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Candan Güdücü, Jörg Liesen, Volker Mehrmann, and Daniel B. Szyld

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Department of Mathematics
Temple University
Philadelphia, PA 19122

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ON NON-HERMITIAN POSITIVE (SEMI)DEFINITE LINEAR ALGEBRAIC SYSTEMS ARISING FROM DISSIPATIVE HAMILTONIAN DAEs *

CANDAN GÜDÜCÜ†, JÖRG LIESEN†, VOLKER MEHRMANN†, AND DANIEL B. SZYLD§

Abstract. We discuss different cases of dissipative Hamiltonian differential-algebraic equations and the linear algebraic systems that arise in their linearization or discretization. For each case we give examples from practical applications. An important feature of the linear algebraic systems is that the (non-Hermitian) system matrix has a positive definite or semidefinite Hermitian part. In the positive definite case we can solve the linear algebraic systems iteratively by Krylov subspace methods based on efficient three-term recurrences. We illustrate the performance of these iterative methods on several examples. The semidefinite case can be challenging and requires additional techniques to deal with “singular part”, while the “positive definite part” can still be treated with the three-term recurrence methods.

Key words. dissipative Hamiltonian system, port-Hamiltonian system, descriptor system, differential-algebraic equation, linear algebraic system, positive semidefinite Hermitian part, Krylov subspace method

AMS subject classifications. 65L80, 65F10, 93A15, 93B11, 93B15

1. Introduction. It is well known that every matrix \( A \in \mathbb{C}^{n,n} \) can be split into its Hermitian and skew-Hermitian parts, i.e.,

\[
A = H + S, \quad H = \frac{1}{2}(A + A^*) \quad \text{and} \quad S = \frac{1}{2}(A - A^*),
\]

where \( A^* \) is the Hermitian transpose (or the transpose in the real case) of \( A \), so that \( H = H^* \) and \( S = -S^* \). This simple, yet fundamental observation has many useful applications. For example, Householder used it in [31, p. 69] to show that all eigenvalues of \( A = H + S \) lie in or on the smallest rectangle with sides parallel to the real and imaginary axes that contains all eigenvalues of \( H \) and of \( S \). This result is attributed to Bendixson [9], and was refined by Wielandt [56]. It shows that if \( H \) is positive definite, then all eigenvalues of \( A \) have a positive real part, and therefore such (in general non-Hermitian) matrices \( A \) are sometimes called positive real. Here we call \( A = H + S \) positive definite or positive semidefinite if \( H \) has the corresponding property.

Our first goal in this paper is to show that, while every matrix \( A \in \mathbb{C}^{n,n} \) trivially splits into \( A = H + S \), there is an important class of practically relevant applications where this splitting occurs naturally and has a physical meaning. The class of applications we consider is given by energy-based modeling using differential algebraic equation (DAE) systems in dissipative Hamiltonian (dH) form, or shortly dHDAE systems. The applicability of this modeling approach has been demonstrated in a variety of application areas such as thermodynamics, electromagnetics, fluid mechanics, chemical processes, and general optimization; see, e.g., [15, 20, 27, 28, 29, 49]. Properties of dHDAE systems have been studied in numerous recent publications; see, e.g., [7, 8, 21, 38, 39, 40, 41, 42, 51].

*Version of November 9, 2021.
†Institute of Mathematics, TU Berlin, Straße des 17. Juni 136, 10623 Berlin, Germany. Email: {guducu,liesen,mehrmann}@math.tu-berlin.de.
§Department of Mathematics, Temple University, 1805 N. Broad Street, Philadelphia, PA 19122, USA. Email: szyld@temple.edu.
We systematically discuss different cases of linear and constant-coefficient dHDAE systems, and we illustrate these cases with examples from practical applications. The linear algebraic systems that arise from the linearization and/or discretization of the dHDAE systems are of the form $A = H + S$, where the Hermitian part $H$ (and hence $A$) is positive definite or at least positive semidefinite.

We also discuss how to solve the linear algebraic systems arising from dHDAE systems. In the positive definite case, Krylov subspace methods based on efficient three-term recurrences can be used. The semidefinite case can be challenging and typically requires additional techniques that deal with the “singular part” of $H$, while the “positive definite part” of $H$ still allows an application of three-term recurrence methods. We show that the formulation of the dHDAE system often leads to a linear algebraic system where the “singular part” of $H$ can be identified without much additional effort. For problems where this is not the case we show how on the linear algebraic level the “singular part” of $H$ can be isolated and dealt with using a unitary congruence transformation to a staircase form, and further via Schur complement reduction to a block diagonal form.

The paper is organized as follows. In Section 2 we introduce the standard form of linear and constant-coefficient dHDAE systems, and in Section 3 we give a systematic overview of the different cases of these systems. In Section 4 we discuss the form of linear algebraic systems arising from the time-discretization of dHDAE systems, and we describe a staircase form for these systems. In Section 5 we discuss iterative methods based on three-term recurrences for the discretized systems, and in Section 6 we present numerical examples with these methods applied to different cases of dHDAE systems. The paper ends with concluding remarks in Section 7.

### 2. Linear dissipative Hamiltonian DAE systems

The standard form of a linear dHDAE system, where for simplicity we consider the case of constant (i.e., time-invariant) coefficients, is given by

$$
\begin{align*}
E \dot{x} &= (J - R)Qx + f, \\
x(t_0) &= x^0,
\end{align*}
$$

see [8, 40], where this class is introduced and studied in the context of control problems for port-Hamiltonian (pH) systems. The physical properties of the modeled system are encoded in the algebraic structure of the coefficient matrices. The matrix $E \in \mathbb{C}^{n \times n}$ is called flow matrix, the skew-Hermitian structure matrix $J \in \mathbb{C}^{n \times n}$ describes the energy flux among energy storage elements, the Hermitian positive semidefinite dissipation matrix $R \in \mathbb{C}^{n \times n}$ describes energy loss and/or dissipation. The energy function or Hamiltonian associated with the system (2.1) is given by the function

$$
\mathcal{H}(x) = \frac{1}{2}(x^* Q^* E x),
$$

and typically, since this is an energy, one has that

$$
E^* Q = Q^* E \geq 0,
$$

where $H \geq 0$ means that the Hermitian matrix $H$ is positive semidefinite. Note that (2.3) implies that $\mathcal{H}(x) \geq 0$ for all states $x$.

Linear dHDAE systems of the form (2.1) often arise directly in mathematical modeling, or as a result of linearization along a stationary solution for general, nonlinear dHDAE systems; see, e.g., [42]. In many applications, furthermore, the matrix $Q$ is
the identity, and if not, it can be turned into an identity for a subsystem; see [41, Section 6.3]. Thus, in the following we restrict ourselves to dHDAE systems of the form

\begin{equation}
E \dot{x} = (J - R)x + f, \quad \text{where} \quad E = E^* \geq 0, \quad J = -J^*, \quad R = R^* \geq 0.
\end{equation}

For analyzing the system (2.4) it is useful to transform it into a \textit{staircase form} that reveals its “positive definite part” and its “singular part”, as well as the common nullspaces (if any) of the different matrices. Such a form was derived using a sequence of spectral and singular value decompositions in [1, Lemma 5], and is adapted here to our notation.

\textbf{Lemma 2.1.} For every dHDAE system of the form (2.4) there exists a unitary (basis transformation) matrix \(\tilde{V} \in \mathbb{C}^{n,n}\), such that the system in the new variable

\[
\tilde{x} = \tilde{V}^* x = \begin{bmatrix}
\tilde{x}_1 \\
\tilde{x}_2 \\
\tilde{x}_3 \\
\tilde{x}_4 \\
\tilde{x}_5 \\
\end{bmatrix}
\]

has the \(5 \times 5\) block form

\begin{align}
\begin{bmatrix}
E_{11} & E_{12} & 0 & 0 & 0 \\
E_{21} & E_{22} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
\dot{\tilde{x}}_1 \\
\dot{\tilde{x}}_2 \\
\dot{\tilde{x}}_3 \\
\dot{\tilde{x}}_4 \\
\dot{\tilde{x}}_5 \\
\end{bmatrix} &=
\begin{bmatrix}
J_{11} - R_{11} & J_{12} - R_{12} & J_{13} - R_{13} & J_{14} & 0 \\
J_{21} - R_{21} & J_{22} - R_{22} & J_{23} - R_{23} & 0 & 0 \\
J_{31} - R_{31} & J_{32} - R_{32} & J_{33} - R_{33} & 0 & 0 \\
J_{41} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
\tilde{x}_1 \\
\tilde{x}_2 \\
\tilde{x}_3 \\
\tilde{x}_4 \\
\tilde{x}_5 \\
\end{bmatrix} +
\begin{bmatrix}
f_1(t) \\
f_2(t) \\
f_3(t) \\
f_4(t) \\
f_5(t) \\
\end{bmatrix},
\end{align}

where \(n_1, n_2, n_3, n_4, n_5 \in \mathbb{N}_0\), and \(n_1 = n_4\). If it is present in (2.5), the matrix

\[
\begin{bmatrix}
E_{11} & E_{12} \\
E_{21} & E_{22} \\
\end{bmatrix}
\]

(or just \(E_{22}\) if \(n_1 = n_4 = 0\)) is Hermitian positive definite, and if they are present in (2.6), the matrices \(J_{33} - R_{33}\) and \(J_{41} = -J_{14}^*\) are nonsingular.

From the staircase form (2.5)–(2.6) we immediately see that the initial value problem (2.4) is uniquely solvable (for consistent initial values and sufficiently often differentiable inhomogeneities \(f\)) if and only if the last block row and column in the matrices (which contain only zeros) do not occur, i.e., if \(n_5 = 0\). If \(n_5 \neq 0\), then \(\tilde{x}_5\) can be chosen arbitrarily. In the following we assume that \(n_5 = 0\), i.e., we assume throughout that (2.4) is uniquely solvable. Equivalently, we assume that the pencil \(\lambda E - (J - R)\) is regular.

As shown in [1, Corollary 1], the differentiation index (i.e., the size of the largest Jordan block associated with the eigenvalue \(\infty\)) of a regular pencil \(\lambda E - (J - R)\) in terms of the staircase form (2.5)–(2.6) is given by

zero if and only if \(n_1 = n_4 = 0\) and \(n_3 = 0\) (or simply \(n_2 = n\)),

one if and only if \(n_1 = n_4 = 0\) and \(n_3 > 0\),

two if and only if \(n_1 = n_4 > 0\).
These are all possible cases that can occur. It is easy to see that the positive definite case \( E = E^* > 0 \) in (2.4) corresponds to a staircase form (2.5)–(2.6) with \( n_2 = n \) and hence to the index zero, regardless of the properties of \( J \) and \( R \). On the other hand, a singular matrix \( E = E^* \geq 0 \) corresponds to an index either one or two, depending on the relation between the matrices \( E, J, R \). Distinguishing between these three cases will be important in our overview in the next section.

In numerical practice, a computation of the form (2.5)–(2.6) for a given dHDAE system requires a sequence of nullspace computations, which can be carried out by singular value decompositions. Unfortunately, these sequences of dependent rank decisions may be very sensitive under perturbations; see, e.g., [13] where the construction of similar staircase forms and the challenges are discussed. Also, these factorizations are often not efficiently computable for large-scale problems. However, as we will demonstrate with several examples in the next section, in many cases the structural properties arising from physical modeling help to make this process easier.

3. Different cases and specific examples. We will now present a systematic overview of different cases of systems of the forms (2.4) or (2.5)–(2.6) that occur in applications, ordered by properties of \( E \) and the index of the (regular) pencil \( \lambda E - (J - R) \). The examples given in this section demonstrate the large variety of applications for dHDAEs.

Case 1: Positive definite \( E \), index zero. The case of \( E = E^* > 0 \) in (2.4), or \( n_2 = n \) in (2.5)–(2.6), is the “simplest” one. This case usually leads to a positive definite Hermitian part of the coefficient matrix in the linear algebraic system; see Section 4 below.

Example 3.1 (index zero). Consider the classical second order representation of a linear damped mechanical system, which is given by

\[
M\ddot{x} + D\dot{x} + Kx = f,
\]

where \( M, D, K \in \mathbb{R}^{n,n} \) are Hermitian matrices with \( M,K > 0 \) and \( D \geq 0 \); see, e.g., [53, Chapter 1]. By introducing the variables, \( \hat{x}_2 = x \) and \( \hat{x}_1 = \dot{x} \), equation (3.1) can be written as

\[
\begin{bmatrix}
M & 0 \\
0 & K
\end{bmatrix}
\begin{bmatrix}
\dot{\hat{x}}_1 \\
\dot{\hat{x}}_2
\end{bmatrix}
= \left(\begin{bmatrix}
0 & -K \\
K & 0
\end{bmatrix} - \begin{bmatrix}
D & 0 \\
0 & 0
\end{bmatrix}\right)
\begin{bmatrix}
\hat{x}_1 \\
\hat{x}_2
\end{bmatrix}
+ \begin{bmatrix}
f \\
0
\end{bmatrix},
\]

which is of the form (2.4) with \( E = \begin{bmatrix} M & 0 \\ 0 & K \end{bmatrix} = E^* > 0 \).

Example 3.2 (index zero). The discretization of the poroelasticity equations that model the deformation of porous media saturated by an incompressible viscous fluid in first order formulation as in [2, Section 3.4] leads to a dHDAE of the form

\[
\begin{bmatrix}
Y & 0 & 0 \\
0 & A & 0 \\
0 & 0 & M
\end{bmatrix}
\begin{bmatrix}
\dot{w} \\
\dot{u} \\
\dot{p}
\end{bmatrix}
= \left(\begin{bmatrix}
0 & -A \\
A & 0 \\
-D & 0
\end{bmatrix} - \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & K
\end{bmatrix}\right)
\begin{bmatrix}
w \\
u \\
p
\end{bmatrix}
+ \begin{bmatrix}
f \\
g
\end{bmatrix},
\]

where \( A,M,Y \) are Hermitian positive definite (where \( Y \) is of very small norm), \( K \) is typically Hermitian positive semidefinite, and \( D \) is general, non-Hermitian. Here \( u \) represents the discretized displacement field, \( w \) the associated discretized velocities, and \( p \) the discretized pressure. Again we have a system of the form (2.4) with \( E = \text{diag}(Y,A,M) = E^* > 0 \).
Case 2: Positive semidefinite $E$, index one. In this case we have a staircase form (2.5)–(2.6) with $n_1 = n_4 = 0$ and $n_3 \neq 0$, which after renumbering the equations and unknowns can be written as

\begin{equation}
\begin{bmatrix}
E_{11} & 0 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
\dot{x}_1 \\
\dot{x}_2
\end{bmatrix}
= \begin{bmatrix}
J_{11} - R_{11} & J_{12} - R_{12} \\
J_{21} - R_{21} & J_{22} - R_{22}
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2
\end{bmatrix}
+ f,
\end{equation}

where $E_{11} = E_{*11} > 0$ and where $J_{22} - R_{22}$ is nonsingular. Note that if it is known in advance that the given dHDAE has index one, the form (3.4) can be obtained from (2.4) by a single (unitary) transformation that “splits off” the nullspace of $E$. Whether the coefficient matrix $A = H + S$ of the corresponding linear algebraic system (after time discretization) in this case has a positive definite or semidefinite Hermitian part $H$ depends on the properties of $R_{22}$. The Hermitian part is of the form $H = E + \frac{\tau}{2} R$ (see Section 4 below), and hence a positive definite $R_{22}$ will lead to a positive definite $H$, which may be (highly) ill-conditioned, since $R$ is multiplied by the potentially small constant $\tau/2$.

**Figure 3.1:** A simple RLC circuit

**Example 3.3 (index one).** Consider the linear RLC circuit shown in Figure 3.1 (see [42, Example 4.1]), which is modeled by the following equations:

\begin{align*}
L\ddot{I} &= -R_L I + V_2 - V_1, \\
C_1 \dot{V}_1 &= I - I_G, \\
C_2 \dot{V}_2 &= -I - I_R, \\
0 &= -R_G I_G + V_1 + E_G, \\
0 &= -R_R I_R + V_2.
\end{align*}

Here $R_G, R_L, R_R > 0$ represent resistances, $L > 0$ inductances, $C_1, C_2 > 0$ capacitances, and $E_G$ a controlled voltage source. The equations can be written in the form (3.4) with $E = \text{diag}(L, C_1, C_2, 0, 0)$, the vector of unknowns $x = [I^*, V_1^*, V_2^*, I_G^*, I_R^*]^*$,

\begin{equation}
J = \begin{bmatrix}
0 & -1 & 1 & 0 & 0 \\
1 & 0 & 0 & -1 & 0 \\
-1 & 0 & 0 & 0 & -1 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0
\end{bmatrix}, \quad R = \begin{bmatrix}
R_L & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & R_G & 0 \\
0 & 0 & 0 & 0 & R_R
\end{bmatrix},
\end{equation}

so that $E_{11} = E_{*11} = \text{diag}(L, C_1, C_2) > 0$, and $J_{22} - R_{22} = -\text{diag}(R_G, R_R)$ is non-singular, and the nullspace of $E$ is displayed directly. Note that most RLC circuits (potentially with millions of equations and unknowns) have this index one structure, but occasionally they have index two [18].
Example 3.4 (index one). The space discretization of the unsteady incompressible Stokes or linearized Navier-Stokes equations via finite element or finite difference methods typically leads to dHDAE systems of the form

$$
\begin{bmatrix}
M & 0 \\
0 & 0
\end{bmatrix} \begin{bmatrix}
\dot{v} \\
\dot{\rho}
\end{bmatrix} = \begin{bmatrix}
A_S & B \\
-B^* & 0
\end{bmatrix} - \begin{bmatrix}
-A_H & 0 \\
0 & -C
\end{bmatrix} \begin{bmatrix}
v \\
p
\end{bmatrix} + \begin{bmatrix}
f \\
g
\end{bmatrix},
$$

where $M = M^* > 0$ is the mass matrix, $A_S = -A_S^*$, $B^*$ is the discretized divergence operator (normalized so that it is of full row rank), $-A_H = -A_H^* > 0$, and $-C = -C^* > 0$ is a stabilization term, typically of small norm; see, e.g., [17]. In the Stokes case we usually have $A_S = 0$. Here $v$ and $p$ denote the discretized velocity and pressure, respectively. In terms of (3.4) we have the Hermitian positive definite matrix $E_{11} = M$, and the nonsingular matrix $J_{22} - R_{22} = -C$.

**Case 3: Positive semidefinite $E$, index two.** In this case we have a staircase form (2.5)–(2.6) with $n_1 = n_2 > 0$.

Example 3.5 (index two). Consider Example 3.2 in the quasi-stationary regime (see [46]), where one usually sets $Y = 0$. After a permutation of the block rows, the system has the form

$$
\begin{bmatrix}
M & 0 & 0 \\
0 & A & 0 \\
0 & 0 & 0
\end{bmatrix} \begin{bmatrix}
\dot{\rho} \\
\dot{u} \\
\dot{w}
\end{bmatrix} = \begin{bmatrix}
0 & 0 & -D \\
0 & 0 & A \\
0 & 0 & 0
\end{bmatrix} \begin{bmatrix}
\dot{v} \\
\dot{g} \\
\dot{f}
\end{bmatrix} - \begin{bmatrix}
K & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix} \begin{bmatrix}
p \\
u \\
0
\end{bmatrix} + \begin{bmatrix}
0 \\
0 \\
f
\end{bmatrix},
$$

with $A = A^*$, $M = M^*$ positive definite. The form (2.5)–(2.6) with $n_3 = 0$ is obtained by performing a QR decomposition of the full row rank matrix $[D^* - A]$, and then transforming the system accordingly.

Example 3.6 (index two). Consider Example 3.4 without stabilization, i.e., with $C = 0$. Let $B^* = U_B \Sigma V_B^*$ be a singular value decomposition with unitary matrices $U_B, V_B$, and a nonsingular diagonal matrix $\Sigma$ (corresponding to the splitting of the space of functions into the subspace of divergence free functions and its orthogonal complement). After a unitary similarity transformation we obtain a staircase form (2.5)–(2.6) with $n_3 = 0$ as follows:

$$
\begin{bmatrix}
M_{11} & M_{12} & 0 \\
M_{21} & M_{22} & 0 \\
0 & 0 & 0
\end{bmatrix} \begin{bmatrix}
\dot{v}_1 \\
\dot{v}_2 \\
\dot{\rho}
\end{bmatrix} = \begin{bmatrix}
A_{11} & A_{12} & \Sigma \\
A_{21} & A_{22} & 0 \\
-\Sigma & 0 & 0
\end{bmatrix} \begin{bmatrix}
\dot{v}_1 \\
\dot{v}_2 \\
\dot{\rho}
\end{bmatrix} + \begin{bmatrix}
\dot{f}_1 \\
\dot{f}_2 \\
0
\end{bmatrix}.
$$

4. **Obtaining and transforming the linear algebraic system.** In order to simulate the dynamical behavior of dHDAEs, time-discretization methods have to be employed. In a general (non-linear) setting this is not an easy task, since the methods have to be implicit and they should be structure preserving. Based on an ansatz derived for standard pH systems in [35], such methods were derived for dHDAE systems in [42]. It was shown, in particular, that Gauss-Legendre collocation methods, like the implicit midpoint rule, are well suited for this purpose.

Here we continue to consider a linear dHDAE system of the form (2.4). Choosing, e.g., a uniform time grid $t_0, \ldots, t_N$ with step size $\tau > 0$, the implicit midpoint rule yields a sequence of linear algebraic systems of the form

$$
\left(E + \frac{\tau}{2}(R - J)\right)x_{k+1} = b(x_k, \tau)
$$
for the time-discrete vectors $x_k = x(t_k)$, $k = 0, 1, 2, \ldots$. The linear algebraic system (4.1) is of the form

\begin{equation}
(4.2) \quad Ax = b \quad \text{with} \quad A = H + S, \quad \text{where} \quad H = E + \frac{\tau}{2} R \quad \text{and} \quad S = -\frac{\tau}{2} J.
\end{equation}

Thus, the splitting $A$ into its Hermitian and skew-Hermitian parts is a natural consequence of the underlying mathematical model. By construction, the Hermitian part is positive definite or positive semidefinite. Moreover, in many cases, for any matrix norm we have $H \rightarrow E$ and $S \rightarrow 0$ as $\tau \rightarrow 0$, so that for small step sizes $\tau$ we can expect that the Hermitian part is dominant. This observation is of interest in the context of iteratively solving (4.2); see Section 5 below.

Iterative methods for solving systems of the form (4.2) are often based on the assumption that $H$ is (positive) definite and hence nonsingular; see Section 5 below for examples. In case of a singular matrix $H$, it is advantageous to identify its “singular part” and treat it separately in the numerical solution algorithm. As shown in Section 3, the mathematical modeling frequently leads to a staircase form (2.5)–(2.6) with block matrices, where the “singular part” of $H$ is readily identified. If this is not possible on the modeling level, one can apply an appropriate reduction (at least in theory, or for small scale practical problems) on the algebraic level. Well-known techniques from the literature that can be applied also in this context include Schur complement constructions or null-space deflation; see, e.g., [12, 25, 54]. We will now show how to transform $A$ into its Hermitian and skew-Hermitian parts is a natural consequence of the underlying mathematical model. By construction, the Hermitian part $A$ is positive definite or positive semidefinite. Moreover, in many cases, for any matrix $A$ we can expect that the Hermitian part is dominant. This observation is of interest in the context of iteratively solving (4.2); see Section 5 below.

The following result is a special case of the controllability staircase form [52]; see also [1]. We present the proof because some of its features will be used later.

**Lemma 4.1.** Consider $A = H + S \in \mathbb{C}^{n \times n}$, where $0 \neq H = H^* \geq 0$ and $0 \neq S = -S^*$. Then there exist a unitary matrix $U \in \mathbb{C}^{n \times n}$, and integers $n_1 \geq n_2 \geq \cdots \geq n_{r-1} > 0$ and $n_r \geq 0$, such that

\begin{equation}
(4.3) \quad U^* H U = \begin{bmatrix}
H_{11} & 0 \\
0 & 0
\end{bmatrix}
\quad \text{and} \quad
U^* S U = \begin{bmatrix}
S_{11} & S_{12} & & 0 \\
S_{21} & S_{22} & \ddots & 0 \\
& \ddots & \ddots & S_{r-2,r-1} \\
0 & \cdots & \cdots & S_{r-1,r-1} 0
\end{bmatrix},
\end{equation}

where $H_{11} = H_{11}^* \in \mathbb{C}^{n_1 \times n_1}$ is positive definite, $S_{ii} = -S_{ii}^* \in \mathbb{C}^{n_i \times n_i}$ for $i = 1, \ldots, r$, and $S_{i,i-1} = -S_{i-1,i}^* = [\Sigma_{i,i-1} 0] \in \mathbb{C}^{n_i \times n_{i-1}}$ with $\Sigma_{i,i-1}$ being nonsingular for $i = 2, \ldots, r-1$.

**Proof.** The result is trivial when $H$ is nonsingular (and thus positive definite), since in this case it holds with $U = I$, $r = 2$, $n_1 = n$, and $n_2 = 0$.

Let $0 \neq H = H^* \geq 0$ be singular. We consider a full rank decomposition of $H$ with a unitary matrix $U_1 \in \mathbb{C}^{n \times n}$,

\begin{equation}
(4.4) \quad U_1^* H U_1 = \begin{bmatrix}
\hat{H}_{11} & 0 \\
0 & 0
\end{bmatrix},
\end{equation}

where we assume that $\hat{H}_{11} = \hat{H}_{11}^* \in \mathbb{C}^{n_1 \times n_1}$, with $1 \leq n_1 < n$, is positive definite. Note that this factorization can be obtained from any rank-revealing factorization (e.g., QR
or SVD) and then applying the orthogonal factor via a congruence transformation. Applying the same unitary similarity transformation to $S$ gives the matrix

\[(4.5) \quad \hat{S} = U_1^* S U_1 = \begin{bmatrix} \hat{S}_{11} & \hat{S}_{12} \\ \hat{S}_{21} & \hat{S}_{22} \end{bmatrix},\]

where $\hat{S}_{11} \in \mathbb{C}^{n_1 \times n_1}$, and $\hat{S}_{21} = -\hat{S}_{12}^*$, since $S$ is skew-Hermitian. If $\hat{S}_{21} = 0$, then we are done. Otherwise, let

$$\hat{S}_{21} = W_2 \begin{bmatrix} \Sigma_{21} & 0 \\ 0 & 0 \end{bmatrix} V_2^*$$

be a singular value decomposition, where $\Sigma_{21}$ is nonsingular (and diagonal), and $W_2 \in \mathbb{C}^{n_1 \times n_1}$ and $V_2 \in \mathbb{C}^{n-n_1 \times n-n_1}$ are unitary. We define $U_2 = \text{diag}(V_2, W_2) \in \mathbb{C}^{n \times n}$, which is unitary. Applying a unitary similarity transformation with this matrix to (4.4) and (4.5) yields

$$U_2^* U_1^* H U_1 U_2 = \begin{bmatrix} V_2^* \hat{H}_{11} V_2 & 0 \\ 0 & 0 \end{bmatrix},$$

where $V_2^* \hat{H}_{11} V_2 \in \mathbb{C}^{n_1 \times n_1}$ is Hermitian positive definite, and

$$U_2^* U_1^* S U_1 U_2 = \begin{bmatrix} V_2^* \hat{S}_{11} V_2 & V_2^* \hat{S}_{12} W_2 \\ W_2^* \hat{S}_{21} V_2 & W_2^* \hat{S}_{22} W_2 \end{bmatrix} = \begin{bmatrix} \tilde{S}_{11} & \tilde{S}_{12} & 0 \\ \tilde{S}_{21} & \tilde{S}_{22} & \tilde{S}_{23} \\ 0 & \tilde{S}_{32} & \tilde{S}_{33} \end{bmatrix}.$$

where $\tilde{S}_{21} = [\Sigma_{21} \ 0]$. If $\tilde{S}_{32} = 0$ or $\tilde{S}_{32} = []$, we are done. Otherwise we continue inductively with the singular value decomposition of $\tilde{S}_{32}$, and after finitely many steps we obtain a decomposition of the required form.

If for a given matrix $A = H + S$ the transformation to the staircase form (4.3) is known, then the equivalent linear algebraic system $(U^*AU)(U^*x) = U^*b$ can be solved using block Gaussian elimination. This amounts to solving a sequence of linear algebraic systems having successive Schur complements as their coefficient matrices. Let us have a closer look at this process.

For simplicity of notation, we set $\tilde{A}_{11} = H_{11} + S_{11}$. By construction, this matrix is (non-Hermitian) positive definite. The set of (non-Hermitian) positive definite matrices is closed under inversion; see, e.g., [34, p. 10]. Hence $\tilde{A}_{11}^{-1}$ exists and is also positive definite. Then in the simplest nontrivial case of the staircase form (namely, $r = 3$) we can write

$$U^*AU = \begin{bmatrix} \tilde{A}_{11} & S_{12} & 0 \\ S_{21} & S_{22} & 0 \\ 0 & 0 & S_{33} \end{bmatrix} = \begin{bmatrix} I & 0 & 0 \\ S_{21} \tilde{A}_{11}^{-1} & I & 0 \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} \tilde{A}_{11} & 0 & 0 \\ 0 & S_{1} & 0 \\ 0 & 0 & S_{33} \end{bmatrix} \begin{bmatrix} I & \tilde{A}_{11}^{-1} S_{12} & 0 \\ 0 & 0 & I \end{bmatrix},$$

where $S_{1} = S_{22} - S_{21} \tilde{A}_{11}^{-1} S_{12}$ is the Schur complement of $\tilde{A}_{11}$ in the top $2 \times 2$ block. Note that the inverses of the first and third matrix in the above factorization of $U^*AU$ are obtained by simply negating the off-diagonal blocks.
Since $\hat{A}_{11}^{-1}$ is positive definite, this matrix can be written as

$$\hat{A}_{11}^{-1} = \hat{H}_{11} + \hat{S}_{11}$$

for some matrices $\hat{H}_{11} = \hat{H}_{11} > 0$ and $\hat{S}_{11} = -\hat{S}_{11}^*$. The Schur complement then is of the form

$$S_1 = S_{22} - S_{21}\hat{A}_{11}^{-1}S_{12} = S_{22} - S_{21}(\hat{H}_{11} + \hat{S}_{11})S_{12} = (S_{21}\hat{H}_{11}S_{21}^*) + (S_{22} + S_{21}\hat{S}_{11}S_{21}^*),$$

where we have used that $S_{12} = -S_{21}^*$. The Hermitian part of the Schur complement is given by

$$S_{21}\hat{H}_{11}S_{21}^* = \Sigma_{21} [I 0] \hat{H}_{11} \left[ \begin{array}{c} I \\ 0 \end{array} \right] \Sigma_{21}^*.$$

By the Cauchy interlacing theorem, the eigenvalues of $[I 0] \hat{H}_{11} \left[ \begin{array}{c} I \\ 0 \end{array} \right]$ strictly interlace the eigenvalues of $\hat{H}_{11}$. Consequently this matrix, and thus the Hermitian part and by definition $S_1$ are positive definite.

Suppose that we have a further block row in the staircase form, i.e., $r = 4$. Then we can write

$$U^*AU = \left[ \begin{array}{cccc}
I & 0 & 0 & 0 \\
S_{21}\hat{A}_{11}^{-1} & I & 0 & 0 \\
0 & 0 & I & 0 \\
0 & 0 & 0 & I
\end{array} \right] \left[ \begin{array}{cccc}
\hat{A}_{11} & 0 & 0 & 0 \\
0 & S_1 & S_{23} & 0 \\
0 & 0 & S_{33} & 0 \\
0 & 0 & 0 & S_{44}
\end{array} \right] \left[ \begin{array}{cccc}
I & \hat{A}_{11}^{-1}S_{12} & 0 & 0 \\
0 & I & 0 & 0 \\
0 & 0 & I & 0 \\
0 & 0 & 0 & I
\end{array} \right],$$

where the Schur complement $S_1$ is positive definite. Using the same idea as above then gives another Schur complement $S_2 = S_{33} - S_{32}S_{11}^{-1}S_{23}$, which again is positive definite. Using this block Gaussian elimination procedure inductively we obtain the following result.

**Lemma 4.2.** In the notation of Lemma 4.1, the matrix $U^*AU$ can be transformed via Schur complement reduction into the block diagonal form

$$\left[ \begin{array}{cccc}
\hat{A}_{11} & S_1 & & \\
& \ddots & & \\
& & S_{r-2} & \\
& & & S_{rr}
\end{array} \right],$$

where $\hat{A}_{11} = H_{11} + S_{11}$ and the Schur complements $S_1, \ldots, S_{r-2}$ are positive definite. Moreover, the skew-Hermitian $S_{rr}$ may not be always present.

Lemma 4.2 shows that the successive formation of Schur complements leads a block diagonal matrix with all but the last block being positive definite, so that the nullspace can be obtained just from the last block.

**Example 4.1.** Consider Example 3.6 with

$$E = \left[ \begin{array}{ccc}
M_{11} & M_{12} & 0 \\
M_{21} & M_{22} & 0 \\
0 & 0 & 0
\end{array} \right], \quad J = \left[ \begin{array}{ccc}
0 & 0 & \Sigma \\
0 & 0 & 0 \\
-\Sigma & 0 & 0
\end{array} \right], \quad R = \left[ \begin{array}{ccc}
-A_{11} & -A_{12} & 0 \\
-A_{21} & -A_{22} & 0 \\
0 & 0 & 0
\end{array} \right].$$
Then $A = H + S$ is already in the staircase form (4.3) with
\[
H_{11} = \begin{bmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22}
\end{bmatrix} + \frac{\tau}{2} \begin{bmatrix}
-A_{11} & -A_{12} \\
-A_{21} & -A_{22}
\end{bmatrix}, \quad S = \begin{bmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{bmatrix} = \begin{bmatrix}
0 & 0 & -\frac{\tau}{2} \Sigma \\
0 & 0 & 0 \\
\frac{\tau}{2} \Sigma & 0 & 0
\end{bmatrix}.
\]

In the notation of Lemma 4.1 we have $r = 3$, and $n_1 \geq n_2 > 0 = n_3$. In order to obtain the block diagonal form of Lemma 4.2 we have to form the Schur complement
\[
S_1 = \frac{\tau^2}{4} [\Sigma \ 0] H_{11}^{-1} [\Sigma] [0]
\]
which is positive definite.

The following corollary follows immediately from Lemma 4.2 and the fact that the Schur complement of a skew-Hermitian matrix is again skew-Hermitian.

**Corollary 4.3.** Every Schur complement of a matrix with positive semidefinite Hermitian part is again a matrix with this property.

In [48] a similar result is shown for symmetric multiple saddle point problems in block tridiagonal form, that is to say, all consecutive Schur complements are positive definite, given that the most upper-left block is positive definite.

5. **Iterative methods for the linear algebraic systems.** In this section we discuss iterative methods for linear algebraic systems of the form $Ax = b$ with $A = H + S$.

A widely known method in this context is the HSS iteration, which was introduced in [5]. Given an initial vector $x^{(0)}$ and some constant $\alpha > 0$, the HSS iteration successively solves linear algebraic systems with the (shifted) Hermitian and skew-Hermitian parts of $A$ by computing
\[
(\alpha I + H)x^{(k+\frac{1}{2})} = (\alpha I - S)x^{(k)} + b,
\]
\[
(\alpha I + S)x^{(k+1)} = (\alpha I - H)x^{(k+\frac{1}{2})} + b,
\]
for $k = 1, 2, \ldots$. There are numerous variants and extensions of the HSS iteration; see, e.g., [3, 4, 5, 6, 10, 36] or [12, Section 10.3] for a summary of some results. As shown in [5, Theorem 2.2], the HSS iteration with exact “inner solves” with $\alpha I + H$ and $\alpha I + S$ converges for every $\alpha > 0$, provided that $H$ (and hence $A$) is positive definite. However, in [11] it was noted that the convergence speed of the HSS iteration is usually too slow to be competitive with other iterative methods, even when $\alpha$ is chosen optimally (in the sense that it minimizes the spectral radius of the iteration matrix). Therefore the HSS iteration is recommended to be used as a preconditioner rather than as an iterative solver.

We will here focus on another approach, introduced in [55] (also see the earlier paper [14]), which suggests to solve, instead of $Ax = b$ with $A = H + S$, the equivalent system
\[
(I + K)x = \hat{b}, \quad \text{where} \quad K = H^{-1}S, \quad \hat{b} = H^{-1}b.
\]

This transformation can be interpreted as a preconditioning of the original system with its Hermitian part, which of course requires that $H$ is nonsingular. If we again assume that $H$ is positive definite, then this matrix defines the $H$-inner product $\langle x, y \rangle_H = y^* H x$. The adjoint of $K$ with respect to the $H$-inner product, or simply the $H$-adjoint, is given by
\[
H^{-1}K^* H = H^{-1}(S^* H^{-1})H = -K,
\]
hence the matrix $K$ is $H$-normal(1), which is a necessary and sufficient condition for $K$ to admit an optimal three-term recurrence for generating an $H$-orthogonal basis of the Krylov subspaces $K_k(K, v)$ for each initial vector $v$; see [37, Theorem 4.6.2]. (Note that, in addition, this implies that $K$ is diagonalizable and its eigenvalues lie on a line in the complex plane.) This fact can be used for constructing Krylov subspace methods based on three-term recurrences for solving the system (5.1). The method of [55] and a minimal residual method of [43] are early and important examples. These methods appear to be neither widely known nor thoroughly studied, with [50] being one of the few publications mentioning both methods. We will therefore summarize some details on their implementation and mathematical properties here.

We first note that in matrix terms the three-term recurrence for generating an $H$-orthogonal basis of $K_k(K, \hat{b})$ yields a Lanczos relation of the form

$$KV_k = V_{k+1}T_{k+1,k},$$

where $\text{Span}(V_k) = K_k(K, \hat{b})$, $V_k^*HV_k = I_k$, and $T_{k+1,k}$ is tridiagonal and skew-Hermitian. Note that $V_k^*SV_k = V_k^*HV_kT_{k+1,k} = T_{k,k}$.

### 5.1. Widlund’s method.

The method of Widlund [55] is an oblique projection method with iterates $x_k^W$ determined by

$$x_k^W \in K_k(K, \hat{b}) \quad \text{such that} \quad r_k^W = b - Ax_k^W \perp K_k(K, \hat{b}).$$

Using the Lanczos relation (5.2), we have $x_k^W = V_ky_k$ for some vector $y_k$ that is computed using the orthogonality property, i.e.,

$$0 = V_k^*r_k^W = V_k^*(b - (H + S)V_ky_k) = V_k^*H\hat{b} - (V_k^*HV_k + V_k^*SV_k)y_k = \|\hat{b}\|_{He1} - (I_k + T_{k,k})y_k.$$

The system $(I_k + T_{k,k})y_k = \|\hat{b}\|_{He1}$ with the $k \times k$ skew-Hermitian matrix $I_k + T_{k,k}$ can be solved efficiently.

In [16, 26, 50] optimality properties are shown for the even and odd subsequences $\{x_{2k}^W\}$ and $\{x_{2k+1}^W\}$, namely that

$$\|x - x_{2k}^W\|_H = \min_{z \in (I - K)K_{2k}(K, \hat{b})} \|x - z\|_H,$$

and similarly for the odd subsequence. The eigenvalues of $K$ are purely imaginary. Let $i[-\lambda, \lambda]$ for some $\lambda > 0$ be the smallest interval that contains these eigenvalues. Then, similar to the CG method [30], the optimality property of Widlund’s method leads to an error bound of the form

$$\|x - x_{2k}^W\|_H \leq 2 \left(\frac{\sqrt{1 + \lambda^2} - 1}{\sqrt{1 + \lambda^2} + 1}\right)^k,$$

and the same bound holds for the sequence $\|x - x_{2k+1}^W\|_H / \|x - x_{1}^W\|_H$; see [16] or [50, Theorem 4.2]. The bound indicates that a “fast” convergence of the method can be expected when $\lambda > 0$ is “small”.

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5.2. Rapoport’s method. The method of Rapoport [43] is a minimal residual method with iterates \( x_k^R \) determined by

\[
x_k^R \in K_k(K, \hat{b}) \quad \text{such that} \quad r_k^R = b - Ax_k^R \perp (I + K)K_k(K, \hat{b}).
\]

Since the Lanczos relation (5.2) can be written as

\[ (I + K)V_k = V_{k+1} \begin{bmatrix} I_k + T_{k,k} \\ t_{k+1,k} e_k \end{bmatrix} = V_{k+1} \tilde{T}_{k+1,k}, \]

we obtain \( x_k^R = V_k y_k \) for some vector \( y_k \) determined by the orthogonality property, i.e.,

\[
0 = ((I + K)V_k)^* r_k^R = \tilde{T}_{k+1,k}^* V_{k+1}^* K (\hat{b} - (I + K)V_k y_k)
= \|\hat{b}\|_H \tilde{T}_{k+1,k}^* e_1 - \tilde{T}_{k+1,k}^* \tilde{T}_{k+1,k} y_k.
\]

Equivalently, \( y_k \) is the solution of the least squares problem

\[
\min_{y_k} \|\| \hat{b}\|_H e_1 - \tilde{T}_{k+1,k} y_k \|_2,
\]

which can again be solved efficiently, since \( \tilde{T}_{k+1,k} \) is tridiagonal.

Since \( A = H(I + K) \), we have \( r_k^R = H(I + K)(x - x_k^R) \), and we can write the orthogonality property in (5.4) as

\[
x - x_k^R \perp_B K_k(I + K, \hat{b}) = K_k(K, \hat{b}),
\]

where \( B \equiv (I + K)^* H(I + K) \) is Hermitian positive definite. Since \( x_k^R \in K_k(K, \hat{b}) \), this is mathematically equivalent to the optimality property

\[
\|x - x_k^R\|_B = \min_{z \in K_k(K, \hat{b})} \|x - z\|_B;
\]

see [37, Theorem 2.3.2]. We thus obtain

\[
\|b - Ax_k^R\|_{H^{-1}} = \|H^{-1}(b - Ax_k^R)\|_H = \|(I + K)(x - x_k^R)\|_H = \|x - x_k^R\|_B = \min_{z \in K_k(K, \hat{b})} \|x - z\|_B
= \min_{z \in K_k(K, \hat{b})} \|\hat{b} - (I + K)z\|_H = \min_{z \in K_k(I + K, \hat{b})} \|\hat{b} - (I + K)z\|_H
= \min_{p(0) \equiv 1 \atop \deg(p) \leq k} \|p(I + K)\hat{b}\|_H = \min_{p(0) \equiv 1 \atop \deg(p) \leq k} \|H^{-1} p(AH^{-1})\hat{b}\|_H
= \min_{p(0) \equiv 1 \atop \deg(p) \leq k} \|p(AH^{-1})\hat{b}\|_{H^{-1}},
\]

where we have used that \( K_k(K, \hat{b}) = K_k(I + K, \hat{b}) \). The matrix \( I + K \) is \( H \)-normal(1), and hence diagonalizable with an \( H \)-unitary matrix of eigenvectors, i.e., \( I + K = YAY^{-1} \) and \( Y^* HY = I \). Note that \( H^{1/2}Y \) is unitary. Using the first expression in
we thus obtain
\[
\|b - Ax_k\|_{H^{-1}} = \min_{\substack{p(0) = 1 \\ \deg(p) \leq k}} \|p(I + K)\hat{b}\|_H \\
= \min_{\substack{p(0) = 1 \\ \deg(p) \leq k}} \|H^{1/2}Yp(\Lambda)Y^{-1}H^{-1}b\|_2 \\
\leq \|(Y^{-1}H^{-1/2})H^{-1/2}b\|_2 \min_{\substack{p(0) = 1 \\ \deg(p) \leq k}} \|H^{1/2}Yp(\Lambda)\|_2 \\
= \|b\|_{H^{-1}} \min_{\substack{p(0) = 1 \\ \deg(p) \leq k}} \|p(\Lambda)\|_2.
\]

The polynomial minimization problem on the spectrum of \(I + K\), which is contained in a complex interval of the form \(1 + i[-\lambda, \lambda]\) for some \(\lambda > 0\), was considered in [19], and it leads to a convergence bound of the form

\[
(5.6) \quad \|b - Ax_k\|_{H^{-1}} \leq \|b\|_{H^{-1}} \min_{\substack{p(0) = 1 \\ \deg(p) \leq k}} \|p(\Lambda)\|_2.
\]

see [50, Theorem 4.3]. As for Widlund’s method, this bound for Rapoport’s method indicates that the convergence is “fast” when \(\lambda > 0\) is “small”.

5.3. Comparison with GMRES. We will now compare the methods of Widlund and Rapoport with GMRES [45]. Recall that the GMRES method applied to \(Ax = b\) and starting with \(x_0 = 0\) has iterates \(x^G_k\) that are determined by

\[x^G_k \in K_k(A, b) \text{ such that } r^G_k = b - Ax^G_k \perp AK_k(A, b),\]

and that the orthogonality property of the method is equivalent to the optimality property

\[
\|r^G_k\|_2 = \min_{z \in K_k(A, b)} \|b - Az\|_2 = \min_{\substack{p(0) = 1 \\ \deg(p) \leq k}} \|p(A)b\|_2.
\]

Note that the GMRES method is well defined when \(A\) is nonsingular, but in contrast to the methods of Widlund and Rapoport it is based on full rather than three-term recurrences.

Analogously, an application of GMRES with \(x_0 = 0\) to the left-preconditioned system \(H^{-1}Ax = b\) has iterates \(x^{LG}_k\) that are characterized by

\[x^{LG}_k \in K_k(H^{-1}A, \hat{b}) \text{ such that } r^{LG}_k = \hat{b} - H^{-1}Ax^{LG}_k \perp H^{-1}AK_k(H^{-1}A, \hat{b}).\]

This method is well defined when \(H\) is nonsingular, but \(H\) does not need to be definite. Note that \(K_k(K, \hat{b}) = K_k(I + K, \hat{b}) = K_k(H^{-1}A, b)\), and hence GMRES applied to the left-preconditioned system uses the same search spaces for the iterates as the methods of Widlund and Rapoport. The optimality property now is given by

\[
(5.7) \quad \|r^{LG}_k\|_2 = \min_{z \in K_k(H^{-1}A, \hat{b})} \|\hat{b} - H^{-1}Az\|_2 = \min_{\substack{p(0) = 1 \\ \deg(p) \leq k}} \|p(H^{-1}A)\hat{b}\|_2 \\
= \min_{\substack{p(0) = 1 \\ \deg(p) \leq k}} \|H^{-1}p(AH^{-1})\hat{b}\|_2 = \min_{\substack{p(0) = 1 \\ \deg(p) \leq k}} \|p(AH^{-1})\hat{b}\|_{H^{-2}}.
\]
we have matrices, and where the minimization problem can be bounded as in (5.6). Moreover, which reminds one of the standard GMRES convergence bound for diagonalizable systems of the form (4.2), which come from different cases discussed in Section 3. Here we do not take these methods into account, since our matrix $K$ is skew-Hermitian with respect to the $H$-inner product, so that methods for usual skew-Hermitian matrices are not directly applicable. Moreover, the methods of Widlund and Rapoport already implement the two most common projection principles in this context, namely oblique and orthogonal projection onto Krylov subspaces.

### Table 5.1: Mathematical characterization and minimization properties of the different methods.

<table>
<thead>
<tr>
<th>Method</th>
<th>Mathematical characterization</th>
<th>Minimization properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Widlund:</td>
<td>$x_k^W \in K_k(K, b)$ such that $r_k^W = b - Ax_k^W$ ⊥ $K_k(K, b)$</td>
<td>$|x - x_{2k}|<em>H = \min</em>{z \in (I - K)K_{2k}(K, b)} |x - z|_H$</td>
</tr>
<tr>
<td>Rapoport:</td>
<td>$x_k^R \in K_k(K, b)$ such that $r_k^R = b - Ax_k^R$ ⊥ $H^{-1}AK_k(K, b)$</td>
<td>$|b - Ax_k^R|<em>{H^{-1}} = \min</em>{z \in K_k(K, b)} |b - Az|<em>{H^{-1}} = \min</em>{\deg(p) \leq k} |p(\Lambda^{-1})b|_{H^{-1}}$</td>
</tr>
<tr>
<td>L-GMRES:</td>
<td>$x_k^{LG} \in K_k(K, b)$ such that $r_k^{LG} = \hat{b} - H^{-1}Ax_k^{LG}$ ⊥ $H^{-1}AK_k(K, b)$</td>
<td>$|b - Ax_k^{LG}|<em>{H^{-2}} = \min</em>{z \in K_k(A, b)} |b - Az|<em>{H^{-2}} = \min</em>{\deg(p) \leq k} |p(A)b|_2$</td>
</tr>
<tr>
<td>GMRES:</td>
<td>$x_k^{G} \in K_k(A, b)$ such that $r_k^{G} = b - Ax_k^{G}$ ⊥ $AK_k(A, b)$</td>
<td>$|b - Ax_k^{G}|<em>2 = \min</em>{z \in K_k(A, b)} |b - Az|<em>2 = \min</em>{\deg(p) \leq k} |p(A)b|_2$</td>
</tr>
</tbody>
</table>

If we again write $I + K = YAY^{-1}$, then the last expression in (5.7) leads to the bound

$$
(5.8) \quad \frac{\|r_k^{\text{LG}}\|_2}{\|b\|_2} \leq \kappa(Y) \min_{\deg(p) \leq k} \|p(A)\|_2,
$$

which reminds one of the standard GMRES convergence bound for diagonalizable matrices, and where the minimization problem can be bounded as in (5.6). Moreover, we have

$$
\|r_k^{\text{LG}}\|_2 = \|\hat{b} - H^{-1}Ax_k^{\text{LG}}\|_2 = \|H^{-1}(b - Ax_k^{\text{LG}})\|_2 = \|b - Ax_k^{\text{LG}}\|_{H^{-2}},
$$

where $b - Ax_k^{\text{LG}}$ can be considered the unpreconditioned residual of the GMRES method applied to the left-preconditioned system.

Table 5.1 contains an overview of the mathematical characterizations and optimality properties of the four methods discussed above, where L-GMRES means GMRES applied to the left preconditioned system.

We point out that several Krylov subspace methods with short recurrences have been proposed in the literature for the solution of linear algebraic systems with (shifted) skew-Hermitian or skew-symmetric matrices; see, e.g., [23, 24, 32, 33]. Here we do not take these methods into account, since our matrix $K$ is skew-Hermitian with respect to the $H$-inner product, so that methods for usual skew-Hermitian matrices are directly applicable. Moreover, the methods of Widlund and Rapoport already implement the two most common projection principles in this context, namely oblique and orthogonal projection onto Krylov subspaces.

### 6. Numerical experiments.

In this section we present numerical experiments with the four iterative methods summarized in Table 5.1 applied to linear algebraic systems of the form (4.2), which come from different cases discussed in Section 3. All experiments were carried out in MATLAB R2021a on a PC with 4 cores (Intel i7-8550U CPU at 1.8 GHz) and 16 GB RAM.
The matrices used in the experiments in Section 6.1 (Brake squeal problem; Case 1; Example 3.1) are directly taken from [22]. The matrices used in the experiments in Section 6.2 (Stokes equation; Case 2; Example 3.4) and Section 6.3 (linearized Navier–Stokes; Case 3; Example 3.6) were generated using reference problems of the IFISS software package [47].

We have implemented the methods of Widlund and Rapoport as stated in [55] and [43], respectively, and our implementation of (preconditioned) GMRES is based on the MGS variant in [44]. The methods of Widlund and Rapoport as well as L-GMRES are based on preconditioning the system (4.2) with the Hermitian part $H$ of $A$, and hence they require solving a linear algebraic system with $H$ in every step. In order to do this solve, we first compute a Cholesky decomposition of $H$, and then solve the two triangular systems by forward and backward substitution in every step. We point out that for a sequence of linear algebraic systems coming from a discretization with constant time steps as in (4.1), only one Cholesky decomposition needs to be computed upfront.

As seen in Table 5.1, the four methods minimize different norms of residual or error. We consider GMRES applied to the non-preconditioned system $Ax = b$ as the reference method. This method minimizes the 2-norm of the residual in every step, and therefore we compare the residuals of all four methods in this norm. In all experiments we start the iterative methods with $x_0 = 0$, and run the iterations until the 2-norm of the relative residual is smaller than $10^{-12}$.

### 6.1. Brake squeal problem (Case 1)

Finite element modeling of a disk brake leads to a second order DAE of the form

$$M \ddot{p} + D \dot{p} + Kp = f,$$

where $p$ is the coefficient vector associated with the displacements of the structure, $f$ is an external force, $M = M^* > 0$ is the mass matrix, $D = D^* \geq 0$ is the damping matrix, and $K = K^* > 0$ is the stiffness matrix; see [8, 22]. The matrices depend on a reference frequency $\omega_{ref}$, and here we use the value $\omega_{ref} = 500$. The resulting first-order formulation gives the state equation of a dHDAE system of the form (3.2). After time discretization we obtain a linear algebraic equation of the form (4.2) with $n = 9338$ and a positive definite Hermitian part.

In the top row of Figure 6.1 we plot the convergence curves (relative residual 2-norm) of the four iterative methods applied (with $x_0 = 0$) to linear algebraic systems corresponding to two different values of the time step, namely $\tau = 0.001$ and $\tau = 0.0001$. We observe that GMRES is outperformed by the methods of Widlund, Rapoport and L-GMRES, which is not surprising, since the latter three are all preconditioned by the dominant Hermitian part. For the value $\tau = 0.001$, the L-GMRES method shows an initial fast decrease of the residual norm (which we did not investigate further), and thus takes fewer steps than the methods of Widlund and Rapoport to reach the stopping criterion. However, as shown in Table 6.1, L-GMRES takes a significantly longer time, which is due to the full recurrences in the algorithm (compared to three-term recurrences in the methods of Widlund and Rapoport). For the smaller value $\tau = 0.0001$, the residual norms of the methods of Widlund, Rapoport and L-GMRES show almost the same behavior, but again L-GMRES is significantly slower.

Figure 6.1 also shows the eigenvalues of $K$ for the two time steps. The smallest (purely imaginary) interval $i[-\lambda, \lambda]$ containing these eigenvalues is given by

$$\lambda \approx 3.4243 \text{ for } \tau = 0.001 \quad \text{and} \quad \lambda \approx 0.3424 \text{ for } \tau = 0.0001.$$
\( \tau = 0.001 \) \hspace{2cm} \( \tau = 0.0001 \)

<table>
<thead>
<tr>
<th>Method</th>
<th>Time</th>
<th># of Iter.</th>
<th>Time</th>
<th># of Iter.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Widlund</td>
<td>3.54</td>
<td>85</td>
<td>0.72</td>
<td>16</td>
</tr>
<tr>
<td>Rapoport</td>
<td>5.19</td>
<td>83</td>
<td>0.91</td>
<td>15</td>
</tr>
<tr>
<td>L-GMRES</td>
<td>31.10</td>
<td>65</td>
<td>10.51</td>
<td>13</td>
</tr>
<tr>
<td>GMRES</td>
<td>6.98</td>
<td>134</td>
<td>10.81</td>
<td>205</td>
</tr>
</tbody>
</table>

Table 6.1: Brake squeal problem. Running times and iteration numbers.

![Graph showing relative residual norms and eigenvalues for different methods with \( \tau = 0.001 \) and \( \tau = 0.0001 \).]

Here the spectrum “shrinks” by approximately a factor of 10 when \( \tau \) is decreased from 0.001 to 0.0001. The convergence bounds (5.3), (5.6), and (5.8) for the methods of Widlund, Rapoport, and L-GMRES indicate a faster convergence in terms of iterative steps of the respective method in this case, and this indeed happens, as can be seen from Figure 6.1 and Table 6.1.

### 6.2. Stokes equation (Case 2)

We consider the incompressible Stokes equation as in Example 3.4, and generate linear algebraic systems using the \( Q1 - Q1 \) finite element approximation of the (unsteady) channel domain problem in IFISS. The systems are of the form

\[
Tx = \begin{bmatrix} A & B \\ -B^* & C \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix} = b,
\]
where $A$ and $C$ are Hermitian positive definite, so that the methods of Widlund and Rapoport are applicable. We use the “grid parameter” 6 in IFISS, which yields matrices $B$ of the size $8450 \times 4225$, and hence $T$ is of the size $12675 \times 12675$. We use a random right hand side $f$ generated by the command `randn` in MATLAB.

Table 6.2 and Figure 6.2 show the numerical results analogous to those reported in Section 6.1. Table 6.2 also shows the computed relative residual norm $\|b-Tx_k\|_2/\|b\|_2$ of the last computed approximate solution $x_k$ of $Tx = b$, where we stopped the GMRES iteration after 250 steps.

In the Stokes problem considered here, the smallest interval $i[-\lambda, \lambda]$ containing the eigenvalues of $K$ is given by

$$\lambda \approx 0.239 \text{ for } \tau = 0.001 \quad \text{and} \quad \lambda \approx 0.036 \text{ for } \tau = 0.0001.$$ 

Thus, the spectrum “shrinks” by approximately a factor of $1/6$ when $\tau$ is decreased from 0.001 to 0.0001. We can see in the iteration numbers in Table 6.2, and in the residual norm curves in Figure 6.2, that the effect of a smaller $\tau$ on the convergence of the methods of Widlund, Rapoport, and L-GMRES is negligible. This can be explained by the fact that already for $\lambda \approx 0.239$, the “convergence factor” on the right hand side of the bounds (5.3) and (5.6) is given by

$$\frac{\sqrt{1+\lambda^2} - 1}{\sqrt{1+\lambda^2} + 1} \approx 0.0139 \quad \text{and} \quad \frac{\lambda}{\sqrt{1+\lambda^2} + 1} \approx 0.1179.$$ 

Thus, the rapid convergence of the methods of Widlund and Rapoport already for $\tau = 0.001$ is explained by these bounds, and for L-GMRES it is indicated by the bound (5.8), which involves the same “convergence factor” as (5.6). Note that although L-GMRES takes a similar number of steps as the methods of Widlund and Rapoport, it takes a longer time, which again is due to the full recurrences compared with three-term recurrences in the methods of Widlund and Rapoport.

### 6.3. Linearized Navier-Stokes equation without stabilization (Case 3).

As a final example we consider the linearized Navier-Stokes equation without stabilization as in Example 3.6, and generate linear algebraic systems using the $Q_2 - Q_1$ finite element discretization of the (unsteady) channel domain problem in IFISS. Now the systems are of the form

$$Tx = \begin{bmatrix} A & B \\ -B^* & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix} = b,$$

where $A$ is non-Hermitian positive definite and $B$ is of full rank. As for the Stokes equation in Section 6.2 we use the “grid parameter” 6, so that $B$ is of size $8450 \times 1089,$
and hence $T$ is of size $9539 \times 9539$. The vector $f$ for the right hand side is also generated by IFISS.

The methods of Widlund and Rapoport are not directly applicable to the system (6.1). However, the system can be solved via Schur complement reduction by applying the four different methods (Widlund, Rapoport, L-GMRES, and GMRES) to the non-Hermitian positive definite systems with $A$, and the positive definite Schur complement $S_1 = B^* A^{-1} B$. In Table 6.3 we show the total time and number of iterative steps required by the four methods for solving the two systems with $A$ and $S_1$, as well as the relative residual norm of the approximate solution of $Tx = b$ obtained in this way. Table 6.3 also shows the performance of GMRES applied to the system $Tx = b$. Here we stopped the iteration after 250 steps, and we report the value of the relative residual norm attained at that point.

Figure 6.3 shows the convergence curves of the four methods applied to $A$ and $S_1$ (top and bottom row), and for $\tau = 0.001$ and $\tau = 0.0001$ (left and right). The (purely imaginary) eigenvalues of the matrix $K$ corresponding to $A$ are contained in the interval $i[-\lambda, \lambda]$ with

$$\lambda \approx 1.0083 \times 10^{-4} \text{ for } \tau = 0.001 \quad \text{and} \quad \lambda \approx 2.3516 \times 10^{-6} \text{ for } \tau = 0.0001,$$

and for the matrix $K$ corresponding to the Schur complement $S_1$ they are contained...
\[ \tau = 0.001 \]

<table>
<thead>
<tr>
<th>Method</th>
<th>Time</th>
<th>| Rel. Res. |</th>
<th># of Iter.</th>
<th>Time</th>
<th>| Rel. Res. |</th>
<th># of Iter.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Widlund</td>
<td>0.116</td>
<td>(1.34 \times 10^{-14})</td>
<td>8</td>
<td>0.128</td>
<td>(1.52 \times 10^{-13})</td>
<td>7</td>
</tr>
<tr>
<td>Rapoport</td>
<td>0.175</td>
<td>(1.34 \times 10^{-14})</td>
<td>6</td>
<td>0.136</td>
<td>(1.52 \times 10^{-15})</td>
<td>5</td>
</tr>
<tr>
<td>L-GMRES</td>
<td>4.190</td>
<td>(1.38 \times 10^{-14})</td>
<td>6</td>
<td>4.477</td>
<td>(1.61 \times 10^{-15})</td>
<td>5</td>
</tr>
<tr>
<td>GMRES</td>
<td>0.248</td>
<td>(2.17 \times 10^{-14})</td>
<td>117</td>
<td>0.324</td>
<td>(2.34 \times 10^{-14})</td>
<td>152</td>
</tr>
<tr>
<td>GMRES (T)</td>
<td>1.133</td>
<td>(4.71 \times 10^{-04})</td>
<td>250</td>
<td>1.157</td>
<td>(6.75 \times 10^{-05})</td>
<td>250</td>
</tr>
</tbody>
</table>

Table 6.3: Linearized Navier-Stokes equation without stabilization. Running times (s), total number of iterations, and relative residual norms at the final step for \(\tau = 0.001\) and \(\tau = 0.0001\).

\[ \tau = 0.001 \]

Fig. 6.3: Linearized Navier-Stokes equation without stabilization. Relative residual norms of the four methods applied to the systems with \(A\) (top row) and \(S_1\) (bottom row) with \(\tau = 0.001\) and \(\tau = 0.0001\) (left and right).

\[ \lambda \approx 7.4483 \times 10^{-5} \text{ for } \tau = 0.001 \quad \text{and} \quad \lambda \approx 9.9225 \times 10^{-7} \text{ for } \tau = 0.0001. \]

Using the values in the bounds (5.3), (5.6), and (5.8) explains the fast convergence of the methods of Widlund and Rapoport as well as L-GMRES applied to the systems with \(A\) and \(S_1\); see Figure 6.3.

7. Concluding remarks. Dissipative Hamiltonian differential-algebraic equation (dHDAE) systems occur in a wide range of energy-based modeling applications, including thermodynamics, electromagnetics, and fluid mechanics. These systems can
be classified using a staircase from, which reveals their differentiation index (either zero, one, or two). We have given a systematic overview of the three different cases. An important common feature is that the matrices arising in the (space and time) discretization of dHDAE systems split naturally into $A = H + S$, where the Hermitian part $H$ is positive definite or positive semidefinite. This feature can be exploited in the numerical solution of the corresponding linear algebraic systems.

A focus of our work has been the case of positive definite $H$, which allows the application of the Krylov subspace methods of Widlund and Rapoport. These methods were derived in the late 1970s, but have rarely been analyzed or even cited in the literature so far. We have summarized their main mathematical properties, and we have presented extensive numerical experiments with linear algebraic systems from different dHDAE application problems. In these experiments the three-term recurrence methods of Widlund and Rapoport have consistently outperformed L-GMRES and (unpreconditioned) GMRES. The behavior we have observed is consistent with the convergence bounds for the methods of Widlund and Rapoport, which indicate a fast convergence for the systems $(I + K)x = b$ when $K = H^{-1}S$ is "small". In time discretizations of dHDAE systems this important feature is virtually "built in", since the skew-Hermitian part of the dHDAE is being multiplied by the (usually) small time step parameter $\tau$.

Overall, we have therefore presented a holistic approach combining energy-based modeling using dHDAE systems, their structure-preserving discretization, and finally a structure-adapted linear algebraic computation.

The case of a positive semidefinite $H$ is challenging. We have shown in Lemma 4.2 that one can identify the "singular part" of $A = H + S$ via a unitary transformation, but this tool in not practical in large scale applications. However, in the mathematical modeling the block structure of the dHDAE frequently exposes the "singular part", and no further transformation is necessary. In such cases, we can apply the methods of Widlund and Rapoport to the "positive definite part" of the problem, and the "singular part" must be solved by other means. A closer analysis of the positive semidefinite case is a subject of future work.

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