Riccati ADI: Existence, uniqueness and new iterative methods

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Abstract

The approximate solution of large-scale algebraic Riccati equations is considered. We are interested in approximate solutions which yield a Riccati residual matrix of a particular small rank. It is assumed that such approximate solutions can be written in factored form $Z Y Z^*$ with a rectangular matrix $Z$ and a small quadratic matrix $Y$. We propose to choose $Z$ such that its columns span a certain rational Krylov subspace. Conditions under which such an approximate solution exists and is unique are determined. It is shown that the proposed method can be interpreted as an oblique projection method. Two new iterative procedures with efficient updates of the solution and the residual factor are derived. With our approach complex system matrices can be handled, realization is provided and parallelization is introduced.

1 Introduction

Consider the continuous-time algebraic Riccati equation

$$0 = \mathcal{R}(X) := A^* X + X A + C^* C - X B B^* X$$

$$= (A^* - X B B^*) X + X (A - B B^* X) + C^* C + X B B^* X$$

(1)

with complex system matrices $A \in \mathbb{C}^{n \times n}$ large and sparse and $B \in \mathbb{C}^{n \times m}$, $C \in \mathbb{C}^{p \times n}$. This Riccati equation occurs in several applications such as linear-quadratic regulator problems of optimal control, in $\mathcal{H}_2$ and $\mathcal{H}_\infty$ control, in balancing-related model order reduction or in Kalman filtering. Due to the quadratic term there may be many solutions of (1), but in most applications one is interested in the unique stabilizing solution. This is the positive semidefinite solution $X$ for which $A - B B^* X$ is stable, i.e. all its eigenvalues are contained in the left half of the complex plane. Existence of this solution is guaranteed if $(A, B)$ is stabilizable and $(C, A)$ is detectable [11, Thm.2.21], [18, Thm. 9.1.2]. If $(C, A)$ is observable, then the sought solution is even positive definite [18, Thm. 9.1.5].
We are concerned with the large-scale setting where direct methods for the solution of (1) are infeasible. In this setting, one is interested in a Hermitian low-rank approximation of the form \( \tilde{X} = ZYZ^* \approx X \) where \( Z \) is a rectangular matrix with only few columns and \( Y \) is a small square Hermitian matrix. This form of approximation gives two degrees of freedom: The approximation space, that is, the space spanned by the columns of \( Z \), and the choice of the approximate solution in this space which is determined by \( Y \). There are several methods which produce such a low-rank approximation; see, e.g. [6] for an overview. Basically, there are three families of methods, described briefly next. All these methods use certain (rational) Krylov subspaces as approximation spaces.

In projection methods, such as the extended [15] and rational Krylov subspace method [25, 24] (denoted *KSM), the factor \( Z \) is chosen such that its columns are an orthonormal basis for a certain (rational) Krylov subspace. The matrix \( Y \) is chosen as the solution of an orthogonal projection of the Riccati equation (1) onto the selected Krylov subspace.

Low-rank Newton-Kleinman methods treat (1) as a nonlinear equation and apply Newton’s method, so in each iteration step a linear matrix equation has to be solved, see e.g. [7] and the references therein. Recently, the projected Newton-Kleinman method was derived in [22] which is a projection scheme where the inner linear solves are performed only implicitly, making this approach competitive to the other methods mentioned here.

The third family are the ADI-type methods which are investigated in this work. They are well known from linear matrix equations and derived from the alternating directions implicit method [26, 19, 17]. In order to be able to apply these methods to large-scale problems, the variant of the ADI iteration for dense matrices is reformulated to obtain a low-rank formulation [19]. However, due to the nonlinearity of the Riccati equations, at first glimpse, this technique seems to be infeasible here. Though there are ADI-type methods for the Riccati equation, e.g. the qADI algorithm [30, 29], the algorithm of Amodei and Buchot [2], the RADI iteration [4] and the Cayley subspace iteration [20]. In fact all these methods produce (at least theoretically) the same approximate solution, which was shown laboriously e.g. in [4, 4]. The term Riccati ADI methods (proposed in [4]) will be used throughout this work to denote the ADI-type methods for Riccati equations. In contrast to the other two families the approximation space is not chosen directly but turns out to be a rational Krylov subspace which is determined by shift parameters, see [4, Prop. 2]. Besides, the residual matrix is of rank \( p \), see e.g. [4, Prop. 1].

As discussed in [4, Sec. 5], the RADI iteration is computationally more efficient than any of the other Riccati ADI methods considered. This method has been formulated for the case of real system matrices \( A, B \) and \( C \) only. It can handle generalized Riccati equations and provides a low-rank formulation \( ZZ^* \) for the approximate solution of (1). The method offers a shift strategy for fast convergence and techniques to reduce the use of complex arithmetic in case of complex shift parameters. In each iteration step the Sherman-Morrison-Woodbury (SMW) formula [14, Chp. 2.1.4] is used to solve the occurring linear system, which becomes expensive in case of a system matrix \( B \) with many
columns, i.e. with large $m$.

Our ADI-type approach is similar to the approach of the projection methods. We decouple the calculation of a basis $Z$ for a certain (rational) Krylov subspace from the calculation of $Y$. That is, we choose $Z$ and consider the approximate solution $\tilde{X} = ZY Z^*$. The matrix $Y$ is determined such that the Riccati residual

$$R(\tilde{X}) = A^* \tilde{X} + \tilde{X} A + C^* C - \tilde{X} BB^* \tilde{X}$$

is of rank $p$. Due to its symmetry and its rank it can be factored into $R(\tilde{X}) = \tilde{R} \tilde{R}^*$ with the Riccati residual factor $\tilde{R} \in \mathbb{C}^{n \times p}$. We call such an approximate solution $\tilde{X} = ZY Z^*$ with a rank $p$ residual an ADI approximate solution.

We answer the following questions: For which (rational) Krylov subspaces with basis $Z$ does a small matrix $Y$ exist such that the Riccati residual $R(ZYZ^*)$ can be factored into rank-$p$ matrices? Is this approximate solution unique? How can it be obtained efficiently?

We show that the ADI approximate solution exists and is unique if the approximation space is a rational Krylov subspace whose poles satisfy a simple condition. Generalized Riccati equations can be handled. It is demonstrated that our Riccati ADI method can be interpreted as an oblique projection method. The projected system matrices are connected to the poles and zeros of a rational function corresponding to the residual factor. We derive two efficient iterative methods, which, due to our uniqueness result, generate the same approximate solution to (1) as the other Riccati ADI methods. When all system matrices are real valued and all poles of the rational Krylov subspace appear in complex conjugated pairs, then we can choose a real basis $Z$ and all involved quantities remain real valued. Our approach allows to parallelize linear systems solves which are necessary to generate the Krylov basis $Z$.

To answer the above questions and derive the new iterative methods we make use of rational Arnoldi decompositions which are introduced in Section 2. In Section 3 conditions for the existence and uniqueness of the ADI approximate solution are derived and the connection to projection methods is presented. New iterative methods based on these theoretical findings are derived in Section 4. Further, realification and parallelization are introduced here. In Section 5 we indicate how to deal with generalized Riccati equations, show how our method simplifies in case of linear matrix equations and mention a shift selection strategy. In the numerical experiments in Section 6 we compare our new iterative methods and demonstrate the effects of parallelization. Concluding remarks are given in Section 7.

1.1 Notation

An underscore is used to indicate matrices with more rows than columns. With a negative index we denote the quadratic lower submatrix $K_{-j} = [0 \ I] K_j$ of such a rectangular matrix. A (block) diagonal matrix with diagonal entries $A_1, \ldots, A_l$ is indicated by $\text{diag}(A_1, \ldots, A_l)$. The set of eigenvalues of a square matrix $A$ is given by $\Lambda(A)$. The matrix $A^*$ is the complex conjugated of the
transposed matrix $A^T$. We use this notation also for real matrices. A linear space $V$ is called $A$-variant if $AV \not\subseteq V$ and $A$-invariant otherwise. With $\mathbb{C}_+$ ($\mathbb{C}_-)$ we indicate the set of complex numbers with positive (negative) real part. For $j \in \mathbb{N}_0$ a polynomial $p$ is given via $p(x) = \sum_{i=0}^{j} a_i x^i$ with coefficients $a_i \in \mathbb{C}$ for $i = 0, \ldots, j$. The degree $\deg(p)$ of the polynomial $p$ is the largest index belonging to a nonzero coefficient. If all coefficients are zero, then the degree is set to $-\infty$. The set of all polynomials with degree at most $j$ is denoted by $\Pi_j$. The $i$-th canonical standard basis vector is denoted $e_i$.

2 Rational Krylov subspaces and rational Arnoldi decompositions

We start with a discussion on (rational) Krylov subspaces. The definitions and theorems in this section are largely based on the work of Berljafa [10, 9]. Given a matrix $A \in \mathbb{C}^{n \times n}$, a vector $b \in \mathbb{C}^n$ and a number $j \in \mathbb{N}$, the polynomial Krylov subspace of order $j$ is defined by

$$\mathcal{K}_j(A, b) := \text{span}\{b, Ab, \ldots, A^{j-1}b\}$$

$$= \{p(A)b \mid p \in \Pi_{j-1}\},$$

the set of all polynomials of degree at most $j - 1$ in $A$ multiplied with $b$. We extend this definition to rational functions instead of only polynomials. Let $q \in \Pi_j$ be a fixed polynomial of degree at most $j$ with no roots in $\Lambda(A)$ so $q(A)$ is invertible. The rational Krylov subspace of order $j$ associated to $q$ is defined by

$$\mathcal{K}_j(A, b, q) := q(A)^{-1}\mathcal{K}_j(A, b)$$

$$= \{q(A)^{-1}p(A)b \mid p \in \Pi_{j-1}\},$$

the set of all rational functions in $A$ multiplied with $b$ with a nominator polynomial of degree at most $j - 1$ and fixed denominator polynomial $q$ of degree equal or less than the order $j$ of the Krylov subspace $\mathcal{K}_j(A, b)$. The polynomial $q$ has roots $s_1, \ldots, s_{\deg(q)} \in \mathbb{C} \setminus \Lambda(A)$. If $\deg(q) < j$ we say it has $j - \deg(q)$ formal roots at infinity. This allows us to characterize the rational Krylov subspace through a set of $j$ roots $s = \{s_1, \ldots, s_j\} \subset \mathbb{C} \cup \{\infty\} \setminus \Lambda(A)$ instead of the polynomial $q$, i.e. we can write $\mathcal{K}_j(A, b, s)$ for $\mathcal{K}_j(A, b, q)$. The roots of $q$ are also called shifts or poles of the rational Krylov subspace.

The polynomial Krylov subspace (2) of order $j$ is a special case of a rational Krylov subspace with $q = 1$, i.e. a rational Krylov subspace of order $j$ with $j$ poles at infinity. On the other extreme, if $q$ has degree $j$, then $q^{-1}p$ is a proper rational function as the degree of $p$ is at most $j - 1$ and so $b \notin \mathcal{K}_j(A, b, q)$ holds. In between these two cases we may apply polynomial long division to decompose the rational Krylov subspace. Let $p \in \Pi_{j-1}$, $q \in \Pi_j$, and set $l = j - \deg(q)$, the number of poles at infinity of a rational Krylov subspace of order $j$ associated to $q$. We find $u \in \Pi_{l-1}$ and $r \in \Pi_{\deg(q)-1}$ with $p = qu + r$ which results in the...
decomposition
\[ K_j(A, b, q) = \{ u(A)b + q(A)^{-1}r(A)b \mid u \in \Pi_{l-1}, r \in \Pi_{\text{deg}(q) - 1} \} \]
\[ = K_l(A, b) + K_{\text{deg}(q)}(A, b, q) \]

of a rational Krylov subspace into a polynomial Krylov subspace of order \( l \) and a rational Krylov subspace of order \( \text{deg}(q) \) without poles at infinity.

In particular it holds \( K_j(A, b) \subset K_j(A, b, s) \) if \( s \) contains the shift infinity at least \( l \) times. More specifically \( b \) is contained in a rational Krylov subspace if the shift infinity occurs at least once. We often omit the term rational in the following.

Consider the general case of an \( A \)-variant Krylov subspace \( K_j(A, b, s) \), that is, \( AK_j(A, b, s) \nsubseteq K_j(A, b, s) \). Then the spaces \( K_j(A, b, s) \) and \( AK_j(A, b, s) \) are of dimension \( j \) and their intersection is of dimension \( j - 1 \), i.e. \( K_j(A, b, s) \) is almost \( A \)-invariant. This implies that the sum of these two spaces is of dimension \( j + 1 \). More specifically it holds
\[ AK_j(A, b, s) = AK_j(A, b, q) \]
\[ = q(A)^{-1}AK_j(A, b) \]
\[ \subset q(A)^{-1}K_{j+1}(A, b) \]
\[ = K_{j+1}(A, b, q) \]
\[ = K_{j+1}(A, b, s \cup \{ \infty \}), \]

with one additional shift infinity in the last line because the order of the polynomial Krylov subspace was increased by one without altering \( q \). We call the latter space with an additional infinite shift augmented Krylov subspace and use the notation \( K_j^+(A, b, s) := K_{j+1}(A, b, s \cup \{ \infty \}) \). It contains rational functions in \( A \) multiplied with \( b \) whose nominator polynomials are of degree at most \( j \) instead of only \( j - 1 \) as in \( (3) \).

Let \( V_{j+1} \) be a basis of the augmented space \( K_j^+(A, b, s) \). As it contains both spaces \( K_j(A, b, s) \) and \( AK_j(A, b, s) \) it is possible to encode the effect of multiplication of \( K_j(A, b, s) \) with \( A \) in a decomposition of the form
\[ AV_{j+1}K_j = V_{j+1}H_j \]

with rectangular matrices \( K_j, H_j \in \mathbb{C}^{(j+1) \times j} \) and
\[ \text{span}\{V_{j+1}K_j\} = K_j(A, b, s), \]
\[ \text{span}\{V_{j+1}H_j\} = AK_j(A, b, s). \]

Decompositions of the form \( (6) \), their connections to Krylov subspaces and their properties play a key role in our discussion on Riccati equations. We therefore introduce some central definitions and results from \cite{10}.

Remark 2.1. We note that our definition \( (3) \) of a rational Krylov subspace differs from the definition in \cite{10} in the order of the involved polynomial Krylov
subspace. The rational Krylov subspaces defined in \cite{10} are equivalent to our augmented Krylov subspace \cite{9}. The reason for the deviation from the literature is that for our purposes Krylov subspaces with only finite shifts are needed, but the augmented Krylov subspaces always contain (at least) one infinite shift. See also \cite{9} Prop. 3.3 and the paragraph preceding it.

**Definition 2.1** (cf. \cite{10} Def. 4.1). Let \( K_j, H_j \in \mathbb{C}^{(j+1) \times j} \) be rectangular matrices. We say that the pencil \((H_j, K_j)\) is regular if the lower \( j \times j \) subpencil \((H_{-j}, K_{-j})\) is regular, i.e., \( \det(zK_{-j} - H_{-j}) \) is not identically equal to zero.

**Definition 2.2** (\cite{10} Def. 4.2). A relation of the form (6) where \( V_{j+1} \) is of full column rank and \((H_{-j}, K_{-j})\) is regular is called a generalized rational Krylov decomposition. The generalized eigenvalues of \((H_{-j}, K_{-j})\) are called poles of the decomposition. If the poles of (6) are outside the spectrum \( \Lambda(A) \), then (6) is called a rational Krylov decomposition (RKD).

If in a (generalized) RKD the matrices \( K_j \) and \( H_j \) are upper Hessenberg matrices then the decomposition is called a (generalized) Arnoldi decomposition (RAD). The columns of \( V_{j+1} \) are called the basis of the decomposition and they span the augmented space of the decomposition (cf. \cite{10} Def. 2.3]). The first column of \( V_{j+1} \) is called starting vector. Every (generalized) RKD can be transformed to a (generalized) RAD with the same starting vector and the same poles using a generalized Schur form of \((A, b, s)\) (see \cite{10} Thm. 4.3]). If \( A \) and \( b \) are real valued and the poles appear in complex conjugated pairs then a general real Schur form of \((H_{-j}, K_{-j})\) can be used to obtain a quasi-RAD, that is \( K_{-j} \) is a real upper triangular matrix and \( H_{-j} \) is a real quasi upper-triangular matrix with 1-by-1 and 2-by-2 blocks on the diagonal (cf. \cite{9} Def. 2.17]). The following theorem guarantees the existence of a RAD for a Krylov subspace \cite{9}.

**Theorem 2.1** (cf. \cite{10} Thm. 2.5). Let \( V_{j+1} \) be a vector space of dimension \( j + 1 \) and \( s \in \mathbb{C} \cup \{ \infty \} \) be a set with \( j \) elements. Then \( \mathcal{V}_{j+1} = \mathcal{K}_j^j(A, b, s) \) holds if and only if there exists a RAD \( AV_{j+1}K_j = V_{j+1}H_j \) with \( K_j, H_j \in \mathbb{C}^{(j+1) \times j} \), starting vector \( b = V_{j+1}e_1 \), poles \( s \) and span\(\{V_{j+1}\} = V_{j+1} \).

Let \( \mathcal{K}_j(A, b, s) \) be a Krylov subspace with associated RKD

\[
AV_{j+1}K_j = V_{j+1}H_j, \tag{8}
\]

Such a RKD can be transformed by a regular matrix \( U \in \mathbb{C}^{(j+1) \times (j+1)} \) into the (generalized) RKD

\[
A\tilde{V}_{j+1}\tilde{K}_j = \tilde{V}_{j+1}\tilde{H}_j \tag{9}
\]

with \( \tilde{V}_{j+1} = V_{j+1}U \), \( \tilde{K}_j = U^{-1}K_j \) and \( \tilde{H}_j = U^{-1}H_j \). The RKD (9) is associated to the same Krylov subspace \( \mathcal{K}_j(A, b, s) \) as (8). In general the starting vector \( \tilde{b} = \tilde{V}_{j+1}e_1 = V_{j+1}Ue_1 \) and the poles \( \Lambda(\tilde{H}_{-j}, \tilde{K}_{-j}) \) are altered through this
transformation and it may happen that the poles coincide with eigenvalues of $A$. Moreover, as $\tilde{b} \in K_j^+(A, b, s)$, there is a polynomial $q \in \Pi_j$ with roots $s$ and a polynomial $\bar{q} \in \Pi_j$ such that $\tilde{b} = q(A)^{-1} \bar{q}(A)b$. Thus, if no root of $\bar{q}$ coincides with an eigenvalue of $A$ then $\bar{q}(A)^{-1} q(A)\tilde{b} = \tilde{b}$ holds. This implies

$$K_j(A, b, q) = q(A)^{-1} K_j(A, b) = \{q(A)^{-1} p(A)\tilde{b} \mid p \in \Pi_{j-1}\}$$

$$= \{q(A)^{-1} p(A)\bar{q}(A)^{-1} q(A)\tilde{b} \mid p \in \Pi_{j-1}\}$$

$$= \{\bar{q}(A)^{-1} p(A)\tilde{b} \mid p \in \Pi_{j-1}\}$$

$$= K_j(A, \tilde{b}, \bar{q}),$$

where we have used the commutativity of rational functions in $A$. Even if a root of $\bar{q}$ coincides with an eigenvalue of $A$ the reverse result holds.

**Theorem 2.2** (cf. [10, Thm. 4.4]). Let $V_{j+1} = K_j^+(A, b, q)$ be $A$-variant. Let $\bar{q} \in \Pi_j$ be a polynomial with roots equal to the poles of the (generalized) RKD $AV_{j+1}K_j = \tilde{V}_{j+1}\tilde{H}_j$. If $V_{j+1}$ spans $V_{j+1}$, then for the starting vector $\tilde{b} = \tilde{V}_{j+1}e_1$, it holds $\tilde{b} = \gamma q(A)^{-1} \bar{q}(A)b$ with a scalar $0 \neq \gamma \in \mathbb{C}$.

Let $0 \neq \tilde{b} \in K_j^+(A, b, q)$ be an arbitrary element of the augmented Krylov subspace with associated RKD (8). Thus, there is a polynomial $\bar{q} \in \Pi_j$ with $\tilde{b} = q(A)^{-1} \bar{q}(A)b$ and a nontrivial vector $u_1$ with $\tilde{b} = V_{j+1}u_1$. Let $U$ be a regular matrix with $Ue_1 = u_1$, so $\tilde{b} = V_{j+1}Ue_1$ holds. Herewith Theorem 2.2 allows us to determine the roots of the nominator polynomial $\bar{q}$ as the poles of the RKD (8), i.e. the generalized eigenvalues of $(\tilde{H}_{-j}, \tilde{K}_{-j})$.

The definition of rational Krylov subspaces and rational Arnoldi decompositions is generalized in [13] to the case where the vector $b \in \mathbb{C}^n$ is replaced by a matrix (or block vector) $b \in \mathbb{C}^{n \times p}$. We recall some of the important definitions. The block Krylov subspace or order $j$ is given by

$$K_j^\square(A, b) = \text{blockspan}\{b, Ab, \ldots, A^{j-1}b\}$$

$$= \left\{\sum_{k=0}^{j-1} A^k b C_k \mid C_k \in \mathbb{C}^{p \times p}\right\}. \tag{10}$$

We only consider the case where the $jp$ columns of $[b \ A b \ \ldots \ A^{j-1}b]$ are linearly independent so the block Krylov subspace (10) has dimension $jp^2$. Every block vector $\sum_{k=0}^{j-1} A^k b C_k \in K_j^\square(A, b)$ corresponds to exactly one matrix polynomial $\sum_{k=0}^{j-1} z^k C_k$.

For the definition of a block rational Krylov subspace we again use a polynomial $q \in \Pi_j$ of degree at most $j$ with no roots in $\Lambda(A)$ and set

$$K_j^\square(A, b, q) = q(A)^{-1} K_j^\square(A, b).$$

As in the non-block part we set $K_j^\square(A, b, s) = K_j^\square(A, b, q)$ with the set $s \subset \mathbb{C} \cup \{\infty\}$ of the $j$ roots of $q$. 

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Before we can define block rational Arnoldi decompositions we need the following definition of a block upper-Hessenberg matrix.

**Definition 2.3** (cf. [13, Def. 2.1]). The block matrix

\[
H_j = \begin{bmatrix}
H_{11} & \cdots & H_{1p} \\
H_{21} & \ddots & H_{2p} \\
\vdots & & \ddots \\
H_{j+1,j} & & & & \ddots \\
& & & & & \ddots \\
& & & & & & \ddots \\
& & & & & & & \ddots \\
& & & & & & & & \ddots \\
& & & & & & & & & \ddots \\
& & & & & & & & & & \ddots \\
& & & & & & & & & & & \ddots \\
\end{bmatrix} \in \mathbb{C}^{(j+1)p \times jp}, \quad H_{ik} \in \mathbb{C}^{p \times p}
\]

is called a block upper-Hessenberg matrix. For block upper-Hessenberg matrices \(H_j\) and \(K_j\) the pencil \((H_j, K_j)\) is called an unreduced block upper-Hessenberg pencil if one of the subdiagonal blocks \(H_{i+1,i}\) or \(K_{i+1,i}\) is nonsingular for every \(i = 1, \ldots, j\).

The next definition generalizes RADs to the block case.

**Definition 2.4** (see [13, Def. 2.2]). Let \(A \in \mathbb{C}^{n \times n}\). A relation of the form

\[
AV_{j+1}K_j = V_{j+1}H_j
\]

is called a block rational Arnoldi decomposition (BRAD) if the following conditions are satisfied:

1. \(V_{j+1}\) is of full column rank,
2. \((H_j, K_j)\) is an unreduced block upper-Hessenberg pencil,
3. \(\alpha_i K_{i+1,i} = \beta_i H_{i+1,i}\) holds for some scalars \(\alpha_i, \beta_i \in \mathbb{C}\) not both zero,
4. the numbers \(\mu_i = \alpha_i/\beta_i\) are outside the spectrum \(\Lambda(A)\)

for \(i = 1, \ldots, j\). The numbers \(\mu_i \in \mathbb{C} \cup \{\infty\}\) are called the poles of the BRAD.

All results presented in the following for Krylov subspaces can be generalized to block Krylov subspaces if not stated otherwise.

### 3 Existence and uniqueness of the Riccati ADI solution

In this section we derive an existence and uniqueness result for the ADI-type solution of the Riccati equation [11]. For ease of presentation, we first consider the case \(C \in \mathbb{C}^{1 \times n}\), i.e. \(p = 1\), and comment on a general \(p \in \mathbb{N}\) in Section 3.2.

Consider an approximate solution of [11] of the form \(X_j = Z_j Y_j Z_j^*\); then the Riccati residual reads

\[
\mathcal{R}(X_j) = A^*Z_j Y_j Z_j^* + Z_j Y_j Z_j^* A + C^*C - Z_j Y_j Z_j^* B B^* Z_j Y_j Z_j^*.
\]

(11)

We intend to use a RAD to rewrite (11) in terms of the basis of an augmented Krylov subspace. This will enable us to derive an equation which makes it possible to obtain \(Y_j\) such that \(\mathcal{R}(X_j)\) is of rank one. Looking at the Riccati
residual from the left we see the terms $A^*Z_j$, $Z_j$ and $C^*$. Due to symmetry, looking from the right we see the adjoint of these terms. Therefore let $Z_j$ be a basis of the Krylov subspace $\mathcal{K}_j(A^*, C^*, s)$ with the matrices $A^*$ and $C^*$ instead of $A$ and $b$ or $b$. Let

$$A^*V_{j+1}K_j = V_{j+1}H_j$$

(12)

be an associated RAD with $Z_j = V_{j+1}K_j$, so $X_j = V_{j+1}K_jV_j^*V_{j+1}^*$ holds. As $C^*$ is an element of the augmented Krylov subspace there exists a vector $v \in \mathbb{C}^{j+1}$ with

$$V_{j+1}v = C^*.$$  (13)

Now, with the help of (12) and (13), we rewrite the Riccati residual for $X_j$ as follows:

$$\mathcal{R}(X_j) = A^*X_j + X_jA + C^*C - X_jBB^*X_j$$

$$= A^*V_{j+1}K_jV_j^*V_{j+1}^* + V_{j+1}K_jY_j^*V_{j+1}^*A + V_{j+1}vv^*V_{j+1}^*$$

$$- V_{j+1}K_jY_j^*V_{j+1}^*BB^*V_{j+1}^*K_jY_j^*V_{j+1}^*$$

$$= V_{j+1}\left( H_jK_j^* + K_jY_jH_j^* + vv^* - K_jY_jS_jK_j^* \right)V_{j+1}^*.$$  (14)

The term in brackets is a quadratic $(j + 1) \times (j + 1)$ matrix. To obtain a $Y_j$ such that the Riccati residual is of rank one we intend to utilize (13) with a special form of the RAD (12).

**Lemma 3.1.** Let $\mathcal{K}_j(A^*, C^*, s)$ be an $A^*$-variant Krylov subspace with $\infty \notin s$. There exists a RAD

$$A^*V_{j+1}K_j = V_{j+1}H_j$$

(15)

associated to this Krylov subspace with $K_j = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $H_j = \begin{bmatrix} h_j \\ H_{j-1} \end{bmatrix}$, an upper triangular matrix $H_{j-1}$ and $V_{j+1} = [C^* \  Z_j]$ with a basis $Z_j$ of $\mathcal{K}_j(A^*, C^*, s)$.

**Proof.** As the Krylov subspace $\mathcal{K}_j(A^*, C^*, s)$ is $A^*$-variant the augmented space $\mathcal{K}_j^+(A^*, C^*, s)$ is of dimension $j + 1$. Thus Theorem 2.1 guarantees the existence of a RAD

$$A^*\tilde{V}_{j+1}K_j = \tilde{V}_{j+1}\tilde{H}_j$$

(16)

associated to $\mathcal{K}_j(A^*, C^*, s)$ with starting vector $C^* \in \text{span}\{V_{j+1}e_1\}$. We aim at constructing an upper triangular matrix $R$ to transform the RAD (15) into the RAD (16) with $V_{j+1} = \tilde{V}_{j+1}R$, $K_j = R^{-1}K_j$ and $H_j = R^{-1}H_j$. This regular $R$ is constructed as follows. Let $\alpha \in \mathbb{C}$ so that $C^* = \tilde{V}_{j+1}\alpha e_1$ and set
\[ R = \begin{bmatrix} ao_1 & \bar{K}_j \end{bmatrix} \] to obtain \( K_j = \begin{bmatrix} 0 \\ I \end{bmatrix} \) and \( V_{j+1}e_1 = C^* \). As we assumed that \( \infty \not\in s \) we have, due to (14) and (7), that \( C^* \not\in K_j(A^*, C^*, s) = \text{span}\{\bar{V}_{j+1}K_j\} \).

Therefore \( e_1 \not\in \text{span}\{K_j\} \) and \( R \) is indeed regular. As \( \bar{K}_j \) is an upper Hessenberg matrix, \( R \) is an upper triangular matrix and so is \( H_{-j} \). Finally, the structure of \( K_j \) and (7) imply that \( Z_j = V_{j+1}K_j \) is a basis of \( \bar{K}_j(A^*, C^*, s) \), which completes the proof. \( \square \)

With the assumptions of Lemma 3.1 let the RAD (13) be given. In particular hereby \( C^* \not\in K_j(A^*, C^*, s) \) is implied. Due to \( V_{j+1} = \begin{bmatrix} C^* & Z_j \end{bmatrix} \) and \( K_j = \begin{bmatrix} 0 \\ I \end{bmatrix} \) we have \( v = e_1 \) in (13) and \( S_j = Z_j^*BB^*Z_j \) in (14). As \( V_{j+1} \) has full rank, we find that the rank of the residual \( \bar{R}(X_j) \) is the same as the rank of the inner matrix

\[
M_j := H_jY_jK_j^* + K_jY_jH_j^* + e_1e_1^* - K_jY_jS_jY_jK_j^*
= \begin{bmatrix} \begin{bmatrix} 0 \ h_jY_j \\ 0 \ H_{-j}Y_j \end{bmatrix} & \begin{bmatrix} 1 \ 0 \\ 0 \ 0 \end{bmatrix} \\ \begin{bmatrix} 0 \ Y_jh_j^* \ Y_jH_{-j}^* \end{bmatrix} & \begin{bmatrix} 0 \ 0 \ 0 \ Y_jS_jY_j \end{bmatrix} \end{bmatrix}
= \begin{bmatrix} 1 \ Y_jh_j^* \ h_jY_j \\ Y_jh_j^* \ h_jY_j \end{bmatrix} H_{-j}Y_j + \begin{bmatrix} 0 \ \begin{bmatrix} 0 \ 0 \ 0 \ Y_jS_jY_j \end{bmatrix} \end{bmatrix} H_{-j}^*Y_j - Y_jS_jY_j
\]

(17)

from (14). Thus we are interested in finding \( Y_j \) such that \( M_j \) is of rank 1. This is the case if and only if

\[
M_j = \begin{bmatrix} 1 \ h_jY_j \\ Y_jh_j^* \ h_jY_j \end{bmatrix}
\]

holds, which is a rank-1 factorization in terms of the first row and column of \( M_j \). From the lower right blocks of (17) and (14) we find that therefore \( Y_j \) must be chosen to be a solution of

\[
0 = H_{-j}Y_j + Y_jH_{-j}^* - Y_jS_jY_j - Y_jh_j^*h_jY_j
= H_{-j}Y_j + Y_jH_{-j}^* - Y_j(S_j + h_j^*h_j)Y_j.
\]

(20)

Assume that there exists a full-rank solution \( Y_j \) of the homogeneous Riccati equation (20), which is desirable as otherwise not all information available in the basis \( Z_j \) is incorporated into the ADI approximate solution \( X_j \). Such a solution exists if and only if the Lyapunov equation

\[
0 = \bar{Y}_jH_{-j} + H_{-j}^*\bar{Y}_j - (S_j + h_j^*h_j)
\]

(21)

is solvable with a full-rank solution, and then \( Y_j = \bar{Y}_j^{-1} \) holds. Thus if the solution of (21) is of full rank and unique, so is the full-rank solution of (20).
The Lyapunov equation (21) is uniquely solvable with a Hermitian solution if and only if \(H_{-j}\) and \(-H_{-j}^*\) have no eigenvalues in common [18 Thm. 5.2.2]. Due to Theorem 2.1 the eigenvalues of \(H_{-j}\) are equal to the shifts \(s\). Therefore the eigenvalue condition \(\Lambda(H_{-j}) \cap \Lambda(-H_{-j}^*) = \emptyset\) is equivalent to the shift condition \(s \cap -s = \emptyset\).

We next proof regularity of the solution \(\hat{Y}_j\) of (21). Assume that \((h_j, H_{-j})\) is unobservable, i.e. the observability matrix \([h_j^* \ H_{-j}^* h_j^* \cdots (H_{-j}^*)^{j-1} h_j^*]^{*}\) is of rank smaller than \(j\). Then due to [3 Thm. 4.26] there exists an vector \(u \neq 0\) with \(h_j u = 0\) and \(H_{-j} u = \mu u\). It holds \(\mu \in s\) as the eigenvalues of \(H_{-j}\) are the poles of the Krylov subspace. Thus we find due to (15)

\[
A^* V_{j+1} H_j u = A^* V_{j+1} \begin{bmatrix} h_j \\ H_{-j} \end{bmatrix} u = A^* V_{j+1} \begin{bmatrix} 0 \\ I \end{bmatrix} \mu u
= \mu V_{j+1} H_j u
\]
i.e. \(V_{j+1} H_j u\) is an eigenvector of \(A^*\) with eigenvalue \(\mu\). This is a contradiction to the definition of rational Krylov subspaces because the poles of the Krylov subspace must be distinct from the eigenvalues of \(A^*\). Thus \((h_j, H_{-j})\) is observable and so \((H_{-j}^*, h_j^*)\) is controllable [3 Thm. 4.23]. This implies controllability of \((H_{-j}^*, [h_j^* Z_j^* B])\) where \([h_j^* Z_j^* B] \begin{bmatrix} h_j \\ B^* Z_j \end{bmatrix} = h_j^* h_j + S_j\) holds with \(S_j\) from (14). Herewith regularity of \(Y_j\) can be shown in full analogy to the proof of [18 Thm. 5.3.1 (b)].

Due to (14) and (15) the residual factor \(R_j\) of the rank-1 residual \(\mathcal{R}(X_j) = R_j R_j^*\) is given by

\[
R_j = V_{j+1} \begin{bmatrix} 1 \\ Y_j h_j^* \end{bmatrix}.
\]

We summarize our findings in the next theorem.

**Theorem 3.1.** Let \(\mathcal{K}_j(A^*, C^*, s)\) be an \(A^*\)-variant Krylov subspace with a basis \(Z_j\). Among all matrices \(Y_j \in \mathbb{C}^{j \times j}\) such that for \(X_j = Z_j Y_j Z_j^*\) the residual \(\mathcal{R}(X_j)\) is of rank one, there exists a unique regular \(Y_j\) if and only if \(\infty \not\in s\) and \(s \cap -s = \emptyset\). Such a unique regular \(Y_j\) is determined by the small scale Lyapunov equation

\[
0 = Y_j^{-1} H_{-j} + H_{-j}^* Y_j^{-1} - (S_j + h_j^* h_j)
\]

(23) where \(H_{-j}\) and \(h_j\) are as in the associated RAD (15) and \(S_j\) is as in (14).

**Proof.** We already constructed the unique rank-1 residual approximation for the case \(\infty \not\in s\) and \(s \cap -s = \emptyset\) preceding this theorem. Now assume \(C^* \in \mathcal{K}_j(A^*, C^*, s)\) which means that \(s\) does contain the pole infinity.

As in the proof of Lemma 3.1 we can transform a RAD \(A^* \bar{V}_{j+1} \bar{K}_j = \bar{V}_{j+1} \bar{H}_j\) associated to \(\mathcal{K}_j(A^*, C^*, s)\) with a regular matrix \(R = \begin{bmatrix} \bar{w} & \bar{K}_j \end{bmatrix}\) to obtain a
RAD with $K_j$ and $H_j$ as in (15), but with a different $V_{j+1}$. Due to $C^* \in K_j(A^*,C^*,s) = \text{span}\{V_{j+1}K_j\}$ there is a $\tilde{v} \in \mathbb{C}^j$ with $C^* = V_{j+1}K_j\tilde{v}$. Thus we have $v = \begin{bmatrix} 0 \\ \tilde{v} \end{bmatrix}$ in (13) because of the special structure of $K_j$. Again from (14) we find that the rank of the residual is the same as the rank of the inner matrix

$$M_j = H_jY_jK_j^* + K_jY_jH_j^* + vv^* - K_jY_jS_jY_jK_j^*$$

$$= \begin{bmatrix} 0 & H_jY_j \\ 0 & H_{-j}Y_j \end{bmatrix} + \begin{bmatrix} 0 & h_j^* \\ 0 & H_{-j}^* \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \tilde{v}v^* \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 0 & Y_jS_jY_j \end{bmatrix}$$

$$= \begin{bmatrix} 0 & h_j^* \\ Y_jh_j^* & \tilde{v}v^* + H_{-j}Y_j + Y_jH_{-j}^* - Y_jS_jY_j \end{bmatrix}.$$ 

Assume this matrix is of rank 1. Then due to the first diagonal entry being zero the first row and column have to be zero, i.e. $Y_jh_j^* = 0$. This is only possible if $Y_j$ is singular or $h_j = 0$. In the latter case the Krylov subspace is $A^*$-invariant. In both cases the assumptions of the theorem are violated and no approximation with the wanted properties exists.

**Remark 3.1.** Under the conditions of Theorem 3.1 with $\infty \notin s$ and $s \cap -s = \emptyset$ there exist many approximate solutions $\tilde{X}_j = Z_j\tilde{Y}Z_j^*$ of (14) resulting in a rank-1 residual if the full-rank condition on $\tilde{Y}$ is omitted. Consider e.g. the trivial solution $\tilde{Y} = 0$ of (20) resulting in the residual factor $C^*$. For other approximations with rank-1 residual consider a subset $\tilde{s} \subset s$ with $\tilde{j}$ elements. Clearly $\tilde{s}$ fulfills the assumptions of Theorem 3.1 and so there exists a rank-$\tilde{j}$ approximate solution $\tilde{X}_j$ resulting in a rank-1 residual. Due to $K_j(A^*,C^*,s) \subset K_j(A^*,C^*,s)$ this solution can be represented by $\tilde{X}_j = Z_j\tilde{Y}Z_j^*$ with a rank-$\tilde{j}$ matrix $\tilde{Y}$. If the shifts in $s$ are pairwise distinct there exist $2^j$ subsets of $s$ and so there are $2^j$ approximate solutions of the form $Z_j\tilde{Y}Z_j^*$ yielding a rank-1 residual.

### 3.1 Obtaining the Riccati ADI solution via projection

We now discuss how the Riccati ADI approximate solution can be interpreted as the solution of a projection of the large scale Riccati equation (1) onto a Krylov subspace. For a general projection method let $Z,W \in \mathbb{C}^{n \times j}$ be matrices of rank $j$, i.e. bases of certain $j$ dimensional subspaces, with regular $Z^*W$. Then $\Pi = Z(W^*Z)^{-1}W^* \in \mathbb{C}^{n \times n}$ is a projection onto $\text{im}(\Pi) = \text{im}(Z)$ along $\ker(\Pi) = \ker(W^*)$. Set $\hat{W} := W(Z^*W)^{-1}$, then $\Pi = Z\hat{W}$ and it holds $\hat{W}^*Z = I$. Let the approximate solution $X_j \approx X$ to the Riccati equation (1) lie in $\text{im}(Z)$ with the representation $X_j = ZY_jZ^*$. Projection of (1) yields the equation

$$\Pi R(X_j)\Pi^* = 0$$

(24)

which is then solved for $Y_j$. Let for instance $Z = W$ be a basis of the Krylov subspace $K_j(A^*,C^*,s)$, so $\Pi = \Pi^*$ is an orthogonal projection onto the Krylov subspace. This is just the approach used in *KSM.
In the following theorem we show how with the assumptions of Theorem 3.1 the Riccati ADI approximation can be obtained as the solution of the projected Riccati equation \((24)\) using an oblique projection. It is a generalization of [27, Sec. 3.2], [28, Rem. 5.16], where a similar statement for the ADI iteration to solve Lyapunov equations is presented.

\textbf{Theorem 3.2.} Let \(K_j(A^*, C^*, s)\) be an \(A^*\)-variant Krylov subspace with shifts \(s \subset \mathbb{C}\) and \(s \cap -\mathbb{R} = \emptyset\). Let \(A^* V_{j+1} = [0 \ I] = V_{j+1} \underbrace{[h_j \ H_{-j}]}_{\Pi}\) be an associated RAD as in Lemma 3.1 with \(V_{j+1} = [C^* \ Z_j]\). Let \(\Pi\) be a projection onto \(\text{im}(Z_j)\) along \(\text{ker}(W^*)\). If the Riccati residual factor \(R_j\) as in \((22)\) is contained in the kernel of the projection \(\Pi\), i.e. \(W \perp R_j\), then the projected equation \((24)\) is equivalent to the small scale Riccati equation \((20)\).

\textit{Proof.} From the orthogonality condition of the residual factor \(R_j = V_{j+1} \begin{bmatrix} 1 & Y_j h_j^* \end{bmatrix}\) we find
\[
0 = \tilde{W}^* R_j = \tilde{W}^* [C^* \ Z_j] \begin{bmatrix} 1 & Y_j h_j^* \end{bmatrix} = \tilde{W}^* (C^* + Z_j Y_j h_j^*),
\]
or equivalently
\[
\tilde{W}^* C^* = -\tilde{W}^* Z_j Y_j h_j^* = -Y_j h_j^*.
\]

Herewith we obtain
\[
\tilde{W}^* V_{j+1} = \tilde{W}^* [C^* \ Z_j] = [\tilde{W}^* C^* \ \tilde{W}^* Z_j] = [-Y_j h_j^* \ I].
\]

As \(Z_j\) is a basis it holds \(\text{ker}(Z_j) = \{0\}\), so with \(\Pi = Z_j \tilde{W}^*\) the projected equation \((24)\) is equivalent to \(\tilde{W}^* \mathcal{R}(X_j) \tilde{W} = 0\). With \((14)\) and \((17)\) we obtain
\[
\tilde{W}^* \mathcal{R}(X_j) \tilde{W} = \tilde{W}^* V_{j+1} \begin{bmatrix} 1 & h_j Y_j \ H_{-j} Y_j + Y_j \ H_{-j}^* - Y_j S_j Y_j \end{bmatrix} V_{j+1}^* \tilde{W} = [-Y_j h_j^* \ I] \begin{bmatrix} 1 & h_j Y_j \ H_{-j} Y_j + Y_j \ H_{-j}^* - Y_j S_j Y_j \end{bmatrix} \begin{bmatrix} -h_j Y_j \ I \end{bmatrix} = -Y_j h_j^* h_j Y_j - Y_j h_j^* h_j Y_j - Y_j h_j^* Y_j + Y_j H_{-j} Y_j + Y_j H_{-j}^* - Y_j S_j Y_j = Y_j h_j^* Y_j + H_{-j} Y_j + Y_j H_{-j}^* - Y_j S_j Y_j.
\]

This is the right hand side of \((20)\) which concludes the proof. \(\Box\)

If in the above theorem \(\Pi\) is an orthogonal projection then \(\text{im}(\Pi) \perp \text{ker}(\Pi)\) holds. It follows that the conditions \(R_j \in \text{ker}(\Pi)\) and \(R_j \perp K_j(A^*, C^*, s)\) are equivalent. Further, the approximations generated by \(*\text{KSM}\) and the Riccati ADI methods coincide.

Although \(\tilde{W}\) is unknown in practice, the projected system matrices \(\tilde{W}^* A^* Z_j\) and \(\tilde{W}^* (A^* - X_j B B^*) Z_j\) can be expressed in terms of parts of the RAD. This relation is established in the next lemma, which will also be useful in the proofs of the subsequent theorems.
Lemma 3.2. Let $K_j(A^*, C^*, s)$ be an $A^*$-variant Krylov subspace. Let
\[
A^* \begin{bmatrix} C^* & Z_j \end{bmatrix} \begin{bmatrix} 0 \\ I \end{bmatrix} = \begin{bmatrix} C^* & Z_j \end{bmatrix} \begin{bmatrix} h_j \\ H_{-j} \end{bmatrix}
\] (25)
be an associated RAD such that (23) holds, i.e.
\[
0 = Y_j^{-1} H_{-j} + H_{-j}^* Y_j^{-1} - (S_j + h_j^* h_j)
\] (26)
as in Theorem 3.1. Let $\Pi$ be a projection onto $\text{im}(Z_j)$ along $\ker(W^*)$ with $\tilde{W} \perp R_j$. Then
\[
\tilde{W}^* A^* Z_j = -Y_j h_j^* h_j + H_{-j}
\]
and
\[
\tilde{W}^* (A^* - X_j BB^*) Z_j = -Y_j H_{-j}^* Y_j^{-1}
\]
hold.

Proof. With $\tilde{W}^* C^* = -Y_j h_j^*$ as in the proof of Theorem 3.2, with $\tilde{W}^* Z_j = I$ and by utilizing the RAD equation (25) we find
\[
-Y_j h_j^* h_j + H_{-j} = \tilde{W}^* C^* h_j + \tilde{W}^* Z_j H_{-j}
\]
\[
= \tilde{W}^* \begin{bmatrix} C^* & Z_j \end{bmatrix} \begin{bmatrix} h_j \\ H_{-j} \end{bmatrix}
\]
\[
= \tilde{W}^* A^* \begin{bmatrix} C^* & Z_j \end{bmatrix} \begin{bmatrix} 0 \\ I \end{bmatrix}
\]
\[
= \tilde{W}^* A^* Z_j.
\]
Multiplication of (26) with $Y_j$ from the left implies
\[
-Y_j h_j^* h_j + H_{-j} = -Y_j H_{-j}^* Y_j^{-1} + Y_j S_j,
\]
which concludes the first part of the proof.

For the second part consider $S_j = Z_j^* BB^* Z_j$ and again $\tilde{W}^* Z_j = I$ to obtain
\[
Y_j S_j = \tilde{W}^* Z_j Y_j S_j
\]
\[
= \tilde{W}^* Z_j Y_j Z_j^* BB^* Z_j
\]
\[
= \tilde{W}^* X_j BB^* Z_j.
\]
Multiplication of (26) with $Y_j$ from the left yields
\[
0 = H_{-j} + Y_j H_{-j}^* Y_j^{-1} - Y_j (S_j + h_j^* h_j).
\]
Thus we have

\[-Y_j H_{-j}^{-1} Y_j^{-1} = H_{-j} - Y_j S_j - Y_j h_j^* h_j \]

\[= \tilde{W}^* A^* Z_j - \tilde{W}^* X_j B B^* Z_j \]

\[= \tilde{W}^* (A^* - X_j B B^*) Z_j \]

with \(-Y_j h_j^* h_j + H_{-j} = \tilde{W}^* A^* Z_j\) from the first part. This concludes the second part of the proof.

The residual factor \(R_j\) from (22) is a linear combination of the columns of \(V_{j+1}\) and so it is an element of the augmented Krylov subspace \(K_j^+(A^*, C^*, s)\), i.e. a rational function in \(A^*\) multiplied with \(C^*\). We aim at specifying this rational function, which turns out to be connected to the eigenvalues of the projected matrix \(\tilde{W}^* A^* Z_j\) as stated in the next theorem.

**Theorem 3.3.** Let the same assumptions as in Lemma 3.2 hold. Additionally let \(K_j^+(A^*, C^*, s)\) be \(A^*\)-variant. Let \(p_j, q_j \in \Pi_j\) be normalized polynomials of degree \(j\) given by

\[p_j(x) = \prod_{i=1}^{j} (x - \lambda_i^{(j)})\]

\[q_j(x) = \prod_{i=1}^{j} (x - s_i)\]

with the eigenvalues \(\{\lambda_i^{(j)}, \ldots, \lambda_j^{(j)}\} = \Lambda(\tilde{W}^* A^* Z_j)\) and the poles \(s_i \in s\) of the Krylov subspace. Then for the residual factor (22)

\[R_j = q_j(A^*)^{-1} p_j(A^*) C^* = \prod_{i=1}^{j} \frac{A^* - \lambda_i^{(j)} I_n}{A^* - s_i I_n} C^*\]

holds.

**Proof.** By construction of the RAD (26) \(Z_j\) is a basis of the Krylov subspace \(K_j(A^*, C^*, s) = K_j(A^*, C^*, q_j)\) and \(q_j\) is normalized. Due to the definition of Krylov subspaces (3) there exists a polynomial \(\tilde{p} \in \Pi_{j-1}\) of degree at most \(j - 1\) with

\[Z_j Y_j h_j^* = q_j(A^*)^{-1} \tilde{p}(A^*) C^*\]

Thus for the residual factor (22)

\[R_j = [C^* Z_j] \left[ \begin{array}{c} 1 \\ Y_j h_j^* \end{array} \right] = C^* + q_j(A^*)^{-1} \tilde{p}(A^*) C^* \]

\[= q_j(A^*)^{-1} (q_j(A^*) + \tilde{p}(A^*)) C^* \]

holds. Set \(p_j = q_j + \tilde{p}\), which is a normalized polynomial because \(q_j\) is normalized and of degree \(j\) and \(\tilde{p}\) is of degree at most \(j - 1\). It remains to specify the roots of
We transform the RAD (25) so that it is a (generalized) RKD with starting vector \( R_j \) and use Theorem 2.2. In order to do so consider the matrix

\[
U = \begin{bmatrix}
1 & 0 \\
Y_j h_j^* & I
\end{bmatrix}
\]

with inverse \( U^{-1} = \begin{bmatrix}
1 & 0 \\
-Y_j h_j^* & I
\end{bmatrix} \).

Transformation of the RAD (25) with \( U \) yields

\[
\begin{bmatrix}
C^* & Z_j
\end{bmatrix} U = \begin{bmatrix}
R_j & Z_j
\end{bmatrix},
\]

\( K_j \) is left unchanged and multiplication of \( U^{-1} \) with \( H_j \) yields

\[
U^{-1} H_j = U^{-1} \begin{bmatrix}
h_j \\
H_{-j}
\end{bmatrix} = \begin{bmatrix}
h_j \\
-Y_j h_j^* h_j + H_{-j}
\end{bmatrix} = \begin{bmatrix}
h_j \\
\tilde{W}^* A^* Z_j
\end{bmatrix},
\]

where the last equality is due to Lemma 3.2. Now Theorem 2.2 implies that \( \{\lambda^{(j)}_1, \ldots, \lambda^{(j)}_j\} = \Lambda(\tilde{W}^* A^* Z_j) \) are the roots of \( p_j \), concluding the proof.

We note that the latter result is the only one in this section for which there is no counterpart in the block case as the elements of block Krylov subspaces (10) correspond to matrix polynomials, which in general cannot be characterized by scalar roots.

We proceed with a theorem which connects the poles of the rational Krylov subspace and the eigenvalues of the projection of the matrix \( A^* - X_j BB^* \). It is a generalization of parts of [20, Thm. 4.4] to oblique projections.

**Theorem 3.4.** With the same assumptions as in Lemma 3.2

\[ \Lambda(\tilde{W}^* (A^* - X_j BB^*) Z_j) = -\pi \]

holds.

**Proof.** Due to Definition 2.2 and Theorem 2.1 the eigenvalues of \( H_{-j} \) are equal to the poles \( s \) and so with Lemma 3.2 and due to similarity

\[
\Lambda(\tilde{W}^* (A^* - X_j BB^*) Z_j) = \Lambda(-Y_j H_{-j}^* Y_j^{-1})
\]

\[= \Lambda(-H_{-j}^*) = -\pi \]

holds, which concludes the proof.

### 3.2 The general case of a matrix \( C^* \in \mathbb{C}^{n \times p} \)

So far we considered the case where \( C^* \) is a vector. We now comment on the general case having a matrix \( C^* \in \mathbb{C}^{n \times p} \) with an arbitrary \( p \in \mathbb{N} \). We aim to construct an approximation \( X_j = Z_j Y_j Z_j^* \) with a regular \( Y_j \) to the solution of the Riccati equation (1) with a rank-\( p \) residual \( R(X_j) = R_j R_j^* \). The residual factor \( R_j \in \mathbb{C}^{n \times p} \) then lies in a block rational Krylov subspace (10) instead of a Krylov subspace (3). To obtain a rank-\( p \) residual we proceed in full analogy
to the rank-1 residual by essentially replacing vectors by block vectors (i.e. matrices with $p$ columns) and scalars by scalar $p$-by-$p$ matrices (i.e. multiples of the $p$-dimensional identity matrix). We briefly comment on the changes to be made to obtain the sought-after approximation. Let a block rational Krylov subspace $K_j^\mathcal{A}(A^*, C^*, s)$ be given with shifts $s = \{\mu_1, \ldots, \mu_j\} \subset \mathbb{C}$ fulfilling $s \cap -s = \emptyset$. Let

$$A^* V_{j+1} K_j = V_{j+1} H_j$$

be an associated BRAD as in Definition [2.4] with full-rank $V_{j+1} = [C^* \ Z_j] \in \mathbb{C}^{n \times jp}$ and block upper Hessenberg matrices

$$K_j = \begin{bmatrix} 0 \\ I \end{bmatrix} \in \mathbb{R}^{(j+1)p \times jp}$$

and

$$H_j = \begin{bmatrix} h_j \\ H_{-j} \end{bmatrix} \in \mathbb{C}^{(j+1)p \times jp}, \text{ with } h_j \in \mathbb{C}^{p \times jp}, \ H_{-j} \in \mathbb{C}^{jp \times jp}$$

in analogy to [15]. In accordance to property [3] of Definition [2.4] the relation $H_{i+1,i} = \mu_i I_p$ must hold for the subdiagonal blocks of $H_j$, which are the diagonal blocks of its quadratic lower submatrix $H_{-j}$. Such a decomposition is constructed iteratively in Section [4]. With the above BRAD [14] holds with the block vector $v = \begin{bmatrix} I_p \\ 0 \end{bmatrix}$ and [21] can be derived in full analogy. The resulting approximation $X_j = Z_j Y_j Z_j^*$ yields a rank-$p$ residual.

4 Two new iterative Riccati ADI methods

Summarizing the approach from Section [3] the ADI approximate solution $X_j = Z_j Y_j Z_j^*$ of the Riccati equation [14] is obtained in two steps: First, generate a Krylov basis $Z_j$ with a corresponding RAD, then solve a small-scale Lyapunov equation for $Y_{j+1}$.

In this section these two steps are combined in an iterative way. The basis of the Krylov subspace is expanded incrementally, simultaneously the solution of the small-scale Lyapunov equation is updated. Due to the importance of the Lyapunov equation [21] we give the following definition.

**Definition 4.1.** For a relation

$$A^* \begin{bmatrix} C^* & Z_j \end{bmatrix} \begin{bmatrix} 0 \\ I \end{bmatrix} = \begin{bmatrix} C^* & Z_j \end{bmatrix} \begin{bmatrix} h_j \\ H_{-j} \end{bmatrix}$$

(27)

the associated $\tilde{Y}$-equation is defined as

$$0 = \tilde{Y} H_{-j} + H_{-j} \tilde{Y} - (S_j + h_j^* h_j)$$

with $S_j = Z_j^* B B^* Z_j$. 

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In the remainder of this work we assume that all shifts have positive real part, i.e. $s \in \mathbb{C}_+$. Hereby it is implied that the shift condition $s \cap -\pi = \emptyset$, $\infty \not\in s$ from Theorem 3.1 is satisfied. Further, in the $Y$-equation all eigenvalues of $H_{-j}$ have positive real part as they are equal to the shifts and $(H_{-j}^*, h_j^*)$ is controllable (cf. the paragraph preceding Theorem 3.1). Due to Thm. 5.3.1 (b) the solution $\hat{Y}$ is positive definite, and so is its inverse $Y_j = \hat{Y}^{-1}$. Thus with a Cholesky decomposition of the small matrix $Y_j$, we find a $\tilde{Z}_j$ spanning the same Krylov space as $Z_j$ with $X_j = Z_jY_jZ_j^* = \tilde{Z}_j\tilde{Z}_j^*$.

The (B)RAD (27) corresponding to $Z_j$ can be altered to obtain a (B)RAD associated to $\tilde{Z}_j$. To our advantage the corresponding $\hat{Y}$-equation is then solved by the identity. The next lemma describes this procedure in detail and is the foundation of our new iterative ADI-type approaches to construct a rank-$p$ residual solution to (1).

**Lemma 4.1.** Let a BRAD of the form (27) be given. Let all shifts $s \in \mathbb{C}_+$ have positive real part such that the associated $\hat{Y}$-equation has a positive definite solution $\hat{Y}_j$. Let $G^*G = \hat{Y}_j$ be a Cholesky decomposition of $\hat{Y}_j$ with upper triangular $G$. Then the approximate solution $X_j = Z_j\hat{Y}_j^{-1}Z_j^*$ yields a rank-$p$ residual $\mathcal{R}(X_j) = R_jR_j^*$ with residual factor $R_j = V_{j+1}\begin{bmatrix} I_p & \hat{Y}_j^{-1}h_j^* \end{bmatrix} \in \mathbb{C}^{n \times p}$. This approximation can be transformed to $X_j = Z_j\hat{Z}_j^*$ with $\hat{Z}_j = Z_jG^{-1}$. Consider the associated transformed BRAD $A^*V_{j+1}\begin{bmatrix} 0 \\
I \end{bmatrix} = \hat{V}_{j+1}\hat{H}_j$ with $\hat{V}_{j+1} = \begin{bmatrix} C^* & \hat{Z}_j \end{bmatrix} = \begin{bmatrix} C^* & Z_j \end{bmatrix}\begin{bmatrix} I_p & 0 \\
0 & G^{-1} \end{bmatrix}$ and $\hat{H}_j = \begin{bmatrix} I_p & 0 \\
0 & G \end{bmatrix}H_jG^{-1}$. It has an associated $\hat{Y}$-equation which is solved by the identity matrix, i.e.

$$0 = \hat{H}_{-j} + \hat{H}_{-j}^* - (\hat{S}_j + \hat{h}_j^*\hat{h}_j)$$

(28)

holds with $\hat{H}_j = \begin{bmatrix} \hat{h}_j \\
\hat{H}_{-j} \end{bmatrix}$ and $\hat{S}_j = \hat{Z}_j^*BB^*\hat{Z}_j = G^{-*}S_jG^{-1}$. With these settings the residual factor can be expressed as $R_j = \hat{V}_{j+1}\begin{bmatrix} I_p \\
\hat{h}_j \end{bmatrix} \in \mathbb{C}^{n \times p}$.

In our iterative procedures after each expansion of the Krylov basis the corresponding BRAD is updated as described in Lemma 4.1. Consider a Krylov subspace $\mathcal{K}_j(A^*, C^*, s)$ with an associated BRAD

$$A^*[C^* Z_j]\begin{bmatrix} 0 \\
I \end{bmatrix} = [C^* Z_j]\begin{bmatrix} h_j \\
H_{-j} \end{bmatrix} = \hat{H}_j$$

(29)

where the associated $\hat{Y}$-equation is solved by the identity i.e. the low-rank residual approximation is given by $X_j = Z_jZ_j^*$ and the residual factor by

$$R_j = [C^* Z_j]\begin{bmatrix} I_p \\
\hat{h}_j \end{bmatrix}.$$
We expand the Krylov subspace $K_j(A^*, C^*, s)$ by adding new poles, resulting in the space $K_j(A^*, C^*, \tilde{s})$ with $s \subset \tilde{s}$. The basis $[C^* Z_j]$ is expanded by a suitable $\tilde{Z}$ to obtain a basis of the expanded space. The BRAD corresponding to the expanded space $K_j(A^*, C^*, \tilde{s})$ thus reads

$$A^* [C^* Z_j \tilde{Z}] \begin{bmatrix} 0 \\ I \end{bmatrix} = [C^* Z_j \tilde{Z}] \tilde{H}_{j+1}. \tag{31}$$

The calculation of the expansion matrix $\tilde{Z}$ corresponding to a new pole $\mu$ is described in detail in the next two subsections. It is obtained through the solution of linear systems with the residual factor on the right hand side. By using different types of system matrices we obtain two iterative procedures: In the Riccati RAD iteration linear systems with matrices of the form $A^* - \mu I_n$ are solved, while in the Lyapunov RAD iteration systems are solved with matrices of the form $A^* - X_j BB^* - \mu I_n$. In Section 4.3 we describe how the involved quantities can be kept real in case of real system matrices and complex shifts and how we can add multiple poles by making use of the solution of independent linear systems, which can be solved in parallel.

### 4.1 The Riccati RAD iteration

For the Riccati RAD iteration (R²ADi) we expand the BRAD (29) with $W_{j+1} = (A^* - \mu I_n)^{-1} R_j$. Rewriting this term we obtain equivalently

$$A^* W_{j+1} = R_j + \mu W_{j+1} = [C^* Z_j W_{j+1}] \begin{bmatrix} I_p \\ h_j^* \\ \mu I_p \end{bmatrix} \tag{32}$$

with the representation of the residual factor $R_j$ as in (30). Set $U_1 = I_p, U_2 = h_j^*$ and $D = \mu I_p$. Then (31) holds with $\tilde{Z} = W_{j+1}$ and the partitioned matrix

$$\tilde{H}_{j+1} = \begin{bmatrix} h_j & U_1 \\ H_{-j} & U_2 \\ 0 & D \end{bmatrix}. \tag{33}$$

We use the variables $U_1, U_2$ with $U_2 = h_j^* U_1$ and $D$ here to keep the derivation of our iterative procedure as general as necessary for the introduction of realisation and parallelization later on. Due to $D = \mu I_p$ we find from Definition 2.4 that the BRAD (29) is expanded with the pole $\mu$.

Our goal is to manipulate the expanded BRAD (31) so that the associated $\tilde{Y}$-equation is again solved by the identity matrix. In order to do so, first we set $\tilde{h} := [h_j \ U_1], \tilde{H}_- := \begin{bmatrix} H_{-j} \\ 0 \\ U_2 \\ D \end{bmatrix}$ and write the $\tilde{Y}$-equation associated to (31).
\[ 0 = \hat{Y} \hat{H}_{-j} + \hat{H}_{-j}^* \hat{Y} - [Z_j \ \bar{Z} ]^* BB^* [Z_j \ \bar{Z}] - \hat{h}^* \hat{h} \]

\[ = \begin{bmatrix} Y_{11} H_{-j} & Y_{12} D + Y_{12} H_{-j}^* Y_{11} \\ Y_{12}^* H_{-j} & Y_{22} U_2 + Y_{22} D^* \end{bmatrix} + \begin{bmatrix} H_{-j}^* Y_{11} \\ U_2^* Y_{11} + D^* Y_{12} \end{bmatrix} \]

\[ \begin{bmatrix} \bar{Z}^* BB^* Z_j \\ \bar{Z}^* BB^* \bar{Z} \\ U_1^* h_j \end{bmatrix}, \]  

(34)

with the partitioned Hermitian solution matrix \( \tilde{Y} = \begin{bmatrix} Y_{11} & Y_{12} \\ Y_{12}^* & Y_{22} \end{bmatrix} \). Now we examine the blocks of (34) separately. The upper left block of (34) yields

\[ 0 = Y_{11} H_{-j} + H_{-j}^* Y_{11} - Z_j^* BB^* Z_j - \hat{h}^* h_j \]

with the solution \( Y_{11} = I \) because this is the \( \tilde{Y} \)-equation associated to (29), which was assumed to be solved by the identity. The lower left block is equal to the conjugated transposed of the upper right block. From the upper right block for \( Y_{12} \) we obtain the Sylvester equation

\[ 0 = U_2 + Y_{12} D + H_{-j}^* Y_{12} - Z_j^* BB^* \bar{Z} - \hat{h}^* U_1 \]

(35)

due to \( U_2 = h_j^* U_1 \). From the lower right block we find that \( Y_{22} \) is the solution of the Lyapunov equation

\[ 0 = Y_{12} U_2 + Y_{22} D + U_2^* Y_{12} + D^* Y_{22} - \bar{Z}^* BB^* \bar{Z} - U_1^* U_1 \]

(36)

Thus, choosing \( Y_{11} = I \) and solving (35) for \( Y_{12} \) and (36) for \( Y_{22} \) yields the matrix \( \hat{Y} \) which solves (34). This \( \hat{Y} \) is used next to transform the BRAD (31) as described in Lemma 4.1. Only the newly added parts in the BRAD (31) are affected by this procedure, namely \( \hat{Z}, U_1, U_2, \) and \( D \).

For the transformation let \( G_{22}^* G_{22} = Y_{22} - Y_{12}^* Y_{12} \) be a Cholesky decomposition. Then

\[ G = \begin{bmatrix} I & Y_{12} \\ 0 & G_{22} \end{bmatrix} \]

is the Cholesky factor of \( \hat{Y} = G^* G \). Now postmultiply the BRAD (31) by

\[ G^{-1} = \begin{bmatrix} I & -Y_{12} G_{22}^{-1} \\ 0 & G_{22}^{-1} \end{bmatrix} \]

and rewrite the resulting equation as

\[ A^* [C^* \ Z_{j+1}] \begin{bmatrix} 0 \\ I \end{bmatrix} = [C^* \ Z_{j+1}] H_{j+1} \]

(37)
with

\[
H_{j+1} = \begin{bmatrix} 1 & 0 \\ 0 & G \end{bmatrix} \tilde{H}_{j+1} G^{-1} = \begin{bmatrix} h_j & \tilde{U}_1 \\ H_{-j} & \tilde{U}_2 \\ 0 & \tilde{D} \end{bmatrix}
\]

where

\[
\tilde{U}_1 = (-h_j Y_{12} + U_1) G_{22}^{-1}
\]
\[
\tilde{U}_2 = (-H_{-j} Y_{12} + U_2 + Y_{12} D) G_{22}^{-1}
\]
\[
\tilde{D} = G_{22} D G_{22}^{-1}
\]

and with

\[
Z_{j+1} = \begin{bmatrix} Z_j & \tilde{Z} \end{bmatrix} G^{-1} = \begin{bmatrix} Z_j & \tilde{Z} \end{bmatrix}
\]

where \( \tilde{Z} = (-Z_j Y_{12} + \tilde{Z}) G_{22}^{-1} \). Due to this manipulation of the BRAD (31), now the \( \tilde{Y} \)-equation associated to the transformed BRAD (37) is solved by the identity matrix, i.e. (28) is satisfied again. For the residual factor we find

\[
R_{j+1} = \begin{bmatrix} C^* & Z_{j+1} \end{bmatrix} \begin{bmatrix} I_p \\ h_{j+1}^* \end{bmatrix} = \begin{bmatrix} C^* & Z_j \end{bmatrix} \begin{bmatrix} I_p \\ h_j^* \end{bmatrix} = R_j + \tilde{Z} \tilde{U}_1^*.
\]

This iterative procedure is summarized in Algorithm 1.

### 4.2 The Lyapunov RADI iteration

We now consider the expansion of the BRAD (29) with \( W_{j+1} = (A^* - X_j BB^* - \mu I_n)^{-1} R_j \). We find equivalently

\[
A^* W_{j+1} = R_j + X_j BB^* W_{j+1} + \mu W_{j+1}
\]
\[
= \begin{bmatrix} C^* & Z_j \end{bmatrix} \begin{bmatrix} I_p \\ h_j^* \end{bmatrix} + Z_j (Z_j^* BB^* W_{j+1}) + \mu W_{j+1}
\]
\[
= \begin{bmatrix} C^* & Z_j \end{bmatrix} \begin{bmatrix} I_p \\ h_j^* + Z_j^* BB^* \tilde{Z} \end{bmatrix}
\]

due to the representation of the residual factor \( R_j \) as in (30) and \( X_j = Z_j Z_j^* \).

Thus (31) holds with \( \tilde{Z} = W_{j+1} \) and

\[
\tilde{H}_{j+1} = \begin{bmatrix} h_j & U_1 \\ H_{-j} & U_2 + Z_j^* BB^* \tilde{Z} \\ 0 & D \end{bmatrix},
\]
Algorithm 1 Riccati RAD iteration (R²ADi)

Input: System matrices $A, B, C$, set of shifts $s \in \mathbb{C}_+$
Output: approximate solution $ZZ^*$, residual factor $R$

1: initialize $Z_0 = [], R_0 = C^*, h_0 = [], H_{-0} = [], s_0 = 0, j = 0$
2: while not converged do
3: obtain new shift(s) $\mu$ from $s$
4: expand RAD, obtain $\tilde{Z}, U_1, U_2, D$ (solve $(A^* - \mu I_n)^{-1}R_j$
5: solve $Y_{12}D + H_{-j}^*Y_{12} - s_j^*(B^*\tilde{Z}) = 0$ for $Y_{12}$
6: solve $Y_{12}^2U_2 + Y_{22}^2D + U_2Y_{12} + D^*Y_{22} - \tilde{Z}^*BB^*\tilde{Z} - U_1^*U_1 = 0$ for $Y_{22}$
7: compute $G_{22} = \text{chol}(Y_{22} - Y_{12}^*Y_{12})$
8: compute $[\tilde{U}_1, \tilde{U}_2, D] = [-h_jY_{12} + U_1, -H_{-j}Y_{12} + U_2 + Y_{12}D, G_{22}D]G_{22}^{-1}$
9: compute $\tilde{Z} = (-Z_jY_{12} + \tilde{Z})G_{22}^{-1}$
10: update $Z_{j+1} = [Z_j, \tilde{Z}], R_{j+1} = R_j + \tilde{Z}U_1^*$
11: update $h_{j+1} = [h_j, \tilde{U}_1], H_{-(j+1)} = \begin{bmatrix} H_{-j} & 0 \\ -U_2 & \tilde{D} \end{bmatrix}$
12: update $s_{j+1} = [s_j, B^*\tilde{Z}]$
13: $j = j + 1$
14: end while
15: $Z = Z_j, R = R_j$

where $U_1 = I_p, U_2 = h_j^*$, and $D = \mu I_p$ holds. Again we use the generic variables $U_1, U_2$ with $U_2 = h_j^*U_1$ and $D$ in preparation for realification and parallelization in Section 4.3. As in the previous subsection $D = \mu I_p$ holds, so the BRAD (29) is expanded with the pole $\mu$ here, too.

We proceed as in Section 4.1 and examine each block of the partitioned $\tilde{Y}$-equation associated to the BRAD (31) in analogy to (34). Due to the additional term $Z_j^*BB^*\tilde{Z}$ in (38) we have to replace every occurrence of $U_2$ in the equations of Section 4.1 with $U_2 + Z_j^*BB^*\tilde{Z}$. Thus we find that in (35) the term $Z_j^*BB^*\tilde{Z}$ cancels out, resulting in the equation

$$0 = Y_{12}D + H_{-j}^*Y_{12}$$

which is solved by $Y_{12} = 0$. By inserting $Y_{12} = 0$ into (36) we obtain $Y_{22}$ as the solution of the Lyapunov equation

$$0 = Y_{22}D + D^*Y_{22} - \tilde{Z}^*BB^*\tilde{Z} - U_1^*U_1.$$  \hspace{1cm} (39)

As at the end of Section 4.1 but now with $Y_{12} = 0$ we obtain

$$A^*[C^* Z_{j+1}] \begin{bmatrix} 0 \\ I \end{bmatrix} = [C^* Z_{j+1}] H_{j+1}$$
Algorithm 2 Lyapunov RADI iteration

**Input:** System matrices \( A, B, C, \) set of shifts \( s \subseteq \mathbb{C}^+ \)

**Output:** approximate solution \( ZZ^* \), residual factor \( R \)

1. initialize \( Z_0 = [], R_0 = C^*, h_0 = [], H_{-0} = [], s_0 = 0, K_0 = 0, j = 0 \)
2. while not converged do
   3. obtain new shift(s) \( \mu \) from \( s \)
   4. expand RAD, obtain \( \tilde{Z}, U_1, U_2, D \) \( \triangleright \) solve \( (A^* - K_j B^* - \mu I_n)^{-1} R_j \)
   5. solve \( Y_{22} D + D^* Y_{22} - \tilde{Z}^* B B^* \tilde{Z} - U_1^* U_1 = 0 \) for \( Y_{22} \)
   6. compute \( G_{22} = \text{cho}(Y_{22}) \)
   7. compute \( [\hat{U}_1, \hat{U}_2, \hat{D}] = [U_1, U_2 + s_j^* (B^* \tilde{Z}), G_{22} D G_{22}^{-1}] \)
   8. compute \( \hat{Z} = \hat{Z} G_{22}^{-1} \)
   9. update \( Z_{j+1} = [Z_j, \hat{Z}], R_{j+1} = R_j + \hat{Z} \hat{U}_1^* \)
   10. update \( h_{j+1} = [h_j, \hat{U}_1], H_{-(j+1)} = \begin{bmatrix} H_{-j} & \hat{U}_2 \\ 0 & \hat{D} \end{bmatrix} \)
   11. update \( s_{j+1} = [s_j, B^* \hat{Z}] \)
   12. update \( K_{j+1} = K_j + \hat{Z} (\hat{Z}^* B) \)
   13. \( j = j + 1 \)
14. end while
15. \( Z = Z_j, R = R_j \)

with \( Z_{j+1} = [Z_j, \hat{Z} G_{22}^{-1}] \) and

\[
H_{j+1} = \begin{bmatrix} 1 & 0 \\ 0 & G \end{bmatrix} \bar{H}_{j+1} G^{-1} = \begin{bmatrix} h_j & U_1 G_{22}^{-1} \\ H_{-j} & (U_2 + Z_j^* B B^* \tilde{Z}) G_{22}^{-1} \\ 0 & G_{22} D G_{22}^{-1} \end{bmatrix},
\]

with \( G = \text{diag}(I, G_{22}) \) and the Cholesky decomposition \( G_{22}^* G_{22} = Y_{22} \). For the residual factor

\[
R_{j+1} = R_j + (\hat{Z} G_{22}^{-1} (U_1 G_{22}^{-1})^*)
= R_j + \hat{Z} Y_{22}^{-1} U_1^*
\]

holds. We summarize this iteration in Algorithm 2.

Note that to obtain \( Z \) and \( R \) in Algorithm 2, it is not necessary to compute and store \( H_j \). When \( \hat{U}_1 \) in line 7 is replaced by \( G_{22}^* U_1^* \), the lines 11, 13, and 14 and the variables \( h_j, H_{-j}, s_j, U_2 \) can be deleted. Nevertheless, having \( H_j \) available might be useful in some situations and only negligible amount of memory and computational time is necessary to create it.

**Remark 4.1.** In general the matrix \( A^* - K_j B^* - \mu I_n \) with the feedback term \( K_j = X_j B \) is a dense matrix due to the term \( K_j B^* \), although \( A^* \) is sparse, making system solves costly. However, as \( K_j B^* \) is of rank \( m \), it was proposed in \cite{4} Sec. 4.2] to use the Sherman-Morrison-Woodbury (SMW) formula to speed
Algorithm 3: Simple RAD expansion

Input: residual factor $R_j = [C^* \ Z_j] \ h_j^*$, shift $\mu \in \mathbb{C} \setminus \Lambda(A^*)$

Output: $\tilde{Z}, U_1, U_2, D$

1: solve $W = (A^* - \mu I_n)^{-1} R_j$ or $W = (A^* - K_j B^* - \mu I_n)^{-1} R_j$
2: $\tilde{Z} = W$
3: $U_1 = I_p, U_2 = h_j^*, D = \mu I_p$

up computations. The formula reads

\[(A^* - K_j B^* - \mu I_n)^{-1} R_j = L + N(I_m - B^* N)^{-1} B^* L \quad (40)\]
\[[L \ N] = (A^* - \mu I_n)^{-1} [R_j \ K_j]. \quad (41)\]

To obtain the solution of (40), first the sparse linear system in (41) is solved for $L$ and $N$, then the right hand side of (40) is used.

Remark 4.2. The procedure derived in this subsection is essentially equivalent to the RADI iteration [4] with mainly two differences. First, instead of an approximation $X_j = Z_j Y_j^{-1} Z_j^*$ with a (block) diagonal matrix $Y_j$ we use a Cholesky factorization of $Y_j^{-1}$ to put it into the factor $Z_j$, resulting in the approximate solution $X_j = Z_j Z_j^*$. Second, the shift parameters $\alpha_j$ in the RADI iteration correspond to the negative poles of our BRADs, therefore the parameters must be chosen as $\mu = -\alpha_j$ to obtain an equivalent approximation.

We further note that for $U_1 = I_p$ and $D = \mu$ as above (39) simplifies to

\[2 \text{Re}(\mu) Y_{22} = I_p + \tilde{Z}^* B B^* \tilde{Z},\]

which is, up to constants, equivalent to line 10 of [4, Alg. 1]. However, we prefer to solve the more general Lyapunov equation (39) because it is more versatile: It allows for realified and parallel RAD expansions which is described in the next subsection.

Due to the Lyapunov equation (39) and the equivalence to the RADI iteration we chose the name Lyapunov RADI iteration for Algorithm 2.

4.3 Parallel and realified expansion of the Krylov basis

In the preceding subsections we have expanded the BRAD (29) with a new pole $\mu$ and obtained the BRAD (31) with

\[\tilde{H}_{j+1} = \begin{bmatrix} h_j & U_1 \\ H_{-j} & 0 \end{bmatrix} \quad \text{or} \quad \tilde{H}_{j+1} = \begin{bmatrix} h_j & U_1 \\ H_{-j} & 0 + Z_j B B^* \tilde{Z} \end{bmatrix} \]

with $D = \mu I_p$ as in (33) and (38). Only one linear system with a shift $\mu$ was solved, which is summarized in Algorithm 3.
be expanded by the two conjugated shifts $\mu$, we consider realification. Let $R$ remain real valued and how the use of complex arithmetic is minimized; in short, $A, B, C$ of real system matrices $\mu$ is expanded with the poles $W$. Hereby we mean expanding the Krylov basis with $W$ as in $\mu$. Parallel expansion of the Krylov basis with the complex block vectors $W$ yields the expanded BRAD $A^* W = R_j + \mu_i W = [C^* Z_j \ W_i] \begin{bmatrix} I_p \\ h_j^* \\ \mu_i I_p \end{bmatrix}$ as in $\mu$. Thus the expanded BRAD (31) with $\tilde{Z} = [W_1 \cdots W_l]$ is given by

$$A^* [C^* Z_j \tilde{Z}] \begin{bmatrix} 0 \\ I \end{bmatrix} = [C^* Z_j \tilde{Z}] \begin{bmatrix} h_j & I_p & \cdots & I_p \\ H_{-j} & h_j^* & \cdots & h_j^* \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mu_i I_p \end{bmatrix}.$$

This procedure is summarized in terms of $U_1, U_2$ with $U_2 = h_j^* U_1$ and $D$ in Algorithm 4. Due to Definition 23 and the structure of $D$ we find that the BRAD is expanded with the poles $\mu_1, \ldots, \mu_l$.

Next we consider the question of how to modify the R$^2$ADI such that in case of real system matrices $A, B, C$ and two complex conjugated shifts the iterates remain real valued and how the use of complex arithmetic is minimized; in short, we consider realification. Let $R_j$ have only real entries and let the BRAD (29) be expanded by the two conjugated shifts $\mu, \mu \in \mathbb{C} \setminus \Lambda(A^*)$, $\mu = a + bi, a, b \in \mathbb{R}$. Set $W = (A^* - \mu I_n)^{-1} R_j$ and so $\overline{W} = (A^* - \overline{\mu I_n})^{-1} R_j$. With $S = \frac{1}{2} \begin{bmatrix} 1 & i \\ 1 & i \end{bmatrix} \otimes I_p$ we see $[W \ \overline{W}] S = [\text{Re}(W) \ \text{Im}(W)]$ and $S^{-1} \begin{bmatrix} I_p \\ \mu I_p \end{bmatrix} \overline{W} = \begin{bmatrix} aI_p \\ bI_p \end{bmatrix}$. Parallel expansion of the Krylov basis with the complex block vectors $W$ and $\overline{W}$ yields the expanded BRAD

$$A^* [C^* Z_j \ W \ \overline{W}] \begin{bmatrix} 0 \\ I \end{bmatrix} = [C^* Z_j \ W \ \overline{W}] \begin{bmatrix} h_j & I_p & I_p \\ H_{-j} & h_j^* & h_j^* \\ 0 & \mu I_p & \overline{\mu I_p} \end{bmatrix}. $$
Algorithm 5 Realified RAD expansion

**Input:** real residual factor \( R_j = [C^* Z_j] [I_p h_j^*] \), shifts \( a + bi = \mu, \bar{\mu} \in \mathbb{C} \setminus \Lambda(A^*) \) with \( b \neq 0 \)

**Output:** \( \tilde{Z}, U_1, U_2, D \)

1: solve \( W = (A^* - \mu I_n)^{-1} R_j \) or \( W = (A^* - K_j B^* - \mu I_n)^{-1} R_j \)

2: \( \tilde{Z} = [\text{Re}(W), \text{Im}(W)] \)

3: \( U_1 = [I_p, 0], U_2 = [h_j^*, 0], D = \begin{bmatrix} a & b \\ -b & a \end{bmatrix} \otimes I_p \)

Transformation of this BRAD with the matrix \( \begin{bmatrix} I & 0 \\ 0 & S \end{bmatrix} \) then yields the equivalent realified BRAD

\[
A^* [C^* Z_j \text{Re}(W), \text{Im}(W)] \begin{bmatrix} 0 \\ I \end{bmatrix} = [C^* Z_j \text{Re}(W), \text{Im}(W)] \begin{bmatrix} h_j & I_p & 0 \\ H_{-j} & h_j^* & 0 \\ 0 & aI_p & bI_p \\ 0 & -bI_p & aI_p \end{bmatrix},
\]

where the Krylov basis is expanded with the real block vectors \( \text{Re}(W) \) and \( \text{Im}(W) \). Note that only one (complex) system solve is necessary for the expansion with the two shifts \( \mu \) and \( \bar{\mu} \). The realified expansion is stated in terms of \( U_1 \), \( U_2 \) with \( U_2 = h_j^* U_1 \) and \( D \) in Algorithm 5.

**Remark 4.3.** Unfortunately after the realification the relation (42) does not fulfill property 3 of Definition 2.4. It therefore does not satisfy the definition of a BRAD anymore. We thus propose the term *quasi BRAD* in analogy to the term quasi RAD. Further, for computational reasons it is beneficial to permute the columns of \( \text{Re}(W) \) and \( \text{Im}(W) \) so that the Krylov basis is expanded by \( [\text{Re}(w_1), \text{Im}(w_1), \ldots, \text{Re}(w_p), \text{Im}(w_p)] \) for \( W = [w_1, \ldots, w_p] \) as then the lower right block \( \begin{bmatrix} a & b \\ -b & a \end{bmatrix} \otimes I_p \) becomes \( I_p \otimes \begin{bmatrix} a & b \\ -b & a \end{bmatrix} \), a block diagonal matrix with 2-by-2 blocks on the diagonal. This permutation makes \( H_{-j} \) in the associated \( \tilde{Y} \)-equation a quasi upper triangular matrix so the Sylvester equation in line 5 of Algorithm 1 can be solved efficiently with established software packages.

The parallel and realified expansion was derived here only for the Riccati RAD iteration. It can be adapted for the Lyapunov RADI iteration by simply incorporating the term \( K_j B^* \) in the linear systems.

## 5 Discussion

As seen in Section 3 the two key assumptions for the existence of the Riccati ADI solution were that the solution factor \( Z \) in the approximate solution is a basis of a certain (block) Krylov subspace and that the Riccati residual is of
rank $p$. Unfortunately, in case of deflation or the lucky case of an exact solution, the residual is of rank smaller than $p$. To avoid these special cases the rank-$p$ condition can be replaced with the requirement that the Riccati residual factor is an element of an augmented (block) Krylov subspace which by definition contains (block) vectors with $p$ columns. However, we did not observe deflation in practice and therefore employed the rank-$p$ condition throughout this work.

We have already stated in the introduction that there are several Riccati ADI methods which have been shown to be equivalent e.g. in [5, 4] by explicitly proving the equivalence of the algorithms. The uniqueness result Theorem 3.1 makes it simpler to proof the equivalence of different Riccati ADI methods. One essentially has to verify that the approximate solution lies in a rational Krylov subspace with a set of poles $s \subset \mathbb{C}$ satisfying $s \cap -s = \emptyset$ and that the Riccati residual is of rank $p$.

### 5.1 Generalized Riccati equations

We consider two generalizations of the Riccati equation (1). We first describe how the generalized Riccati equation

$$A^*XE + E^*XA + C^*C - E^*BB^*XE = 0$$

with an additional regular system matrix $E \in \mathbb{C}^{n \times n}$ affects our iteration. This equation is not solved directly. Instead, as in [4, Sec. 4.4], the equivalent Riccati equation

$$E^{-*}A^*X + XAE^{-1} + E^{-*}C^*CE^{-1} - XBB^*X = 0$$

is considered. It has the same structure as (1) where the system matrices $A$ and the initial residual factor $C^*$ are replaced by $AE^{-1}$ and $E^{-*}C^*$. It can therefore be solved with the methods described in the preceding sections. In an efficient iteration inverting $E$ is avoided by utilizing the relation

$$(AE^{-1})^* - \mu I_n)^{-1}E^{-*}R = (A^* - \mu E^*)^{-1}R$$

with a residual factor $R$ of (43). This requires the following modifications in the algorithms presented. All linear systems have to be shifted by a multiple of $E^*$ instead of $I_n$, i.e. the systems $(A^* - \mu E^*)^{-1}R_j$ respectively $(A^* - K_jB^* - \mu E^*)^{-1}R_j$ have to be solved. Further, the residual and feedback updates have to be multiplied with $E^*$ to convert these quantities corresponding to (43) into ones corresponding to (44). For instance, the residual update in line 10 of Algorithm 1 has to be replaced by $R_{i+1} = R_j + E^*ZU_1^*$ and the feedback update in line 12 of Algorithm 2 must be replaced by $K_{j+1} = K_j + E^*Z(\bar{Z}^*B)$. In all other algorithms these lines have to be modified alike.

Our approach can also be applied to the nonsymmetric Riccati equation

$$A^*_1X + XA_2 + C_1^*C_2 - XB_2B_1^*X = 0$$

(45)
with $A_i \in \mathbb{C}^{n_i \times n_i}$, $B_i \in \mathbb{C}^{n_i \times m_i}$, and $C_i \in \mathbb{C}^{p \times n_i}$ for $i = 1, 2$ and $X \in \mathbb{C}^{n_1 \times n_2}$. It can be solved in analogy to the symmetric Riccati equation as follows. Consider the two decompositions

$$A_i^* [C_i^* Z_i] K_i = [C_i^* Z_i] H_i$$

for $i = 1, 2$, with $K_i = \begin{bmatrix} 0 & I \end{bmatrix}$ and $H_i = \begin{bmatrix} h_i & H_i^{-1} \end{bmatrix}$ similar to Lemma 3.1 and with the same number of columns in $Z_1$ and $Z_2$. Then in analogy to (14) we can rewrite the residual (45) for the approximate solution $X = Z_1 Y Z_2^*$ as

$$[C_1^* Z_1] \left( H_1 Y K_2^* + K_1 Y H_2^* + \begin{bmatrix} I_p & 0 \\ 0 & 0 \end{bmatrix} - K_1 Y S Y K_2^* \right) [C_2^* Z_2]^*$$

due to $Z_i = [C_i^* Z_i] K_i$ and with $S = Z_2^* B_i^* B_i Z_1$. The associated $Y$-equation as in (21) which determines $Y = Y^{-1}$ so that a rank-$p$ residual is obtained has to be adapted accordingly and results in the Sylvester equation

$$0 = \tilde{Y} H_{-1} + H_{-2}^* \tilde{Y} - (S + h_2^* h_1)$$

and the approximate solution $X = Z_1 Y Z_2^*$ of (45). Of course also the derivation of the iterative procedure in Section 4 can be transferred to the nonsymmetric Riccati equation. We briefly mention where such a procedure differs from Algorithm 1. On the one hand, clearly two RADs have to be created instead of one, doubling the computational effort for the solution of linear systems. On the other hand, the associated $Y$-equation becomes the Sylvester equation (46) and is in general solved by a non Hermitian matrix. Therefore the upper right and lower left block of the solution $\tilde{Y}$ of (46) as in (31) are not connected via conjugated transposition and two Sylvester equations like (35) have to be solved. Further, the Lyapunov equation (36) becomes a Sylvester equation and yields a non Hermitian solution, such that no Cholesky decomposition exists. However, the matrix $Y$ can be decomposed in arbitrary ways, e.g. trivially into $Y = Y I = I Y$ resulting in $(Z_1 Y) Z_2^*$ and $Z_1 (Y Z_2^*)$. Another possible decomposition is a $LDU$ factorization with $L$ and $U$ being (block) triangular matrices with ones on the diagonal and a $D$ being a (block) diagonal matrix. For parallelization and realification no further changes are necessary as both happens in the algorithms for the RAD expansion.

### 5.2 Linear matrix equations

All results in this work immediately transfer to Lyapunov equations which are a special case of the Riccati equation (14) with $B = 0$ and so $S_j = Z_j^* B B^* Z = 0$. The $R^2$ADi and Lyapunov RADI iteration both simplify considerably. In the $R^2$ADi there is no need for the multiplication of $Y_{12}$ with the previous Krylov basis and in the Lyapunov RADI iteration there is no need for the SMW formula any more and both algorithms become equivalent.

It is notable that even for the linear Lyapunov equations the projected equation (24) respectively (20) is a Riccati equation, i.e. a quadratic matrix equation.
This was also found in [11, Sec. IV] for large scale Sylvester equations. However, as this small scale Riccati equation is homogeneous, the equivalent small scale Lyapunov equation (21) can be solved for the inverse of the solution instead. The discussion in Section 4.2 implies that this solution is a (block) diagonal matrix.

Also the residual formula from Theorem 3.3 simplifies considerably. It becomes

\[ R_j = \frac{\prod_{i=1}^{j} (A^* + s_i I)}{\prod_{i=1}^{j} (A^* - s_i I)} C^* \]

as \( \Lambda(\tilde{W}^*A^*Z_j) = \Lambda(-Y_j H_{-j}^*Y_j^{-1}) = \Lambda(-H_{-j}^*) = -s \) holds due to Lemma 3.2 and \( B = 0 \). This means that the roots remain constant from step to step in the iteration, other than in the quadratic case.

5.3 Shift selection

For a good approximate solution the choice of the poles of the rational Krylov subspace used in the approximate solution \( X_j \) is crucial. Many shift strategies exist, but their description is beyond the scope of this work. Here we only describe, in concise form and in our notation, the residual Hamiltonian shift strategy from [4, Sec. 4.5.1] which we use in our numerical experiments. For a detailed discussion of this and other shift strategies we refer to [4, Sec. 4.5].

The residual Hamiltonian shift strategy makes use of the eigenvalues of the Hamiltonian matrix

\[ \mathcal{H}^{\text{proj}} = \begin{bmatrix} U^* \hat{A} U & U^* BB^* U \\ U^* R_j R_j^* U & -U^* \hat{A} U \end{bmatrix} \]

where \( \hat{A} = A - BB^* X_j \) holds and \( U \) is an orthonormal matrix which spans the same space as the last \( l \) columns of \( Z_j \), where \( l \) is a parameter of choice. Let \( \hat{\lambda} \) be an eigenvalue of \( \mathcal{H}^{\text{proj}} \) with the corresponding eigenvector \( \begin{bmatrix} \hat{r} \\ \hat{q} \end{bmatrix} \). The next shift is chosen as \( \mu = -\hat{\lambda} \) where \( \hat{\lambda} \) maximizes the expression \( \|\hat{q}(\hat{q}^* \hat{r})^{-1} \hat{q}^*\| \) as a heuristic for fast convergence.

6 Numerical experiments

We perform numerical experiments to compare the Riccati RAD iteration as in Algorithm 1 with the Lyapunov RADI iteration as in Algorithm 2 and show the effects of our parallel approach. The algorithms were implemented including the modifications described in Section 5.1 to handle generalized Riccati equations (43) with \( E \) and with realification and the possibility to use parallelization as described in Section 4.3. Our implementations of both algorithms share large parts of their code, which allows for a fair performance comparison. We compared the resulting approximate solutions of our implementations with the
M-M.E.S.S.-2.0 \cite{M.E.S.S.} RADI implementation and only found differences in the order of the machine precision. Therefore we only state results for the R$^2$ADI and the Lyapunov RADI iteration.

The convergence of the iteration considerably depends on the choice of shifts which determine the Krylov subspace used for the approximate solution. We used the M-M.E.S.S.-2.0 implementation of the RADI iteration with the shift strategy residual Hamiltonian shifts as described in Section 5.3 (denoted gen-ham-opti in M-M.E.S.S.-2.0) and parameter $l = 6p$ to precompute the shifts which were then used in our numerical experiments. The RADI iteration was stopped when the relative residual norm $rac{\|R_jR_j^*\|_2}{\|CC^*\|_2}$ became smaller than $10^{-9}$. Due to the precomputed shifts the Riccati ADI solution is fixed. This allows us to employ our parallelization approach and compare the accuracy of approximate solutions obtained with different numbers of parallel threads. However, as shifts are precomputed, no timings for the shift calculation are presented, although this may contribute considerably to the iteration time. For a discussion of the effects of different shift strategies and different Riccati ADI methods we refer to the numerical experiments in \cite[Sec. 5]{4}.

We used the following three examples. The rail example (ID 1445, \cite{8}) describes the semi-discretization of a heat transfer process for optimal cooling of steel profiles. It consists of symmetric negative/positive definite $A, E$ and was used with $n = 79841$, $m = 7$ and $p = 6$. It is denoted by rail79k. The second example is the chip0 example (ID 1428, \cite{21}), a finite element model of a chip cooled by convection. Its system matrices have sizes $n = 20082$, $m = 1$ and $p = 5$. Both originate from the Oberwolfach Benchmark Collection \cite{16}. Further, we used the example lung2, modeling processes in the human lung, with $n = 109460$, and $E = I$ from the UF Sparse Matrix Collection \cite{12}. We employed this example with the negated system matrix $-A$, $m = p = 10$ and $C = B^*$ chosen at random. All these examples are real valued, so all iteration steps were executed with realification in case of complex shifts.
6.1 Comparison of R²ADI and Lyapunov RADI iteration

All numerical experiments in this subsection were executed using MATLAB 2019a on an Intel® Core™ i7-5600U CPU @ 2.60 GHz with 12 GB RAM.

In Figure 1 the convergence behaviour for the three examples is displayed. In Table 1 we display the computational time for the different parts of the two algorithms compared. The expansion of the RADs is the most expensive part due to the necessary solves of linear systems. In the R²ADI we additionally have to multiply the current Krylov basis with the variable $Y_{12}$ in line 9 of Algorithm 1. All other parts of the iterations are aggregated under misc.

Figure 2 shows the cost for the RAD expansion and the $ZY_{12}$ multiplication in every step of the iterations. While the cost for solving the linear systems is almost constant during the iteration (the spikes are due to the more expensive solves with complex shifts), the $ZY_{12}$ multiplication becomes more expensive from step to step as the number of columns in the Krylov basis $Z$ grows by $p$ columns in every step. We can also observe that the Lyapunov RADI iteration needs more time for the linear solves, as due to the SMW formula equations with $m + p$ right hand sides have to be solved instead of only $p$ right hand sides in the R²ADI. For instance in the lung2 example with $m = 10$ the additional costs for the SMW formula make system solves 60% more expensive than in the R²ADI, while in the chip0 example with $m = 1$ the additional costs are only little.

Due to the linearly increasing cost of the $ZY_{12}$ multiplication it is advantageous to switch from the R²ADI to the Lyapunov RADI iteration as soon as the steps of the Lyapunov RADI iteration become cheaper than the steps of R²ADI. However, in all examples considered here the cheaper system solves in the R²ADI compensate for the additional time needed for the $ZY_{12}$ multiplication.

6.2 Effect of parallelization in R²ADI

For the experiments in this subsection we used MATLAB 2018b on four Intel® Xeon® CPU E7-4880 v2 @ 2.50 GHz with altogether 60 CPU cores and 1 TB RAM. For the parallel expansion of the RADs the parfor command in MATLAB was utilized. All calculations were performed with the Riccati RAD iteration Algorithm 1.

To parallelize the system solves, multiple shifts have to be available. This is the case here as all shifts were precomputed, which allows us to compare the

| subsp. | R²ADI | Lyap. RADI |
|-------|-------|------------|
|       | dim.  | RAD exp.  | $ZY_{12}$ mul. | misc. | total | RAD exp. | misc. | total |
| rail79k | 252   | 7.8       | 0.5            | 0.8   | 9.1    | 8.8      | 0.8   | 9.6   |
| chip0  | 180   | 32.8      | 0.1            | 0.1   | 33.0   | 34.9     | 0.1   | 35.0  |
| lung2  | 300   | 10.0      | 0.4            | 1.0   | 11.4   | 16.0     | 1.0   | 17.0  |

Table 1: Times in seconds for different parts of the iterations.
performance and accuracy of the parallel with the serial approach. In practice the shifts are calculated one after another during the iteration as described in Section 5.3. An efficient shift strategy which obtains multiple shifts per iteration step has yet to be found.

In Figure 3 the necessary times for the iteration and speedup factors are plotted against the number of parallel system solves in the RAD expansion step. The speedup factor is the iteration time for an iteration without parallelization and a for loop divided by the iteration time needed with parallel system solves and MATLABs parfor loop. Due to the overhead introduced by the parfor command the serial iteration with a for loop is faster than the same serial iteration with the parfor loop. Thus the speedup factor for one thread is smaller than one. Further, only the system solves are executed in parallel but not the ZY₁₂ multiplication and miscellaneous tasks. As they take up to about 15%
of the calculation time in the rail79k and lung2 examples the possible maximal speedup is quite limited. Indeed we observe a moderate speedup for the rail79k and lung2 examples. For the chip0 example the speedup is higher. The factor for four parallel threads is 3.0 and it increases to 4.4 when eight parallel threads are used.

Besides the performance gain we also investigate the accuracy of the parallel calculations. We therefore compare the parallel iterates with the serial iterates. Let a subscript \( (k) \) denote the number of parallel threads utilized to obtain the variable. We calculated the relative deviation of the residuals obtained with \( k \) parallel threads from the residual obtained with the serial iteration, i.e.

\[
\frac{\| R_{(1)} - R_{(k)} \|_2}{\| R_{(1)} \|_2}.
\]

The second quantity we use to indicate the accuracy is the relative deviation of the parallel approximants \( X_{(k)} \) from the serial approximant \( X_{(1)} \)

\[
\frac{\| X_{(1)} - X_{(k)} \|_2}{\| X_{(1)} \|_2}.
\]

A direct calculation of the norms of the involved matrices is infeasible due to the large dimensions. We thus exploit the factorized form of the residual and the approximants, i.e. \( R_{(k)} = R_{(k)} R^*_{(k)} \) and \( X_{(k)} = Z_{(k)} Z^*_{(k)} \). Let \( QS = [Z_{(1)} \ Z_{(k)}] \) be an economy-size QR decomposition with upper triangular \( S \). Then due to the unitary invariance of the norm it holds

\[
\| X_{(1)} - X_{(k)} \|_2 = \left\| S \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} S^* \right\|_2
\]

and only the norm of a small matrix must be computed. For the denominator we use the formula \( \| Z_{(k)} Z^*_{(k)} \|_2 = \| Z^*_{(k)} Z_{(k)} \|_2 \). We proceed in the same way for the residual deviation.

The results are displayed in Figure 4. We observe that the relative deviations from the residual are below \( 10^{-5} \) for all examples. The relative deviation of the
final approximation is even smaller than $10^{-12}$ for all examples and fewer than twenty parallel threads. All in all the effects of parallelization to the accuracy of the results appear to be very little. Thus parallel system solves are a reasonable technique to speed up computations.

7 Conclusion

In this work we have introduced a new approach for the ADI-type approximation of complex large-scale algebraic Riccati equations. We made use of rational Krylov decompositions to rewrite the Riccati residual. By imposing a rank condition on this formulation of the residual we obtained a small scale Lyapunov equation, which characterizes the sought solution. It was shown that the Riccati ADI approximate solution exists and is unique under a simple condition for the shifts. Uniqueness of the solution implies the equivalence of all previously known Riccati ADI methods and our new approach. Further, we revealed that the Riccati ADI solution can be interpreted as an oblique projection onto a rational Krylov subspace if the kernel of the projection contains the Riccati residual factor. The residual factor is a rational function. The poles and zeros of this function were connected to the eigenvalues of projected system matrices.

We introduced two new iterative methods to calculate the Riccati ADI solution. Both make use of the fact that the solution of the small scale Lyapunov equation can be updated efficiently. In our first iterative method, the Riccati RAD iteration, only system solves with matrices of the form $A^* - \mu I$ and the residual factor are necessary. The second method derived, the Lyapunov RADI iteration, contains the RADI iteration as a special case. Here, system solves with a matrix of the form $A^* - KB^* - \mu I$ and the residual factor are necessary. In both algorithms the extension of the Krylov subspace was decoupled from the rest of the iteration, which made parallelization and, in case of real system matrices, realification possible easily.

The numerical experiments show the competitiveness of our new approach.
They indicate that it is beneficial to start with the $R^2$ADI and switch to the Lyapunov RADI iteration for best performance whenever the $R^2$ADI becomes too expensive due to the linear increasing cost of the $ZY_{12}$ multiplication. Parallel system solves scale well with the number of parallel threads if they dominate the iteration, even though there seems to be a large overhead due to the use of MATLABs `parfor` command. The accuracy of the solution obtained with parallelization is remarkably good in all numerical examples, even for as many as 20 parallel solves. However, to make the parallel approach work in practice, a shift strategy has to be found which generates multiple shifts during the iteration.

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