part of the mesh.

5 Numerical experiments

For all experiments, we consider the transverse-electric (TE) polarization of linear Maxwell's equations in a homogeneous medium $\Omega = (0, 1)^2$ with $\mu = \epsilon = 1$, i.e.,

$$\partial_t E_x = \partial_y H_z - J_x, \quad \Omega \times (0, T), \quad (5.1a)$$

$$\partial_t E_y = -\partial_x H_z - J_y, \quad \Omega \times (0, T), \quad (5.1b)$$

$$\partial_t H_z = \partial_y E_x - \partial_x E_y, \quad \Omega \times (0, T), \quad (5.1c)$$

$$E(0) = E^0, \quad H(0) = H^0, \quad \Omega, \quad (5.1d)$$

$$E \times \mathbf{n} = 0, \quad \partial\Omega \times (0, T). \quad (5.1e)$$

The codes to reproduce our results are available at

<https://github.com/MalikScheifinger/HigherOrderLTI>

The software is based on the FEM library `deal.II` [2] version 9.7 and the Maxwell toolbox `TiMaxdG` [6].

5.1 Illustration of Theorems 4.3 and 4.5

We consider a dG discretization with polynomials of degree two and fix

$$\alpha = \left(\frac{1}{24} + i \frac{\sqrt{3}}{24} \right) \tau^2, \quad \gamma = \alpha_R = \frac{1}{24} \tau^2, \quad (5.2)$$

for the system matrix $\mathbf{A}$ in (3.13) and the preconditioner $\mathbf{B}$ in (4.9), respectively. This choice follows from $\alpha_i = \tau^2 \lambda_i^2$ in (3.11), with λ_i one of the two complex conjugate eigenvalues of the RK matrix $\mathbf{Q}$ of the two-stage implicit Gauß–Legendre method. The parameter $\gamma = \alpha_R$ is the choice suggested in (4.18). The spatial domain is discretized by a uniform coarse mesh which is then locally refined at the center, yielding a coarse mesh width $h_c = 0.117851$ and fine mesh widths $h_f^{(2)} = 0.0294628$, $h_f^{(3)} = 0.0147314$, and $h_f^{(4)} = 0.0073657$, where the superscript denotes the local refinement level. Local refinement level three is illustrated in Figure 1.

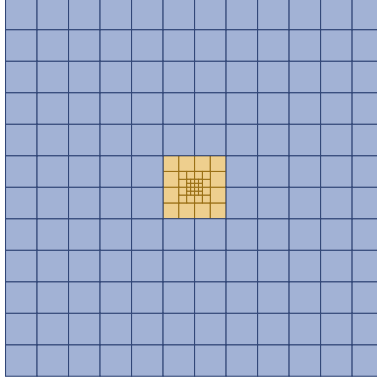


Figure 1: Mesh with local refinement level three at the center of the domain.

Figure 2 shows the spectrum of $\mathbf{A}$ from (3.13), the field of values of the preconditioned matrix $\tilde{\mathbf{A}}$ from (4.10b), and the quadrilateral bounds Q and R from (4.13a) and (4.13b), for time step size $\tau = 0.05$ and local refinement level three. By the inverse estimate used in the proof of

Corollary 4.4, the eigenvalues of $\mathbf{A}$ scale like $h_{\min}^{-1}$. The spectrum of the unpreconditioned system is therefore governed by the fine elements and spreads out as the mesh is refined.

Next, we apply the QMR method to the system (3.13), with and without the preconditioner (4.9). To obtain an algebraic test problem with known solution, we choose a random vector as the exact solution $\mathbf{x}$ of the linear system (3.13) and define the right-hand side $\mathbf{b}$ by applying the matrix $\mathbf{A}$ to it. This allows us to compare the relative L^2 -error of the QMR iterates directly. Figure 3 shows the results. For a fixed tolerance, the number of preconditioned QMR iterations is almost independent of the local refinement level, whereas the number of QMR iterations grows with it, as predicted by Theorem 4.5 together with Corollary 4.4.

The bound of Theorem 4.3 is fine-mesh-independent but not tight when τ is small relative to the fine mesh width, where the linear system is only mildly stiff. In this regime the fine-mesh dependence of the superset enters solely through the term $\Gamma_\gamma^e - 1/\Gamma_\gamma^i$ of R in (4.13b): the factor $1/\Gamma_\gamma^i$ with Γ_γ^i from (4.12) is not negligible at on the coarsest level of refinement and vanishes only as the fine mesh is refined, so R grows toward its level-independent limit. Figure 4 shows this effect for $\tau = 0.01$: preconditioned QMR still improves the convergence, and the iteration count increases with the local refinement level while remaining bounded by the fine-mesh-independent superset $\mathcal{S}$ of Theorem 4.3. Figure 5 illustrates the same dependence geometrically, where Q is identical for all levels and only R grows. Such small time steps are not used in practice for the coarse spatial discretizations considered here: once the time discretization error drops below the spatial discretization error, decreasing τ further does not reduce the total error.

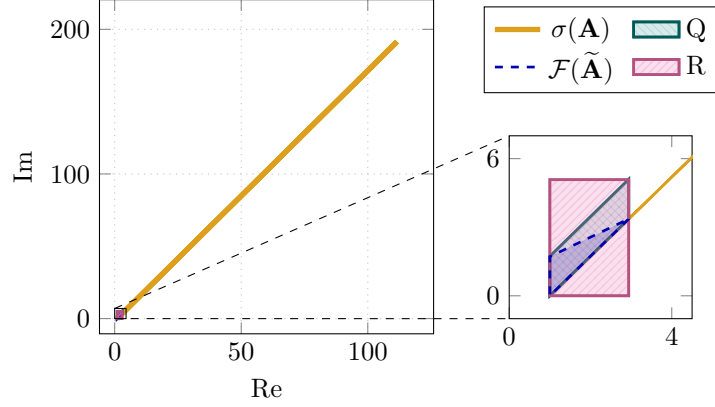


Figure 2: Spectrum $\sigma(\mathbf{A})$ (orange), field of values $\mathcal{F}(\tilde{\mathbf{A}})$ of the preconditioned matrix (blue, dashed), and quadrilateral bounds Q (teal) and R (magenta) with α chosen as in (5.2) and $\tau = 0.05$, local refinement level three. The inset shows a zoom near the origin.

5.2 Runtime comparison

In this section, we compare the methods with respect to runtime and time integration accuracy. We use the same TE model problem, but now choose a manufactured solution which is a polynomial of degree seven in each variable. The spatial discretization uses dG polynomials of degree four. Thus, the exact solution is not represented exactly by the spatial discretization, and the measured error contains the full discretization error. To further reduce the effect of superconvergence, we randomly perturb the mesh. The locally refined mesh has $h_f = 0.00184142$, $h_c = 0.0147314$, and $N = 693\,900$. The L^2 -error is evaluated at the final time $T = 1$.

Figure 6 compares Gauß RK methods with two (purple) and three (orange) stages, with

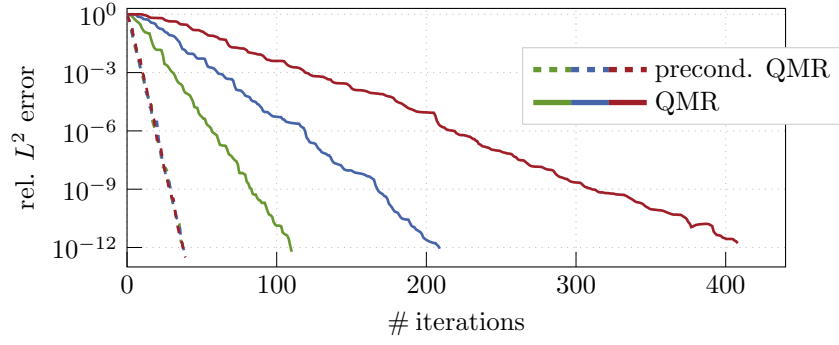


Figure 3: Relative L^2 error versus iteration count for QMR (solid) and preconditioned QMR (dashed) applied to (3.13) with α chosen as in (5.2) and $\tau = 0.05$. Colors denote local refinement levels: 2 (green), 3 (blue), 4 (red).

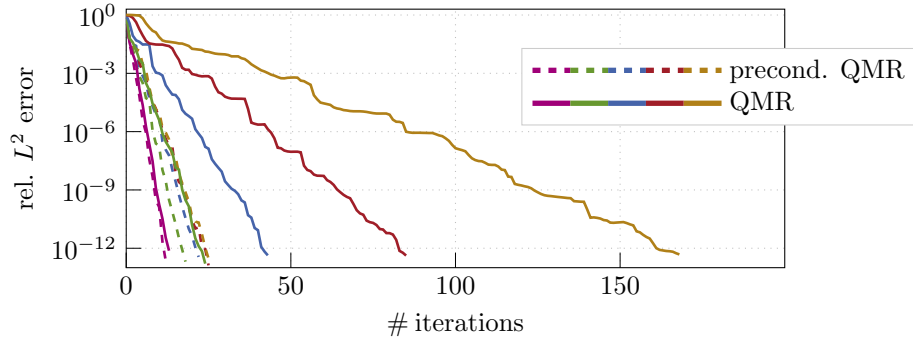


Figure 4: Relative L^2 error versus iteration count for QMR (solid) and preconditioned QMR (dashed) applied to (3.13) with α chosen as in (5.2) and $\tau = 0.01$. Colors denote local refinement levels: 1 (purple), 2 (green), 3 (blue), 4 (red), 5 (orange).

(dashed) and without (solid) preconditioner (4.9), the locally implicit method [33] (blue), a local time-stepping method [32] (green), and the popular low-storage Runge–Kutta method LSRK(12,4) [35] (red). The local time-stepping method uses a Chebyshev-type iteration on the local system instead of solving a linear system like the locally implicit method, thus resulting in a fully explicit method. The degree of the Chebyshev polynomial must be chosen large enough to obtain a CFL condition independent of the stiff part of the system. For the two- and three-stage Gauß RK methods, the preconditioner significantly reduces the runtime at comparable errors. The savings come from the reduced number of QMR iterations for the preconditioned system (4.10a), while the application of the preconditioner (4.9) only requires solves on the fine part and its neighboring coarse elements. The locally implicit and local time-stepping methods are efficient for admissible time stepsizes, but are still restricted by a CFL condition on the coarse mesh and become unstable for larger time stepsizes. Moreover, LSRK(12,4) is only stable for time stepsizes so small that the spatial error dominates. Though it is faster than the unpreconditioned Gauß RK methods, it is slower than the preconditioned variants at nearly the same full discretization accuracy. The Gauß RK methods are unconditionally stable and therefore remain applicable for all time stepsizes.

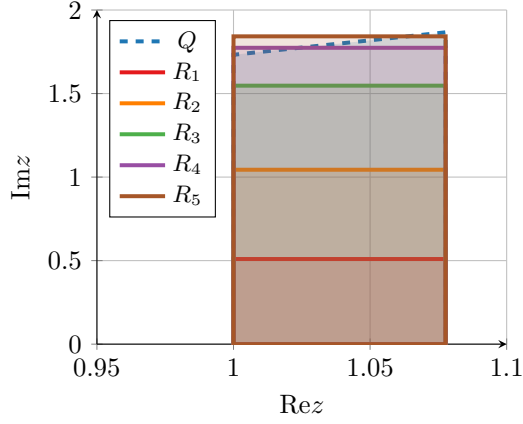


Figure 5: Quadrilateral bounds Q (blue, dashed, identical for all levels) and R_k (solid) for local refinement levels $k = 1, \dots, 5$ (red, orange, green, purple, brown) for preconditioned system (4.10b) with (5.2) and $\tau = 0.01$.

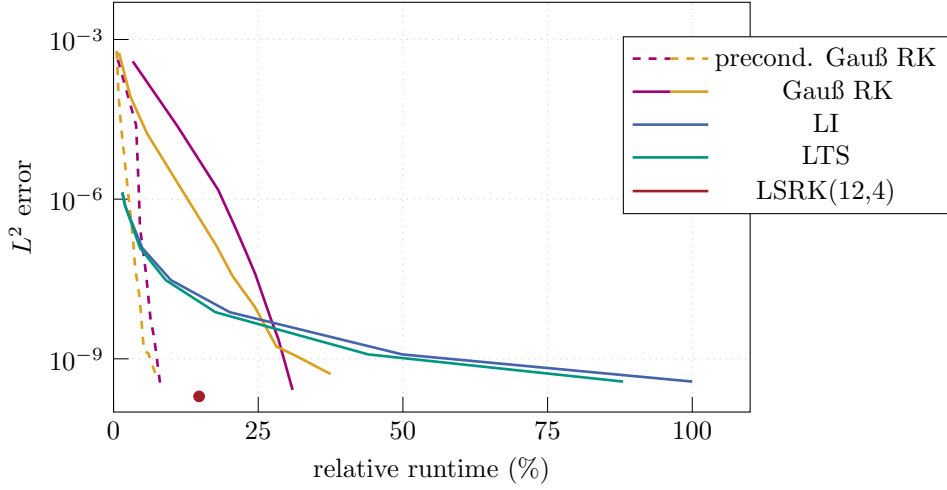


Figure 6: L^2 error at final time $T = 1$ versus relative runtime for Gauß RK with two stages (purple) and three stages (orange), with preconditioner (4.9) (dashed) and without (solid); the locally implicit method (blue); the local time-stepping method (green); and LSRK(12,4) (red marker).

6 Conclusion

In this paper, we proposed and analyzed computationally efficient implicit higher-order time integration methods for solving linear Friedrichs' systems on locally refined spatial grids which consist of a small number of fine and a large number of coarse mesh elements. This is achieved by constructing a preconditioned Krylov subspace method to solve the linear systems arising in each time step of the implicit scheme. Our main result shows that the number of Krylov steps to achieve the desired accuracy can be bounded independently of the fine mesh.

Although we focused on linear Friedrichs' systems, our ideas carry over to nonlinear Friedrichs problems like nonlinear Maxwell's equations, where linear systems of the same type appear in

each iteration of a (simplified) Newton method. Moreover, instead of Gauß collocation methods other implicit time integration schemes might be employed and the preconditioner can also be combined with rational Krylov subspace methods.

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