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On semi-convergence of Hermitian and skew-Hermitian splitting methods for singular linear systems

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Abstract For the singular, non-Hermitian, and positive semidefinite systems of linear equations, we derive necessary and sufficient conditions for guaranteeing the semi-convergence of the Hermitian and skew-Hermitian splitting (HSS) iteration methods. We then investigate the semi-convergence factor and estimate its upper bound for the HSS iteration method. If the semi-convergence condition is satisfied, it is shown that the semi-convergence rate is the same as that of the HSS iteration method applied to a linear system with the coefficient matrix equal to the compression of the original matrix on the range space of its Hermitian part, that is, the matrix obtained from the original matrix by restricting the domain and projecting the range space to the range space of the Hermitian part. In particular, an upper bound is obtained in terms of the largest and the smallest nonzero eigenvalues of the Hermitian part of the coefficient matrix. In addition, applications of the HSS iteration method as a preconditioner for Krylov subspace methods such as GMRES are investigated in detail, and several examples are used to illustrate the theoretical results and examine the numerical

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effectiveness of the HSS iteration method served either as a preconditioner for GMRES or as a solver.

Keywords Singular linear system · Non-Hermitian matrix · Positive semidefinite matrix · Hermitian and skew-Hermitian splitting · Splitting iteration method · Semi-convergence · Preconditioning matrix · Krylov subspace method

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1 Introduction

We consider an iterative solution of the large, sparse, *non-Hermitian* and, possibly, *singular* system of linear equations

$$Ax = b, \qquad A \in \mathbf{C}^{n\times n}, \quad A \neq A^*, \quad \text{and} \quad x, b \in \mathbf{C}^n, \tag{1.1}$$

where A^* denotes the conjugate transpose of the complex matrix A; see [17–19,25].

Based on the *Hermitian and skew-Hermitian* (**HS**) splitting

$$A = \mathcal{H}(A) + \mathcal{S}(A), \text{ with } \mathcal{H}(A) = \frac{1}{2}(A + A^*) \text{ and } \mathcal{S}(A) = \frac{1}{2}(A - A^*),$$

Bai et al. [7] established the following *Hermitian and skew-Hermitian splitting* (HSS) iteration method for solving the non-Hermitian system of linear equations (1.1).

The HSS Iteration Method. Given an initial guess $x^{(0)} \in \mathbf{C}^n$, compute $x^{(k)}$ for $k = 0, 1, 2, \ldots$ using the following iteration scheme until $\{x^{(k)}\}$ satisfies the stopping criterion:

$$\begin{cases} (\alpha I + \mathcal{H}(A))x^{(k+\frac{1}{2})} = (\alpha I - \mathcal{S}(A))x^{(k)} + b, \\ (\alpha I + \mathcal{S}(A))x^{(k+1)} \ = (\alpha I - \mathcal{H}(A))x^{(k+\frac{1}{2})} + b, \end{cases}$$

where α is a given positive constant and $I \in \mathbf{C}^{n\times n}$ the identity matrix.

When the coefficient matrix $A \in \mathbf{C}^{n\times n}$ is positive definite, i.e., its Hermitian part $\mathcal{H}(A) \in \mathbf{C}^{n\times n}$ is Hermitian positive definite, Bai et al. proved in [7] that the HSS iteration converges unconditionally to the exact solution of the system of linear equations (1.1), with the bound on the rate of convergence about the same as that of the conjugate gradient method when applied to the Hermitian matrix $\mathcal{H}(A)$: indeed by the *mixing-up effect* described in [14, Sect. 2.1.3] the given bounds of convergence rates could be very pessimistic, as already observed in [7]. Moreover, **an upper bound** of the contraction factor is obtained in terms of the largest and the smallest nonzero eigenvalues of $\mathcal{H}(A)$. Numerical experiments have shown that the HSS iteration method is efficient and robust for solving non-Hermitian positive definite linear systems.

When the coefficient matrix $A \in \mathbf{C}^{n\times n}$ is nonsingular and positive semidefinite, i.e., its Hermitian part $\mathcal{H}(A) \in \mathbf{C}^{n\times n}$ is Hermitian positive semidefinite, Bai et al. [5]

proved that the HSS iteration is convergent if and only if A does not have a (reducing) eigenvalue of the form $\imath\xi$ with $\xi \in \mathbf{R}$ and $\imath$ the imaginary unit, or equivalently, the null space of $\mathcal{H}(A)$, denoted as $\text{null}(\mathcal{H}(A))$, does not contain an eigenvector of $\mathcal{S}(A)$. This result immediately leads to a necessary and sufficient condition for guaranteeing the unconditional convergence of the HSS iteration method when it is used to solve the saddle-point problem

$$Ax \equiv \begin{pmatrix} B & E \\ -E^* & C \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix} \equiv b,$$

where $B \in \mathbf{C}^{p\times p}$ is positive definite, $C \in \mathbf{C}^{q\times q}$ is Hermitian positive semidefinite, $E \in \mathbf{C}^{p\times q}$ is of full column rank, and $p \geq q$. Note that the convergence theorem given in Benzi and Golub [12] is a special case of this result; see also [3,10] and references therein.

In this paper, we give a necessary and sufficient condition for an arbitrary *singular*, non-Hermitian, and positive *semidefinite* linear system so that the HSS iteration method will lead to a semi-convergent iteration sequence. In particular, this result immediately gives a necessary and sufficient condition for guaranteeing the semi-convergence of the HSS iteration method applied to the saddle-point problem of a singular and positive semidefinite coefficient matrix. We then investigate the semi-convergence factor and estimate its upper bound for the HSS iteration method. It is shown that the semi-convergence rate of the HSS iteration method is about the same as that of the conjugate gradient method applied to the symmetrized linear system of the coefficient matrix being $\mathcal{H}(A)$. Moreover, **an upper bound** of the semi-convergence factor is obtained in terms of the largest and the smallest nonzero eigenvalues of $\mathcal{H}(A)$. In addition, we investigate the preconditioning property of the HSS preconditioner induced from the HSS iteration method and, in particular, we discuss the semi-convergence behavior of the HSS-preconditioned GMRES method. Several examples arising from the finite difference discretizations of second-order differential equations of periodic boundary conditions are used to illustrate the theoretical results and examine the computational effectiveness of the HSS iteration method served either as a preconditioner for GMRES or as a solver.

2 Notations and concepts

For a matrix $W \in \mathbf{C}^{n\times n}$, $\text{rank}(W)$ and $\text{index}(W)$ are used to represent its rank and index, respectively. For two matrices A_1 and A_2 of suitable dimensions, we use $A_1 \oplus A_2$ to denote their direct sum, i.e.,

$$A_1 \oplus A_2 = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}.$$

Assume that a matrix $A \in \mathbf{C}^{n\times n}$ can be split as

$$A = M - N, \tag{2.2}$$

with $M \in \mathbf{C}^{n\times n}$ nonsingular. Then we can construct a splitting iteration method as

$$x^{(k+1)} = Tx^{(k)} + c, \quad k = 0, 1, 2, \dots, \tag{2.3}$$

where $T = M^{-1}N$ is the iteration matrix, and $c = M^{-1}b$. Obviously, a vector $x \in \mathbf{C}^n$ is a solution of the linear system (1.1) if and only if $(I - T)x = c$; see [13,18].

The convergence and semi-convergence of the iterative scheme (2.3) have been studied extensively; see, e.g., [11,13,22,24]. When A is singular, then 1 is an eigenvalue of the iteration matrix T. Moreover, when the spectral radius of the iteration matrix T is equal to one, i.e., $\rho(T) = 1$, the following two conditions are necessary and sufficient for guaranteeing the semi-convergence of the iterative method (2.3):

(a) The elementary divisors of the iteration matrix T associated with its eigenvalue $\mu = 1$ are linear;
(b) If $\mu \in \sigma(T)$, the spectrum of the iteration matrix T, satisfying $|\mu| = 1$, then $\mu = 1$, i.e., $\vartheta(T) < 1$, where

$$\vartheta(T) \equiv \max\{|\mu| \mid \mu \in \sigma(T), \quad \mu \neq 1\}.$$

We remark that for a nonsingular matrix A, the semi-convergence concept of the correspondingly induced matrix splitting or iteration matrix coincides with the standard convergence concept.

From [13] we know that the splitting (2.2) or the corresponding iteration matrix T is called semi-convergent, if the iteration (2.3) is semi-convergent. In this case, we define $\vartheta(T)$ as the semi-convergence factor of the iteration (2.3).

The HSS iteration method can be rewritten in matrix-vector form as

$$x^{(k+1)} = T(\alpha)x^{(k)} + G(\alpha)b, \qquad k = 0, 1, 2, \dots, \tag{2.4}$$

where

$$T(\alpha) = (\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{H}(A))(\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{S}(A)) \tag{2.5}$$

and

$$G(\alpha) = 2\alpha(\alpha I + \mathcal{S}(A))^{-1}(\alpha I + \mathcal{H}(A))^{-1}.$$

Here, $T(\alpha)$ is the iteration matrix of the HSS iteration method. Note that $T(\alpha)$ is similar to the matrix

$$L(\alpha) = (\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))(\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A)). \tag{2.6}$$

In fact, (2.4) may also result from the splitting

$$A = M(\alpha) - N(\alpha)$$

of the coefficient matrix A, with

$$\begin{cases} M(\alpha) = \frac{1}{2\alpha}(\alpha I + \mathcal{H}(A))(\alpha I + \mathcal{S}(A)), \\ N(\alpha) = \frac{1}{2\alpha}(\alpha I - \mathcal{H}(A))(\alpha I - \mathcal{S}(A)). \end{cases}$$

Evidently, the HSS iteration method can naturally induce a preconditioner $M(\alpha)$ to the matrix A. This preconditioner is called as the HSS preconditioner; see [3,10,12]. For other types of preconditioners about a non-Hermitian matrix, we refer to [15,16, 19,25].

3 The semi-convergence of the HSS iteration method

We first reveal a basic relationship between a singular matrix and its Hermitian and skew-Hermitian parts.

Lemma 3.1 *Let $A \in \mathbf{C}^{n\times n}$ be a singular and positive semidefinite matrix, and $\mathcal{H}(A)$ and $\mathcal{S}(A)$ be its Hermitian and skew-Hermitian parts, respectively. Then*

$$\text{null}(A) = \text{null}(\mathcal{H}(A)) \cap \text{null}(\mathcal{S}(A)).$$

Proof Evidently,

$$\text{null}(\mathcal{H}(A)) \cap \text{null}(\mathcal{S}(A)) \subseteq \text{null}(A).$$

Hence, we only need to demonstrate the inclusion relationship

$$\text{null}(A) \subseteq \text{null}(\mathcal{H}(A)) \cap \text{null}(\mathcal{S}(A)).$$

In fact, for an $x \in \text{null}(A)$ we have

$$0 = Ax = \mathcal{H}(A)x + \mathcal{S}(A)x. \tag{3.7}$$

Let

$$x^*\mathcal{H}(A)x + x^*\mathcal{S}(A)x = \mu + \imath\nu,$$

with $\mu, \nu \in \mathbf{R}$. Then

$$x^*\mathcal{H}(A)x = \mu = 0.$$

Since $\mathcal{H}(A)$ is Hermitian positive semidefinite, $x^*\mathcal{H}(A)x = 0$ implies $\mathcal{H}(A)x = 0$. Thus, by using (3.7), we immediately get $\mathcal{S}(A)x = Ax - \mathcal{H}(A)x = 0$. Hence, $x \in \text{null}(\mathcal{H}(A)) \cap \text{null}(\mathcal{S}(A))$. □

From Lemma 3.1, we get the following conclusion.

Corollary 3.2 *Consider the saddle-point matrix*

$$A = \begin{pmatrix} B & E \\ -E^* & C \end{pmatrix}, \tag{3.8}$$

where $B \in \mathbf{C}^{p\times p}$, $C \in \mathbf{C}^{q\times q}$ are Hermitian positive semidefinite, $E \in \mathbf{C}^{p\times q}$ is rectangular, and $p \geq q$, with $p+q=n$. If the matrix $A \in \mathbf{C}^{n\times n}$ is singular, then at least one of the sets $\mathrm{null}(B) \cap \mathrm{null}(E^*)$ *and* $\mathrm{null}(C) \cap \mathrm{null}(E)$ *is not trivial, i.e., the dimension of one of the two sets is at least one.*

Let $T \in \mathbf{C}^{n\times n}$ satisfy $\|T\|_2 \leq 1$. Then for any $x \in \mathbf{C}^n$, $Tx = x$ if and only if $T^*x = x$. To see this, suppose $Tx = x$ and $T^*x = ax + y$ such that $x^*y = 0$ and $\|ax\|_2 \leq \|T^*x\|_2 \leq \|x\|_2$. Without loss of generality, we may assume that $\|x\|_2 = 1$. Then $1 = x^*T^*Tx = x^*T^*x = a$. Thus, $1 = a$ and $y = 0$, i.e., $T^*x = x$. The converse can be verified readily. As a result, the index of $I - T$ is one. Since the HSS iteration matrix $T(\alpha)$ of a singular positive semidefinite matrix leads to $\|L(\alpha)\|_2 = 1$, with $L(\alpha)$ being defined in (2.6), and since two similar matrices have the same index, we see that the matrix $I - T(\alpha)$ has index 1. We can say more about the stationary vectors of $T(\alpha)$.

Theorem 3.3 *Let $A \in \mathbf{C}^{n\times n}$ be a singular and positive semidefinite matrix, $\mathcal{H}(A)$ and $\mathcal{S}(A)$ be its Hermitian and skew-Hermitian parts, respectively, and $T(\alpha)$ be the iteration matrix of the HSS iteration method defined in* (2.5). *Then* $\mathrm{index}(I - T(\alpha)) = 1$. *Furthermore, $x \in \mathbf{C}^n$ satisfies $L(\alpha)x = x$ if and only if $Ax = 0 = A^*x$, where $L(\alpha)$ is defined in* (2.6).

Proof Suppose $L(\alpha)x = x$. Then

$$\|(\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))y\|_2 = \|y\|_2,$$

where

$$y = (\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))x.$$

Here we have used the fact that

$$\mathcal{Q}_A(\alpha) = (\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))$$

is a Cayley transform and is, thus, a unitary matrix. Since $(\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))$ is Hermitian with eigenvalues lying in $(-1, 1]$, we see that $(\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))y = y$, equivalently, $\mathcal{H}(A)y = 0$. It then follows that

$$\begin{aligned} L(\alpha)x &= (\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))(\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))x \\ &= (\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))y \\ &= (\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))x. \end{aligned}$$

Thus, $(\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))x = x$, equivalently, $\mathcal{S}(A)x = 0$. It then follows that $y = \mathcal{Q}_A(\alpha)x = x$ and $\mathcal{H}(A)x = 0$. Consequently, $Ax = 0 = A^*x$. The converse can be readily verified. □

Using Lemma 3.1 and Theorem 3.3, we can now establish the semi-convergence theorem for the HSS iteration method.

Theorem 3.4 *Let $A \in \mathbf{C}^{n\times n}$ be a singular and positive semidefinite matrix, and $\mathcal{H}(A)$ and $\mathcal{S}(A)$ be its Hermitian and skew-Hermitian parts, respectively. Then the following conditions are equivalent:*

(a) *The HSS iteration sequence $\{x^{(k)}\}$, starting from any initial vector $x^{(0)} \in \mathbf{C}^n$, is semi-convergent to a solution of the system of linear equations (1.1), i.e., $\vartheta(T(\alpha)) < 1$, $\forall\alpha > 0$;*
(b) $\mathrm{null}(A) = \mathrm{null}(\mathcal{H}(A))$;
(c) *A is unitarily similar to $\widehat{A} \oplus 0$ such that $\mathcal{H}(\widehat{A})$ is positive definite, i.e., $\widehat{A}$ is the compression of A on the range space of $\mathcal{H}(A)$.*

Proof We will verify the implications: (a)⇒ (b) ⇒ (c) ⇒ (a).

(a) ⇒ (b): It follows from Lemma 3.1 that $\mathrm{null}(A) = \mathrm{null}(\mathcal{H}(A))$ if and only if $\mathrm{null}(\mathcal{H}(A)) \subseteq \mathrm{null}(\mathcal{S}(A))$, or equivalently, $\mathrm{null}(\mathcal{S}(A))^{\perp} \subseteq \mathrm{null}(\mathcal{H}(A))^{\perp}$, where

$$\begin{cases} \mathrm{null}(\mathcal{H}(A))^{\perp} = \mathrm{span}\{x \mid \mathcal{H}(A)x = \lambda x, \quad \lambda > 0\} \quad \text{and} \\ \mathrm{null}(\mathcal{S}(A))^{\perp} = \mathrm{span}\{x \mid \mathcal{S}(A)x \ = \imath\xi x, \quad \xi \in \mathbf{R}\backslash\{0\}\} \end{cases}$$

are the orthogonal complement spaces of $\mathrm{null}(\mathcal{H}(A))$ and $\mathrm{null}(\mathcal{S}(A))$, respectively.

If we suppose that $\mathrm{null}(A) \neq \mathrm{null}(\mathcal{H}(A))$, then there exists a nonzero vector $x \in \mathbf{C}^n$ such that

$$x \in \mathrm{null}(\mathcal{S}(A))^{\perp} \quad \text{but} \quad x \notin \mathrm{null}(\mathcal{H}(A))^{\perp}.$$

Then x satisfies

$$\mathcal{H}(A)x = 0 \quad \text{and} \quad \mathcal{S}(A)x = \imath\xi x, \quad \text{with} \quad \xi \in \mathbf{R}\backslash\{0\}.$$

Therefore, by direct computations we have

$$T(\alpha)x = (\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{H}(A))(\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{S}(A))x = \frac{\alpha - \imath\xi}{\alpha + \imath\xi}x.$$

This shows that $\mu := \frac{\alpha-\imath\xi}{\alpha+\imath\xi}$ is an eigenvalue of $T(\alpha)$. As $\xi \neq 0$, we see that $\mu \neq 1$. But $|\mu| = 1$. Hence, $\vartheta(T(\alpha)) = 1$, which contradicts the condition $\vartheta(T(\alpha)) < 1$. As a result, it must hold that $\mathrm{null}(A) = \mathrm{null}(\mathcal{H}(A))$.

(b) ⇒ (c): Suppose $\mathcal{H}(A)$ is unitarily similar to $D\oplus 0$, where D is a diagonal matrix with positive entries. Then A is unitarily similar to

$$\widetilde{A} = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} + \imath \begin{pmatrix} G_{11} & G_{12} \\ G_{12}^* & G_{22} \end{pmatrix}$$

such that G_{11} and G_{22} are Hermitian, G_{11} and D have the same size. Note that $R := D + \imath G_{11}$ is invertible because $y^* R y$ has positive real part for any nonzero vector y and thus there is no eigenvector corresponding to the eigenvalue 0. Let

$$\widetilde{R} = \begin{pmatrix} I & 0 \\ -\imath G_{12}^* R^{-1} & I \end{pmatrix}.$$

Then

$$\widetilde{R}\widetilde{A} = \begin{pmatrix} R & \imath G_{12} \\ 0 & \imath G_{22} + G_{12}^* R^{-1} G_{12} \end{pmatrix}.$$

If (b) holds, then A and $\mathcal{H}(A)$ have the same rank. Hence

$$\imath G_{22} + G_{12}^* R^{-1} G_{12} = 0. \tag{3.9}$$

Suppose $G_{12} \neq 0$. Then there is a vector y such that $R^{-1} G_{12} y = z \neq 0$. It follows that the complex number

$$y^* G_{12}^* R^{-1} G_{12} y = y^* G_{12}^* R^{-*} R^* R^{-1} G_{12} y = z^* (D - \imath G_{11}) z$$

has a positive real part $z^* D z$. Since $y^* (\imath G_{22}) y$ is pure imaginary, we see that

$$y^* (\imath G_{22} + G_{12}^* R^{-1} G_{12}) y \neq 0,$$

which contradicts (3.9). By (3.9), if $G_{12} = 0$, then $G_{22} = 0$ as well. Thus, condition (c) holds.

(c) $\Rightarrow$ (a): Suppose (c) holds. Then there exists a unitary matrix $U \in \mathbf{C}^{n \times n}$ such that

$$A = U(\widehat{A} \oplus 0) U^* = U(\mathcal{H}(\widehat{A}) \oplus 0) U^* + U(\mathcal{S}(\widehat{A}) \oplus 0) U^*.$$

Hence, after straightforward operations we see that $T(\alpha)$ is unitarily similar to $\widehat{T}(\alpha) \oplus I$, where $\widehat{T}(\alpha)$ associated with $\widehat{A}$ has spectral radius less than one. So, condition (a) holds. $\square$

We can also give an independent proof for the implication (b) $\Rightarrow$ (a), which is useful for revealing more algebraic properties of the HSS iteration matrix $T(\alpha)$. This proof is given as follows. Let $\lambda \in \sigma(T(\alpha))$. Then $\lambda \in \sigma(L(\alpha))$, too, where $L(\alpha)$ is defined in (2.6). Let $x \in \mathbf{C}^n$, with $\|x\|_2 = 1$, be an eigenvector of the matrix $L(\alpha)$ corresponding to its eigenvalue λ, i.e., $L(\alpha) x = \lambda x$. Since Lemma 3.1 and condition (b) readily imply $\text{null}(\mathcal{H}(A)) \subseteq \text{null}(\mathcal{S}(A))$, we can use Theorem 3.3 to complete the proof by discussing the module of λ according to the following three cases.

Case (i) $x \in \text{null}(\mathcal{H}(A))$. For this case, we have $\mathcal{H}(A) x = 0$ and $\mathcal{S}(A) x = 0$. By direct computations we can obtain $L(\alpha) x = x$. Hence, $\lambda = 1$.

Case (ii) $x \in \text{null}(\mathcal{S}(A))$, but $x \notin \text{null}(\mathcal{H}(A))$. For this case, we have $\mathcal{H}(A)x \neq 0$ and $\mathcal{S}(A)x = 0$. By direct computations we can obtain $L(\alpha)x = (\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))x$. Hence, $\lambda \in \sigma((\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A)))$. Clearly, λ is real and satisfies $|\lambda| \leq 1$. We can further conclude that $|\lambda| < 1$, since $\lambda = 1$ implies $\mathcal{H}(A)x = 0$ while $\lambda = -1$ implies $x = 0$, which are both impossible.
Case (iii) $x \notin \text{null}(\mathcal{S}(A))$. For this case, we have $\mathcal{H}(A)x \neq 0$ and $\mathcal{S}(A)x \neq 0$. From $L(\alpha)x = \lambda x$ we can obtain

$$\lambda = x^*(\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))(\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))x.$$

It then follows from this formula and $(\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))$ being a unitary matrix that

$$\begin{aligned} |\lambda| &\leq \|(\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))x\|_2 \|(\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))x\|_2 \\ &= \|(\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))x\|_2. \end{aligned} \tag{3.10}$$

Let

$$\mathcal{H}(A) = U \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} U^*$$

be the spectral decomposition of the Hermitian positive semidefinite matrix $\mathcal{H}(A)$, where $U \in \mathbf{C}^{n\times n}$ is a unitary matrix and D is a diagonal matrix with positive diagonal entries. If we decompose the vector $\widetilde{x} = U^* x$ into $\widetilde{x} = \begin{pmatrix} \widetilde{y} \\ \widetilde{z} \end{pmatrix}$ according to the spectral decomposition of the matrix $\mathcal{H}(A)$, then by recalling that $\mathcal{H}(A)x \neq 0$ we see that $D\widetilde{y} \neq 0$.

By making use of (3.10) we can obtain

$$\begin{aligned} |\lambda| &\leq \left\| U \begin{pmatrix} (\alpha I + D)^{-1}(\alpha I - D) & 0 \\ 0 & I \end{pmatrix} U^* x \right\|_2 \\ &= \left(\|(\alpha I + D)^{-1}(\alpha I - D)\widetilde{y}\|_2^2 + \|\widetilde{z}\|_2^2 \right)^{1/2} \\ &< \left(\|\widetilde{y}\|_2^2 + \|\widetilde{z}\|_2^2 \right)^{1/2} \\ &= \|x\|_2 \\ &= 1. \end{aligned}$$

In summary, Cases (i)-(iii) show that $\vartheta(T(\alpha)) < 1$.

The following result follows from Theorem 3.4 and Lemma 3.1.

Corollary 3.5 *Let $A \in \mathbf{C}^{n\times n}$ be a singular and positive semidefinite matrix, and $\mathcal{H}(A)$ and $\mathcal{S}(A)$ be its Hermitian and skew-Hermitian parts, respectively. Then the HSS iteration sequence $\{x^{(k)}\}$, starting from any initial vector $x^{(0)} \in \mathbf{C}^n$, is semi-convergent to a solution of the system of linear equations (1.1) if and only if* $\text{null}(\mathcal{H}(A)) \subseteq \text{null}(\mathcal{S}(A))$.

Corollary 3.5 immediately leads to the following semi-convergence theorem for the HSS iteration method applied to the saddle-point problem of the coefficient matrix (3.8).

Theorem 3.6 *The HSS iteration method for the singular saddle-point matrix* (3.8) *is semi-convergent if and only if any one of the following conditions holds true:*

(a) $\mathrm{null}(B) \subseteq \mathrm{null}(E^*)$ *and* $\mathrm{null}(C) \subseteq \mathrm{null}(E)$*;*
(b) *There exist unitary matrices U and V such that*

$$(U \oplus V)^* A (U \oplus V) = \begin{pmatrix} \widehat{B} & 0 & \widehat{E} & 0 \\ 0 & 0 & 0 & 0 \\ -\widehat{E}^* & 0 & \widehat{C} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

whenever $U^* B U = \widehat{B} \oplus 0$ *and* $V^* C V = \widehat{C} \oplus 0$.

Proof Assume that the HSS iteration method of the singular saddle-point matrix (3.8) is semi-convergent. Then by Corollary 3.5, we know that condition (a) holds true.

Suppose (a) holds true. If $U^* B U = \widehat{B} \oplus 0$ and $V^* C V = \widehat{C} \oplus 0$, then the columns of U in the null space of B also belong to the null space of E^* and the columns of V in the null space of C also belong to the null space of E. Thus, $(U \oplus V)^* A (U \oplus V)$ has the form described in (b).

Suppose (b) holds true. Choose U and V so that $\widehat{B}$ and $\widehat{C}$ are positive definite. Then $(U \oplus V)^* A (U \oplus V)$ is permutationally similar to $\widehat{A} \oplus 0$ such that $(\widehat{A} + \widehat{A}^*)/2 = \widehat{B} \oplus \widehat{C}$ is positive definite. By Theorem 3.4, the HSS iteration method for the singular saddle-point matrix (3.8) is semi-convergent. □

We remark that in condition (b) of Theorem 3.6 we can choose U and V so that $\widehat{B}$ and $\widehat{C}$ are positive definite as shown in the proof.

Furthermore, from the proof of Theorem 3.4, Theorem 3.6, and the definition of the semi-convergence factor we can obtain the following corollaries.

Corollary 3.7 *Let $A \in \mathbf{C}^{n \times n}$ be a singular and positive semidefinite matrix, and its Hermitian and skew-Hermitian parts $\mathcal{H}(A)$ and $\mathcal{S}(A)$ satisfy* $\mathrm{null}(\mathcal{H}(A)) \subseteq \mathrm{null}(\mathcal{S}(A))$. *Then the HSS iteration is semi-convergent and its semi-convergence factor $\vartheta(T(\alpha))$ is bounded by*

$$\theta(T(\alpha)) = \sup_{x \in \mathrm{null}(\mathcal{H}(A))^\perp} \frac{|x^*(\alpha I + \mathcal{H}(A))^{-1}(\alpha I - \mathcal{H}(A))(\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))x|}{x^* x}.$$

Proof Notice that the HSS iteration is semi-convergent and $\sigma(L(\alpha)) = \sigma(T(\alpha))$, where $T(\alpha)$ and $L(\alpha)$ are defined in (2.5) and (2.6), respectively. From the proof of Theorem 3.4 we see that $\mu \in \sigma(T(\alpha)) \backslash \{1\}$ satisfying $|\mu| < 1$ if and only if its corresponding eigenvector $x \in \mathbf{C}^n$ of the matrix $L(\alpha)$ satisfies $x \notin \mathrm{null}(\mathcal{H}(A))$, or $x \in \mathrm{null}(\mathcal{H}(A))^\perp$. Now, from $L(\alpha)x = \mu x$ we can see that $\mu = \frac{x^* L(\alpha) x}{x^* x}$ and

$$
\begin{aligned}
\vartheta(T(\alpha)) &= \max\{|\mu| \mid \mu \in \sigma(T(\alpha))\backslash\{1\}\} = \vartheta(L(\alpha)) \\
&\leq \sup_{x\in \mathrm{null}(\mathcal{H}(A))^{\perp}} \frac{|x^*(\alpha I+\mathcal{H}(A))^{-1}(\alpha I-\mathcal{H}(A))(\alpha I+\mathcal{S}(A))^{-1}(\alpha I-\mathcal{S}(A))x|}{x^*x} \\
&= \theta(T(\alpha)).
\end{aligned}
$$

□

Corollary 3.8 *Let $A \in \mathbf{C}^{n\times n}$ be the singular saddle-point matrix (3.8), and B, C and E satisfy* $\mathrm{null}(B) \subseteq \mathrm{null}(E^*)$ *and* $\mathrm{null}(C) \subseteq \mathrm{null}(E)$. *Then the HSS iteration for the singular saddle-point matrix (3.8) is semi-convergent and its semi-convergence factor $\vartheta(T(\alpha))$ is bounded by*

$$
\theta(T(\alpha)) = \sup_{x\in \mathrm{null}(\mathcal{H}(\widehat{A}))^{\perp}} \frac{|x^*(\alpha I+\mathcal{H}(\widehat{A}))^{-1}(\alpha I-\mathcal{H}(\widehat{A}))(\alpha I+\mathcal{S}(\widehat{A}))^{-1}(\alpha I-\mathcal{S}(\widehat{A}))x|}{x^*x},
$$

where

$$
\widehat{A} = \begin{pmatrix} \widehat{B} & \widehat{E} \\ -\widehat{E}^* & \widehat{C} \end{pmatrix},
$$

with $\widehat{B}$, $\widehat{C}$ and $\widehat{E}$ being the matrices defined as in Theorem 3.6 (b).

Proof From Theorem 3.6 (b) we have

$$
P(U \oplus V)^* A (U \oplus V) P = \begin{pmatrix} \widehat{A} & 0 \\ 0 & 0 \end{pmatrix},
$$

where

$$
P = \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{pmatrix}
$$

is a permutation matrix. It follows that the HSS iteration matrix $T(\alpha)$ is unitarily similar to $\widehat{T}(\alpha) \oplus I$, where $\widehat{T}(\alpha)$ is the HSS iteration matrix associated with the matrix $\widehat{A}$. Now, by making use of Corollary 3.7, after straightforward computations we can immediately obtain the result what we were proving. □

We remark that the $\theta(T(\alpha))$ given in Corollaries 3.7–3.8 are the best-possible upper bounds about the semi-convergence factors of the HSS iteration methods for a general singular positive-semidefinite matrix and a singular saddle-point matrix.

Note that Theorem 3.4(c) implies that the semi-convergence behavior of the HSS iteration method for the singular system of linear equations (1.1) with the coefficient matrix $A \in \mathbf{C}^{n\times n}$ being positive semi-definite is algebraically equivalent to its convergence behavior for the nonsingular system of linear equations $\widehat{A}\widehat{x} = \widehat{b}$ with the coefficient matrix $\widehat{A} \in \mathbf{C}^{n\times n}$, a compression of A on to the range space of $\mathcal{H}(A)$, being positive definite. Therefore, according to [14] the so-called *mixing-up effect* may occur for the semi-convergence of the HSS iteration method. That is to say, under suitable assumptions of non-normality of A and strong cluster[1] of the nonzero eigenvalues of $\mathcal{H}(A)$, the actual semi-convergence rate of the HSS iteration method is related to a certain average of the moduli of the eigenvalues excluding 1 of the iteration matrix $T(\alpha)$ instead of the semi-convergence factor $\vartheta(T(\alpha))$, or more specifically, the reduction rate of the HSS iteration errors can be bounded by a constant factor that is close to the square root of the geometric mean of the singular values excluding 1 of the iteration matrix $T(\alpha)$. We refer to Section 2.1.3 in [14] for a detailed discussion about this important and useful phenomenon.

4 Optimization of the semi-convergence factor

In this section, we are going to find an iteration parameter $\alpha_{\rm opt} > 0$ such that the semi-convergence factor $\vartheta(T(\alpha))$ of the HSS iteration achieves the minimum. To this end, we first investigate the property of its best-possible upper bound $\theta(T(\alpha))$ and derive a further simpler upper bound $\varrho(\alpha)$ for $\theta(T(\alpha))$.

Based on Corollary 3.7, we can obtain

$$\begin{aligned}
\theta(T(\alpha)) &= \sup_{x\in \mathrm{null}(\mathcal{H}(A))^\perp} \frac{|x^*(\alpha I+\mathcal{H}(A))^{-1}(\alpha I-\mathcal{H}(A))(\alpha I+\mathcal{S}(A))^{-1}(\alpha I-\mathcal{S}(A))x|}{x^*x}\\
&\le \sup_{x\in \mathrm{null}(\mathcal{H}(A))^\perp} \frac{\|(\alpha I+\mathcal{H}(A))^{-1}(\alpha I-\mathcal{H}(A))x\|_2\|(\alpha I+\mathcal{S}(A))^{-1}(\alpha I-\mathcal{S}(A))x\|_2}{\|x\|_2^2}\\
&\le \sup_{x\in \mathrm{null}(\mathcal{H}(A))^\perp} \frac{\|(\alpha I+\mathcal{H}(A))^{-1}(\alpha I-\mathcal{H}(A))x\|_2}{\|x\|_2}\\
&= \max_{\lambda\in\sigma(\mathcal{H}(A))\setminus\{0\}} \left|\frac{\alpha-\lambda}{\alpha+\lambda}\right|\\
&:= \varrho(\alpha).
\end{aligned}$$

Here, we have used the fact that $\mathcal{Q}_A(\alpha) := (\alpha I + \mathcal{S}(A))^{-1}(\alpha I - \mathcal{S}(A))$ is a Cayley transform and, hence, is unitary. Because computing a minimal point $\alpha_{\rm opt}$ of $\vartheta(T(\alpha))$ is difficult usually, we turn to minimize the upper bound $\varrho(\alpha)$ of $\theta(T(\alpha))$ or $\vartheta(T(\alpha))$ instead. The obtained result is described as follows.

Theorem 4.1 *Let $A \in \mathbf{C}^{n\times n}$ be a singular and positive semidefinite matrix, $\mathcal{H}(A)$ and $\mathcal{S}(A)$ be its Hermitian and skew-Hermitian parts satisfying* $\mathrm{null}(\mathcal{H}(A)) \subseteq \mathrm{null}(\mathcal{S}(A))$*, and $\gamma_{\min}$ and $\gamma_{\max}$ be the minimum and the maximum nonzero eigenvalues of the matrix $\mathcal{H}(A)$, respectively. Then*

[1] For the notion of strong cluster of eigenvalues of a matrix, we refer to Definition 3.1 in [14].

$$\alpha_\star \equiv \arg\min_{\alpha}\left\{\max_{\gamma_{\min}\le\lambda\le\gamma_{\max}}\left|\frac{\alpha-\lambda}{\alpha+\lambda}\right|\right\} = \sqrt{\gamma_{\min}\gamma_{\max}}$$

and

$$\varrho(\alpha_\star) = \frac{\sqrt{\gamma_{\max}}-\sqrt{\gamma_{\min}}}{\sqrt{\gamma_{\max}}+\sqrt{\gamma_{\min}}} = \frac{\sqrt{\kappa(\mathcal{H}(A))}-1}{\sqrt{\kappa(\mathcal{H}(A))}+1},$$

where $\kappa(\mathcal{H}(A)) := \gamma_{\max}/\gamma_{\min}$ *is defined as the spectral condition number of* $\mathcal{H}(A)$.

Proof Now,

$$\varrho(\alpha) = \max\left\{\left|\frac{\alpha-\gamma_{\min}}{\alpha+\gamma_{\min}}\right|, \quad \left|\frac{\alpha-\gamma_{\max}}{\alpha+\gamma_{\max}}\right|\right\}.$$

If $\alpha_\star$ is a minimum point of $\varrho(\alpha)$, then it must satisfy $\alpha_\star-\gamma_{\min}>0$, $\alpha_\star-\gamma_{\max}<0$, and

$$\frac{\alpha_\star-\gamma_{\min}}{\alpha_\star+\gamma_{\min}} = \frac{\gamma_{\max}-\alpha_\star}{\gamma_{\max}+\alpha_\star}.$$

Therefore,

$$\alpha_\star = \sqrt{\gamma_{\min}\gamma_{\max}},$$

and the result follows. □

We emphasize that in Theorem 4.1 the optimal parameter $\alpha_\star$ only minimizes the upper bound $\varrho(\alpha)$ of the semi-convergence factor $\vartheta(T(\alpha))$ of the HSS iteration matrix $T(\alpha)$, but does not minimize the semi-convergence factor itself. Also, Theorem 4.1 shows that when the optimal parameter $\alpha_\star$ is used, the upper bound of the semi-convergence rate of the HSS iteration is about the same as that of the conjugate gradient method applied to the Hermitian positive semidefinite linear system with the coefficient matrix being $\mathcal{H}(A)$, and it does become the same when, in particular, the coefficient matrix A is Hermitian. It should be mentioned that when the coefficient matrix A is normal, we have $\mathcal{H}(A)\mathcal{S}(A) = \mathcal{S}(A)\mathcal{H}(A)$ and, therefore, $\vartheta(T(\alpha)) = \theta(T(\alpha)) = \varrho(\alpha)$. The optimal parameter $\alpha_\star$ then minimizes all of these quantities.

For the singular saddle-point matrix $A \in \mathbf{C}^{n\times n}$ in (3.8), if there exist unitary matrices U and V such that

$$(U\oplus V)^* A (U\oplus V) = \begin{pmatrix} \lambda_1 I_r & 0 & \widehat{E} & 0 \\ 0 & 0 & 0 & 0 \\ -\widehat{E}^* & 0 & \lambda_2 I_s & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

whenever $U^*BU = \lambda_1 I_r \oplus 0$ and $V^*CV = \lambda_2 I_s \oplus 0$, with $\lambda_1 > 0$ and $\lambda_2 \geq 0$, we can make use of Corollary 3.8, and Theorem 4.1 and Remark 4.3 in [4] to obtain the exact formulas for the optimal iteration parameter and the optimal semi-convergence factor of the corresponding HSS iteration method.

5 Connections to Krylov subspace methods

In general, we consider a system of linear equations

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \qquad \mathbf{A} \in \mathbf{C}^{n\times n}, \quad \mathbf{x}, \mathbf{b} \in \mathbf{C}^n, \tag{5.11}$$

with the coefficient matrix $\mathbf{A}$ being either singular or nonsingular, $\mathbf{x}$ being the unknown vector, and $\mathbf{b}$ being the known vector such that the system of linear equations (5.11) is consistent, i.e., $\mathbf{b} \in \text{range}(\mathbf{A}) := \text{span}\{\mathbf{A}\mathbf{x} \mid \mathbf{x} \in \mathbf{C}^n\}$.

Let $\mathbf{x}^{(0)} \in \mathbf{C}^n$ be the initial approximation to the exact solution $\mathbf{x}_\star$ of the system of linear equations (5.11) and $\mathbf{r}^{(0)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(0)}$ be the initial residual. Then the Krylov subspace of dimension m associated with $\mathbf{A}$ and $\mathbf{r}^{(0)}$ can be defined as

$$\mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)}) = \text{span}\{\mathbf{r}^{(0)}, \mathbf{A}\mathbf{r}^{(0)}, \mathbf{A}^2\mathbf{r}^{(0)}, \ldots, \mathbf{A}^{m-1}\mathbf{r}^{(0)}\}.$$

A Krylov subspace method generates an iterative sequence $\{\mathbf{x}^{(k)}\} \subset \mathbf{C}^n$ by finding the m-th approximate solution $\mathbf{x}^{(m)}$ from $\mathbf{x}^{(0)} + \mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$ under certain minimization or (oblique) orthogonal projection rule. It is easily seen that the m-th residual $\mathbf{r}^{(m)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(m)}$ has the natural expression $\mathbf{r}^{(m)} = \mathbb{P}_m(\mathbf{A})\mathbf{r}^{(0)}$, where $\mathbb{P}_m(\lambda)$ is a polynomial of degree at most m such that $\mathbb{P}_m(0) = 1$. We denote the set of all such polynomials $\mathbb{P}_m$ by $\mathcal{P}_m$.

In particular, when the matrix $\mathbf{A} \in \mathbf{C}^{n\times n}$ is singular and is of index 1, by applying the Jordan canonical form theorem we know that there exists a nonsingular matrix $\mathbf{V}_c \in \mathbf{C}^{n\times n}$ such that

$$\mathbf{A} = \mathbf{V}_c^{-1}(\mathbf{A}_c \oplus 0)\mathbf{V}_c, \tag{5.12}$$

where $\mathbf{A}_c \in \mathbf{C}^{p\times p}$, a compression of the matrix $\mathbf{A}$ on the range space of $\mathbf{A}$, is nonsingular, with p the dimension of range$(\mathbf{A})$. It then follows that

$$\mathbb{P}_m(\mathbf{A}) = \mathbf{V}_c^{-1}(\mathbb{P}_m(\mathbf{A}_c) \oplus 0)\mathbf{V}_c. \tag{5.13}$$

If we further restrict the matrix $\mathbf{A} \in \mathbf{C}^{n\times n}$ to be positive semidefinite and specify the Krylov subspace method to be GMRES, then $\mathbf{A}_c$ is a positive definite matrix and $\mathbf{r}^{(m)}$ is determined according to

$$\|\mathbf{r}^{(m)}\|_2 = \min_{\mathbb{P}_m \in \mathcal{P}_m} \|\mathbb{P}_m(\mathbf{A})\mathbf{r}^{(0)}\|_2.$$

By making use of (5.13) we can easily obtain the estimate

$$\frac{\|\mathbf{r}^{(m)}\|_2}{\|\mathbf{r}^{(0)}\|_2} \leq \kappa(\mathbf{V}_c) \min_{\mathbb{P}_m \in \mathcal{P}_m} \|\mathbb{P}_m(\mathbf{A}_c)\|_2, \tag{5.14}$$

where $\kappa(\mathbf{V}_c) := \|\mathbf{V}_c\|_2 \|\mathbf{V}_c^{-1}\|_2$. Note from (5.12) that $\sigma(\mathbf{A}_c) = \sigma(\mathbf{A})\backslash\{0\}$ and $\mathbf{A}_c$ is diagonalizable if and only if so is $\mathbf{A}$. Therefore, if the matrix $\mathbf{A}$ is diagonalizable by the nonsingular matrix $\mathbf{V} \in \mathbf{C}^{n\times n}$, i.e., $\mathbf{A} = \mathbf{V}^{-1}\Lambda\mathbf{V}$ with Λ being the diagonal matrix of the eigenvalues of $\mathbf{A}$, and if all nonzero eigenvalues of the matrix $\mathbf{A}$ are contained in the ellipse $\mathcal{E}(\mathbf{c}, \mathbf{d}, \mathbf{a})$ with center $\mathbf{c}$, focal distance $\mathbf{d}$, and semi-major axis $\mathbf{a}$, which locates on the right-half complex plane and excludes the origin, then by making use of (5.14) and Corollary 6.33 in [23] we have

$$\frac{\|\mathbf{r}^{(m)}\|_2}{\|\mathbf{r}^{(0)}\|_2} \lesssim \kappa(\mathbf{V}) \left(\frac{\mathbf{a} + \sqrt{\mathbf{a}^2 - \mathbf{d}^2}}{\mathbf{c} + \sqrt{\mathbf{c}^2 - \mathbf{d}^2}} \right)^m .$$

So, the asymptotic convergence factor of GMRES, defined as $\overline{\lim}_{m\to+\infty} \left(\frac{\|\mathbf{r}^{(m)}\|_2}{\|\mathbf{r}^{(0)}\|_2} \right)^{1/m}$, is given by $\frac{\mathbf{a}+\sqrt{\mathbf{a}^2-\mathbf{d}^2}}{\mathbf{c}+\sqrt{\mathbf{c}^2-\mathbf{d}^2}}$. In particular, if all nonzero eigenvalues of the matrix $\mathbf{A} \in \mathbf{C}^{n\times n}$ are located in the circle $\mathcal{C}(\mathbf{c}, \varrho)$ centered at $\mathbf{c}$ with radius ϱ, which excludes the origin, then

$$\frac{\|\mathbf{r}^{(m)}\|_2}{\|\mathbf{r}^{(0)}\|_2} \lesssim \kappa(\mathbf{V}) \left(\frac{\varrho}{|\mathbf{c}|} \right)^m$$

and, hence, the asymptotic convergence factor of GMRES is now reduced to $\frac{\varrho}{|\mathbf{c}|}$.

Now, we consider the HSS iteration method associated with the system of linear equations (1.1), for which the coefficient matrix $A \in \mathbf{C}^{n\times n}$ is assumed to be singular and positive semidefinite. The HSS splitting matrix

$$M(\alpha) = \frac{1}{2\alpha}(\alpha I + \mathcal{H}(A))(\alpha I + \mathcal{S}(A))$$

naturally leads to a preconditioner, called the HSS preconditioner, for the matrix A. Here, we remark that the matrix $\alpha I + \mathcal{H}(A)$ is Hermitian positive definite and the matrix $\alpha I + \mathcal{S}(A)$ is positive definite even if A is singular and positive semidefinite. The HSS-preconditioned linear system is then given by

$$\mathbf{A}(\alpha)\mathbf{x} = \mathbf{b}(\alpha), \qquad \text{with} \quad \mathbf{A}(\alpha) = M(\alpha)^{-1}A \quad \text{and} \quad \mathbf{b}(\alpha) = M(\alpha)^{-1}b.$$

Note that $\mathbf{A}(\alpha) = I - T(\alpha)$, where $T(\alpha)$ is the HSS iteration matrix. Because Theorem 3.3 has shown $\text{index}(\mathbf{A}(\alpha)) = 1$, from Theorem 3.4 and [13, Lemma 6.9] we know that there exists a nonsingular matrix $\mathbf{V}_c(\alpha) \in \mathbf{C}^{n\times n}$ such that

$$\mathbf{A}(\alpha) = \mathbf{V}_c(\alpha)^{-1}(\mathbf{A}_c(\alpha) \oplus 0)\mathbf{V}_c(\alpha),$$

where $\mathbf{A}_c(\alpha) \in \mathbf{C}^{p\times p}$, a compression of the matrix $\mathbf{A}(\alpha)$ on the range space of $\mathcal{H}(\mathbf{A}(\alpha))$, is positive definite, with p the dimension of range$(\mathbf{A}(\alpha))$. By utilizing the above investigation, we can obtain the following semi-convergence result about the GMRES method preconditioned by the HSS iteration.

Theorem 5.1 *Let $A \in \mathbf{C}^{n\times n}$ be a singular and positive semidefinite matrix, and $\mathcal{H}(A)$ and $\mathcal{S}(A)$ be its Hermitian and skew-Hermitian parts, respectively. Assume* $\text{null}(A) = \text{null}(\mathcal{H}(A))$. *Then the following results hold true:*

(a) *The HSS-preconditioned GMRES(m) iteration (abbreviated as HSS-GMRES(m)) is semi-convergent to a solution of the system of linear equations* (1.1) *for any positive integer $m \ge 1$ and any initial vector $x^{(0)} \in \mathbf{C}^n$, where GMRES(m) represents the restarted GMRES method with m as the number of restarting steps;*
(b) *The HSS-preconditioned GMRES iteration (abbreviated as HSS-GMRES) sequence $\{x^{(k)}\}$, starting from any initial vector $x^{(0)} \in \mathbf{C}^n$, is semi-convergent, with the asymptotic semi-convergence factor $\vartheta(T(\alpha))$ being bounded by $\theta(T(\alpha))$, which is defined in Corollary* 3.7. *Moreover, $\theta(T(\alpha))$ is bounded by $\varrho(\alpha)$ defined in Sect.* 4, *which attains the minimum value $\frac{\sqrt{\kappa(\mathcal{H}(A))}-1}{\sqrt{\kappa(\mathcal{H}(A))}+1}$ when $\alpha \equiv \alpha_\star = \sqrt{\gamma_{\min}\gamma_{\max}}$, where $\gamma_{\min}$ and $\gamma_{\max}$ are, respectively, the minimum and the maximum nonzero eigenvalues of the matrix $\mathcal{H}(A)$, and $\kappa(\mathcal{H}(A)) = \gamma_{\max}/\gamma_{\min}$.*

Proof Theorem 3.4 has shown that A is unitarily similar to $\widehat{A} \oplus 0$ such that $\mathcal{H}(\widehat{A})$ is positive definite, i.e., $\widehat{A}$ is the compression of A on to the range space of $\mathcal{H}(A)$. Hence, there exists a unitary matrix $U \in \mathbf{C}^{n\times n}$ such that $A = U^*(\widehat{A} \oplus 0)U$ and

$$M(\alpha) = U^*(\widehat{M}(\alpha) \oplus I)U,$$

where

$$\widehat{M}(\alpha) = \frac{1}{2\alpha}(\alpha I + \mathcal{H}(\widehat{A}))(\alpha I + \mathcal{S}(\widehat{A})).$$

It follows that

$$\mathbf{A}(\alpha) = M(\alpha)^{-1}A = U^*((\widehat{M}(\alpha)^{-1}\widehat{A}) \oplus 0)U = U^*(\mathbf{A}_c(\alpha) \oplus 0)U,$$

where $\mathbf{A}_c(\alpha) := \widehat{M}(\alpha)^{-1}\widehat{A}$. Therefore, (a) is a straightforward corollary of Theorem 6.30 in [23] and the unitary property of the matrix $U \in \mathbf{C}^{n\times n}$, and (b) can be directly deduced from Theorem 4.1 and the general investigation about the asymptotic semi-convergence factor of the GMRES method for the singular system of linear equations (5.11) given in the first part of this section. □

6 Several examples

We consider the one-dimensional second-order differential equation satisfying the periodic boundary condition as follows:

$$\begin{cases} \frac{d^2u}{dx^2} + \gamma \frac{du}{dx} = -f(x), & x \in (0,1), \\ u(0) = u(1). \end{cases}$$

When this differential equation is discretized by the centered finite difference scheme with the equidistant stepsize $h = \frac{1}{n+1}$, we can get the system of linear equations

$$\begin{cases} (-1+R_e)u_{i-1} + 2u_i + (-1-R_e)u_{i+1} = h^2 f_i, & i = 1, 2, \ldots, n, \\ u_0 = u_n, \quad u_1 = u_{n+1}, \end{cases}$$

where $R_e = \frac{\gamma h}{2}$ is the mesh Reynolds number, and $u_i = u(ih)$ and $f_i = f(ih)$. In matrix-vector form, it gives the system of linear equations (1.1), in which

$$A = \begin{pmatrix} 2 & -1-R_e & 0 & 0 & \cdots & 0 & 0 & -1+R_e \\ -1+R_e & 2 & -1-R_e & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1+R_e & 2 & -1-R_e & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ldots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 & -1-R_e & 0 \\ 0 & 0 & 0 & 0 & \cdots & -1+R_e & 2 & -1-R_e \\ -1-R_e & 0 & 0 & 0 & \cdots & 0 & -1+R_e & 2 \end{pmatrix}, \tag{6.15}$$

and

$$x = (u_1, u_2, \ldots, u_n)^T, \quad b = (h^2 f_1, h^2 f_2, \ldots, h^2 f_n)^T.$$

By straightforward computations we can obtain

$$\operatorname{rank}(A) = n-1 \quad \text{and} \quad \operatorname{null}(A) = \operatorname{span}\{\mathbf{1}\},$$

where $\mathbf{1}$ is the column vector of ones. Hence, $A \in \mathbf{R}^{n\times n}$ is a singular matrix. Evidently, the symmetric and the skew-symmetric parts of the matrix $A \in \mathbf{R}^{n\times n}$ in (6.15) is given by

$$\mathcal{H}(A) = \begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ldots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ -1 & 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix}$$

and

$$\mathcal{S}(A) = \begin{pmatrix} 0 & -R_e & 0 & 0 & \cdots & 0 & 0 & R_e \\ R_e & 0 & -R_e & 0 & \cdots & 0 & 0 & 0 \\ 0 & R_e & 0 & -R_e & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & -R_e & 0 \\ 0 & 0 & 0 & 0 & \cdots & R_e & 0 & -R_e \\ -R_e & 0 & 0 & 0 & \cdots & 0 & R_e & 0 \end{pmatrix},$$

respectively, and $\mathcal{H}(A) \in \mathbf{R}^{n \times n}$ is a symmetric positive semidefinite matrix. It then follows that $A \in \mathbf{R}^{n \times n}$ is a singular and positive semidefinite matrix. Again, by direct computations we can obtain

$$\operatorname{rank}(\mathcal{H}(A)) = n - 1, \qquad \operatorname{null}(\mathcal{H}(A)) = \operatorname{span}\{\mathbf{1}\},$$

as well as

$$\operatorname{rank}(\mathcal{S}(A)) = \begin{cases} n-2, & \text{for } n \text{ even}, \\ n-1, & \text{for } n \text{ odd}, \end{cases}$$

and

$$\operatorname{null}(\mathcal{S}(A)) = \begin{cases} \operatorname{span}\{\mathbf{1}, \phi\}, & \text{for } n \text{ even}, \\ \operatorname{span}\{\mathbf{1}\}, & \text{for } n \text{ odd}, \end{cases}$$

where $\phi = (1, 0, 1, 0, \ldots, 1, 0)^T \in \mathbf{R}^n$.

Clearly, it holds that $\operatorname{null}(A) = \operatorname{null}(\mathcal{H}(A))$. So, by making use of Theorem 3.4 we can conclude that the HSS iteration method is semi-convergent to a solution of the system of linear equations (1.1) with its coefficient matrix being given by (6.15).

Moreover, because both $\mathcal{H}(A)$ and $\mathcal{S}(A)$ are circulant matrices, they can be diagonalized by the n-by-n Fourier matrix F_n, whose (j,k)-th entry is equal to $\frac{1}{\sqrt{n}} e^{\imath 2\pi (j-1)(k-1)/n}$, $j, k = 1, 2, \ldots, n$. That is to say, it holds that

$$\mathcal{H}(A) = F_n^* \Lambda_n^{(H)} F_n \quad \text{and} \quad \mathcal{S}(A) = F_n^* \Lambda_n^{(S)} F_n,$$

where

$$\Lambda_n^{(\xi)} = \operatorname{diag}(\lambda_1^{(\xi)}, \lambda_2^{(\xi)}, \ldots, \lambda_n^{(\xi)}), \qquad \xi = H, S,$$

with

$$\lambda_k^{(H)} = 2\left(1 - \cos\left(\frac{2\pi(k-1)}{n}\right)\right) \quad \text{and} \quad \lambda_k^{(S)} = -\imath \cdot 2R_e \sin\left(\frac{2\pi(k-1)}{n}\right), \quad k = 1, 2, \ldots, n.$$

By concrete computations, we know that the HSS iteration matrix is given by

$$T(\alpha) = F_n^* \Lambda_n F_n, \quad \text{with} \quad \Lambda_n = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n),$$

where

$$\lambda_k = \frac{\left(\alpha + \imath \cdot 2R_e \sin\left(\frac{2\pi(k-1)}{n}\right)\right)\left(\alpha - 2\left(1 - \cos\left(\frac{2\pi(k-1)}{n}\right)\right)\right)}{\left(\alpha - \imath \cdot 2R_e \sin\left(\frac{2\pi(k-1)}{n}\right)\right)\left(\alpha + 2\left(1 - \cos\left(\frac{2\pi(k-1)}{n}\right)\right)\right)}, \quad k = 1, 2, \ldots, n.$$

Hence, we have

$$\begin{aligned}
\vartheta(T(\alpha)) &= \max_{2\le k\le n} \left| \frac{\left(\alpha + \imath \cdot 2R_e \sin\left(\frac{2\pi(k-1)}{n}\right)\right)\left(\alpha - 2\left(1 - \cos\left(\frac{2\pi(k-1)}{n}\right)\right)\right)}{\left(\alpha - \imath \cdot 2R_e \sin\left(\frac{2\pi(k-1)}{n}\right)\right)\left(\alpha + 2\left(1 - \cos\left(\frac{2\pi(k-1)}{n}\right)\right)\right)} \right| \\
&= \max_{2\le k\le n} \left| \frac{\alpha - 2\left(1 - \cos\left(\frac{2\pi(k-1)}{n}\right)\right)}{\alpha + 2\left(1 - \cos\left(\frac{2\pi(k-1)}{n}\right)\right)} \right| \\
&= \begin{cases} \max\left\{ \left| \frac{\alpha-2\left(1-\cos\left(\frac{2\pi}{n}\right)\right)}{\alpha+2\left(1-\cos\left(\frac{2\pi}{n}\right)\right)} \right|, \quad \left| \frac{\alpha-4}{\alpha+4} \right| \right\}, & \text{for } n \text{ even}, \\ \max\left\{ \left| \frac{\alpha-2\left(1-\cos\left(\frac{2\pi}{n}\right)\right)}{\alpha+2\left(1-\cos\left(\frac{2\pi}{n}\right)\right)} \right|, \quad \left| \frac{\alpha-2(1+\cos(\frac{\pi}{n}))}{\alpha+2(1+\cos(\frac{\pi}{n}))} \right| \right\}, & \text{for } n \text{ odd}. \end{cases}
\end{aligned}$$

It then follows that $\vartheta(T(\alpha))$ attains its minimum at the minimal point

$$\alpha_{\text{opt}} = \begin{cases} 4\sin\left(\frac{\pi}{n}\right), & \text{for } n \text{ even}, \\ 4\sin\left(\frac{\pi}{n}\right)\cos\left(\frac{\pi}{2n}\right), & \text{for } n \text{ odd}, \end{cases}$$

and the optimal semi-convergence factor of the HSS iteration method is correspondingly given by

$$\vartheta(T(\alpha_{\text{opt}})) = \begin{cases} \frac{1-\sin(\frac{\pi}{n})}{1+\sin(\frac{\pi}{n})}, & \text{for } n \text{ even}, \\ \frac{1-2\sin(\frac{\pi}{2n})}{1+2\sin(\frac{\pi}{2n})}, & \text{for } n \text{ odd}. \end{cases}$$

When the HSS preconditioner is employed to accelerate the GMRES method, from Theorem 5.1 we see that the resulted HSS-GMRES iteration sequence is semi-convergent with the optimal asymptotic semi-convergence factor $\frac{1-\sin(\frac{\pi}{n})}{1+\sin(\frac{\pi}{n})}$ and $\frac{1-2\sin(\frac{\pi}{2n})}{1+2\sin(\frac{\pi}{2n})}$, for n being even and odd, respectively.

The above results can be easily extended to the system of linear equations (1.1) with the singular and positive semidefinite real n-by-n coefficient matrix

$$A = \begin{pmatrix} \Delta & -(1+R_e)I & 0 & 0 & \cdots & 0 & -(1-R_e)I \\ -(1-R_e)I & \Delta & -(1+R_e)I & 0 & \cdots & 0 & 0 \\ 0 & -(1-R_e)I & \Delta & -(1+R_e)I & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \Delta & -(1+R_e)I \\ -(1+R_e)I & 0 & 0 & 0 & \cdots & -(1-R_e)I & \Delta \end{pmatrix},$$

where $\Delta \in \mathbf{R}^{m\times m}$ is given by

$$\Delta = \begin{pmatrix} 4 & -1-R_e & 0 & 0 & \cdots & 0 & 0 & -1+R_e \\ -1+R_e & 4 & -1-R_e & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1+R_e & 4 & -1-R_e & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1+R_e & 4 & -1-R_e \\ -1-R_e & 0 & 0 & 0 & \cdots & 0 & -1+R_e & 4 \end{pmatrix},$$

which arises from the centered finite difference discretization with the equidistant step-size $h = \frac{1}{m+1}$ and $n = m^2$ of the following two-dimensional second-order differential equation satisfying the periodic boundary conditions:

$$\begin{cases} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \gamma\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y}\right) = -f(x,y), & x, y \in (0,1)\times(0,1), \\ u(x,0) = u(x,1), & x \in (0,1), \\ u(0,y) = u(1,y), & y \in (0,1). \end{cases}$$

More generally, we consider the one-dimensional variable-coefficient second-order differential equation satisfying the periodic boundary condition as follows:

$$\begin{cases} \frac{d}{dx}\left(c(x)\frac{du}{dx}\right) + \gamma\frac{du}{dx} = -f(x), & x \in (0,1), \\ u(0) = u(1), \end{cases}$$

where $c(x)$ is a given positive and continuously differentiable function defined on $(0,1)$. When the second-order term is approximated by an average of the forward and the backward finite differences and the first-order term is approximated by the centered finite difference, both using the equidistant stepsize $h = \frac{1}{n+1}$, we can get the system of linear equations

$$\begin{cases} -(c_{i-\frac{1}{2}} - R_e)u_{i-1} + (c_{i-\frac{1}{2}} + c_{i+\frac{1}{2}})u_i - (c_{i+\frac{1}{2}} + R_e)u_{i+1} = h^2 f_i, & i = 1, 2, \ldots, n, \\ u_0 = u_n, \quad u_1 = u_{n+1}, \end{cases}$$

where $R_e = \frac{\gamma h}{2}$ is the mesh Reynolds number, $u_i = u(ih)$, $f_i = f(ih)$ and $c_{i\pm\frac{1}{2}} = c(x_i \pm \frac{1}{2}h)$, for $i = 1, 2, \ldots, n$. In matrix-vector form, it gives the system of linear equations (1.1), in which $A = (a_{ij}) \in \mathbf{R}^{n\times n}$ is a singular and positive semidefinite matrix defined as

$$a_{ij} = \begin{cases} -(c_{i-\frac{1}{2}} - R_e), & \text{for} \quad j = i-1 \quad \text{and} \quad i = 2, 3, \ldots, n, \\ c_{i-\frac{1}{2}} + c_{i+\frac{1}{2}}, & \text{for} \quad j = i \quad \text{and} \quad i = 1, 2, \ldots, n, \\ -(c_{i+\frac{1}{2}} + R_e), & \text{for} \quad j = i+1 \quad \text{and} \quad i = 1, 2, \ldots, n-1, \\ -(c_{i-\frac{1}{2}} - R_e), & \text{for} \quad i = 1 \quad \text{and} \quad j = n, \\ -(c_{i+\frac{1}{2}} + R_e), & \text{for} \quad i = n \quad \text{and} \quad j = 1, \\ 0, & \text{otherwise}; \end{cases} \tag{6.16}$$

see [20] for a general and detailed derivation. By straightforward computations we can obtain

$$\operatorname{rank}(A) = \operatorname{rank}(\mathcal{H}(A)) = n-1 \quad \text{and} \quad \operatorname{null}(A) = \operatorname{null}(\mathcal{H}(A)) = \operatorname{span}\{\mathbf{1}\}.$$

Hence, by making use of Theorem 3.4 again we can conclude that the HSS iteration method is semi-convergent to a solution of the system of linear equations (1.1) with its coefficient matrix being given by (6.16).

We remark that when $c(x) \equiv 1$, the matrix A given in (6.16) reduces to the one given in (6.15). In addition, the above results can be easily extended to the system of linear equations (1.1) with the singular and positive semidefinite coefficient matrix $A \in \mathbf{R}^{n\times n}$, which arises from an analogous finite difference discretization scheme with the equidistant stepsize $h = \frac{1}{m+1}$ and $n = m^2$ of the following two-dimensional separable variable-coefficient second-order differential equation satisfying the periodic boundary conditions:

$$\begin{cases} \frac{\partial}{\partial x}\left(c_x(x)\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(c_y(y)\frac{\partial u}{\partial y}\right) + \gamma\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y}\right) = -f(x, y), & x, y \in (0, 1) \times (0, 1), \\ u(x, 0) = u(x, 1), & x \in (0, 1), \\ u(0, y) = u(1, y), & y \in (0, 1), \end{cases}$$

where $c_x(x)$ and $c_y(y)$ are given positive and continuously differentiable functions defined on $(0, 1)$, with respect to the variables x and y, respectively.

7 Numerical results

In this section, we solve the singular and positive semidefinite system of linear equations (1.1) by the HSS iteration method or the HSS-GMRES iteration method, in order to show numerically the feasibility and effectiveness of these two methods in the sense of iteration step (denoted as "IT"), elapsed CPU time in seconds (denoted as "CPU"), and relative residual error (denoted as "RES") defined by

$$\text{RES} = \frac{\|b - Ax^{(k)}\|_2}{\|b - Ax^{(0)}\|_2},$$

where the coefficient matrix $A \in \mathbf{R}^{n\times n}$, with $n = m^2$, is obtained from the finite difference discretization with equidistant stepsize $h = \frac{1}{m}$ of the two-dimensional variable-coefficient second-order differential equation satisfying the periodic boundary conditions:

$$\begin{cases} -\frac{\partial}{\partial x}\left(c(x,y)\frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(c(x,y)\frac{\partial u}{\partial y}\right) + \gamma\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y}\right) = f(x,y), & x, y \in (0,1)\times(0,1), \\ u(x,0) = u(x,1), & x \in (0,1), \\ u(0,y) = u(1,y), & y \in (0,1), \end{cases} \tag{7.17}$$

with

$$c(x,y) = 2 + \frac{1}{2}\left(\sin(2\pi x) + \sin(2\pi y)\right)$$

a given positive and continuously differentiable function defined on (0, 1), and the right-hand side vector is taken to be $b = Ax_\star$, with $x_\star = (1, 2, \ldots, n)^T \in \mathbf{R}^n$ being the exact solution.

More specifically, the system of linear equations to be solved is of the form

$$\begin{aligned} &-\left(c_{i\left(j-\frac{1}{2}\right)} + R_e\right) u_{i(j-1)} - \left(c_{\left(i-\frac{1}{2}\right)j} + R_e\right) u_{(i-1)j} \\ &\quad + \left(c_{\left(i-\frac{1}{2}\right)j} + c_{\left(i+\frac{1}{2}\right)j} + c_{i\left(j-\frac{1}{2}\right)} + c_{i\left(j+\frac{1}{2}\right)}\right) u_{ij} \\ &- \left(c_{\left(i+\frac{1}{2}\right)j} - R_e\right) u_{(i+1)j} - \left(c_{i\left(j+\frac{1}{2}\right)} - R_e\right) u_{i(j+1)} = h^2 f_{ij}, \quad i, j = 1, 2, \ldots, m, \end{aligned}$$

with

$$u_{i0} = u_{im}, \quad u_{i1} = u_{i(m+1)}, \quad u_{0j} = u_{mj}, \quad u_{1j} = u_{(m+1)j}, \qquad i, j = 1, 2, \ldots, m,$$

Table 1 The iteration parameter α

n	256	576	1024
α	1.1036	0.7384	0.5545

Table 2 Numerical results for $n = 256$ ($m = 16$) and different γ

γ	HSS			GMRES			HSS-GMRES		
	IT	CPU	RES	IT	CPU	RES	IT	CPU	RES
10	45	0.141	9.752E−7	112	0.031	1.950E−7	32	0.109	3.286E−10
10^2	44	0.141	7.712E−7	240	0.063	9.789E−7	48	0.125	2.520E−8
10^3	48	0.141	9.570E−7	592	0.125	9.123E−7	32	0.078	7.865E−8
10^4	50	0.156	9.772E−7	1072	0.219	9.956E−7	32	0.094	1.715E−9
10^5	51	0.156	8.232E−7	8288	1.719	9.967E−7	32	0.094	1.431E−9
10^6	51	0.156	8.263E−7	48944	10.141	9.994E−7	32	0.078	1.423E−9

and

$$\begin{cases} c_{ij} = c(ih, jh), \quad c_{\left(i\pm\frac{1}{2}\right)j} = c\left(\left(i \pm \frac{1}{2}\right)h, jh\right), \\ c_{i\left(j\pm\frac{1}{2}\right)} = c\left(ih, \left(j \pm \frac{1}{2}\right)h\right), \\ u_{ij} = u(ih, jh), \quad f_{ij} = f(ih, jh), \end{cases} \qquad i, j = 1, 2, \ldots, m,$$

where $R_e = \frac{\gamma h}{2}$ is the mesh Reynolds number.

In our implementations, the iteration parameter α is chosen to be the optimal one that minimizes the semi-convergence factor of the HSS iteration matrix $T(\alpha)$, for the finite difference matrix of the differential equation (7.17) when the coefficient $c(x, y)$ is constantly unit, i.e., $c(x, y) \equiv 1$. That is to say, $\alpha = 4\sqrt{2}\sin\left(\frac{\pi}{m}\right)$; see Table 1. In addition, all iterations are started from the initial vector $x^{(0)} = 0$ and terminated once the current iterate satisfies RES $\le 10^{-6}$, and all codes are run in MATLAB (version 6.5) with machine precision 10^{-16} on a Pentium IV personal computer.

In Tables 2, 3, 4, for different values of γ we list the iteration steps, CPU times and the relative residual errors for the HSS, the GMRES and the HSS-GMRES methods, when the problem sizes are equal to 256, 576 and 1024, respectively. From these tables, we see that all of these three methods can compute satisfactory approximations to the solution $x_\star$ of the referred system of linear equations.

As a solver, HSS costs much less iteration step and CPU time than GMRES. In addition, for fixed n and increasing γ, or for fixed γ and increasing n, both iteration step and CPU time of HSS increase mildly. However, for fixed n and increasing γ, the iteration step and CPU time of GMRES increase very quickly; and for fixed γ and increasing n, the CPU time of GMRES increase very rapidly, while the iteration step of GMRES is increasing for small γ (say, for $\gamma \le 10^3$) but decreasing for large γ (say, for $\gamma \ge 10^4$). Hence, HSS outperforms GMRES for all implementations in the sense of iteration step and CPU time.

Table 3 Numerical results for $n = 576$ ($m = 24$) and different γ

γ	HSS			GMRES			HSS-GMRES		
	IT	CPU	RES	IT	CPU	RES	IT	CPU	RES
10	68	1.047	8.593E−7	176	0.219	6.672E−7	32	0.469	1.145E−8
10^2	66	0.969	8.340E−7	368	0.438	9.223E−7	48	0.594	7.172E−7
10^3	67	1.000	8.817E−7	976	1.125	9.517E−7	48	0.594	1.641E−7
10^4	75	1.094	8.881E−7	544	0.625	9.591E−7	32	0.422	7.587E−8
10^5	75	1.078	9.893E−7	5392	6.125	9.969E−7	32	0.422	6.819E−8
10^6	75	1.094	9.987E−7	36672	42.109	9.986E−7	32	0.438	8.449E−8

Table 4 Numerical results for $n = 1024$ ($m = 32$) and different γ

γ	HSS			GMRES			HSS-GMRES		
	IT	CPU	RES	IT	CPU	RES	IT	CPU	RES
10	90	3.109	9.422E−7	240	1.375	6.281E−7	32	1.078	1.105E−7
10^2	88	3.047	8.937E−7	608	3.469	8.591E−7	64	1.703	5.741E−8
10^3	87	3.016	8.854E−7	1312	7.469	9.758E−7	64	1.703	1.495E−7
10^4	98	3.328	9.006E−7	880	5.016	9.290E−7	32	1.109	3.317E−7
10^5	99	3.391	9.913E−7	4976	28.328	9.870E−7	32	1.109	2.364E−7
10^6	100	3.406	9.048E−7	28992	164.531	9.984E−7	32	1.109	2.362E−7

As a preconditioner, HSS can considerably accelerate the convergence rate of GMRES, as HSS-GMRES requires much less iteration step and CPU time than GMRES. Moreover, for fixed n and increasing γ, the iteration step and CPU time of HSS-GMRES change moderately, in particular, the iteration step is indeed almost fixed. Also, HSS-GMRES costs much less iteration step and CPU time than HSS.

Therefore, as both solver and preconditioner, the HSS iteration method is very robust and effective for solving singular and positive semidefinite system of linear equations.

In addition, we examine the feasibility and efficiency of the HSS and the HSS-GMRES iteration methods for solving singular and positive semidefinite systems of linear equations with their coefficient matrices being complex.

To this end, we take the coefficient matrix of the system of linear equations (1.1) to be $A = W + \imath T \in \mathbf{C}^{n\times n}$, where $n = m^2$,

$$T = \frac{\gamma}{2m}(I \otimes U_c + U_c \otimes I), \qquad W = I \otimes V_c + V_c \otimes I,$$

m is a positive integer, γ is a positive constant, and $\otimes$ is the Kronecker product symbol, with

$$U = \text{pentadiag}(-1, -1, 4, -1, -1) \in \mathbf{R}^{m\times m}, \qquad V = \text{tridiag}(-1, 2, -1) \in \mathbf{R}^{m\times m}$$

Table 5 Numerical results for $n = 4096$ ($m = 64$) and different γ

γ	HSS			GMRES			HSS-GMRES		
	IT	CPU	RES	IT	CPU	RES	IT	CPU	RES
10^2	146	6.920	9.726E−07	5127	33.090	9.994E−07	32	1.640	4.581E−07
10^3	148	7.000	9.436E−07	1861	11.310	9.952E−07	28	1.440	5.599E−07
10^4	148	6.990	9.449E−07	821	5.350	9.894E−07	28	1.440	7.723E−07
10^5	148	7.050	9.449E−07	931	5.700	9.583E−07	28	1.430	6.997E−07
10^6	148	6.990	9.449E−07	967	6.270	9.420E−07	28	1.440	6.332E−07
10^7	148	7.060	9.449E−07	1215	7.550	8.993E−07	28	1.440	7.358E−07

being penta-diagonal and tridiagonal matrices,

$$U_c = U - (e_1 e_{m-1}^T + e_{m-1} e_1^T + e_a e_m^T + e_m e_a^T), \quad V_c = V - e_1 e_m^T - e_m e_1^T,$$

and

$$\begin{aligned} e_a &= (1, 1, 0, \dots, 0)^T \in \mathbf{R}^m, \quad e_{m-1} = (0, \dots, 0, 1, 0)^T \in \mathbf{R}^m, \\ e_m &= (0, \dots, 0, 1)^T \in \mathbf{R}^m. \end{aligned}$$

We take the right-hand side vector $b \in \mathbf{R}^n$ to be $b = Ax_\star$, with $x_\star = (1, 2, \dots, n)^T \in \mathbf{R}^n$ being the exact solution of the system of linear equations (1.1).

Although this example is an artificially constructed one, it is quite challenging for iterative solvers. By straightforward computations we can obtain

$$\text{null}(A) = \text{null}(\mathcal{H}(A)).$$

Hence, by making use of Theorem 3.4 we can conclude that the HSS iteration method is semi-convergent to a solution of the referred system of linear equations.

In our implementations, we adopt the same starting vector and stopping criterion as the above. We also choose the iteration parameter α such that the semi-convergence factor of the HSS iteration matrix $T(\alpha)$ is minimized; such an optimal α is exactly given by $\alpha = 4\sqrt{2}\sin\left(\frac{\pi}{m}\right)$.

In Tables 5, 6, 7, for different γ we list the iteration steps, CPU times and the relative residual errors for the HSS, the GMRES and the HSS-GMRES methods, when the problem sizes are equal to 4096, 6400 and 9216. The numerical results in these tables show much analogous computational phenomenon to our previous observations. Hence, as both solver and preconditioner, the HSS iteration method is very robust and effective for solving singular and positive semidefinite systems of linear equations even when their coefficient matrices are complex.

Table 6 Numerical results for $n = 6400$ ($m = 80$) and different γ

γ	HSS			GMRES			HSS-GMRES		
	IT	CPU	RES	IT	CPU	RES	IT	CPU	RES
10^2	176	15.580	9.525E−07	6651	75.780	9.994E−07	36	3.520	7.692E−07
10^3	178	15.950	9.961E−07	3511	39.610	9.944E−07	32	3.060	5.220E−07
10^4	178	15.800	9.981E−07	1985	22.750	9.151E−07	32	3.070	4.966E−07
10^5	178	15.660	9.982E−07	1929	21.490	9.516E−07	32	3.060	4.838E−07
10^6	178	15.760	9.982E−07	1983	22.330	8.991E−07	31	2.970	7.865E−07
10^7	178	15.690	9.982E−07	2166	24.150	9.931E−07	32	3.060	4.981E−07

Table 7 Numerical results for $n = 9216$ ($m = 96$) and different γ

γ	HSS			GMRES			HSS-GMRES		
	IT	CPU	RES	IT	CPU	RES	IT	CPU	RES
10^2	204	31.470	9.629E−07	6851	117.220	9.992E−07	40	6.710	9.307E−07
10^3	208	32.180	9.815E−07	5706	97.550	9.999E−07	35	5.820	7.088E−07
10^4	208	32.030	9.844E−07	2885	49.260	9.894E−07	35	5.870	5.971E−07
10^5	208	32.110	9.844E−07	3151	53.840	9.855E−07	35	5.890	6.015E−07
10^6	208	32.180	9.844E−07	3185	53.890	9.999E−07	34	5.670	9.038E−07
10^7	208	32.140	9.844E−07	3359	57.330	9.997E−07	35	5.830	6.004E−07

8 Concluding remarks

As a solver for the singular system of linear equations (1.1) with a positive semi-definite coefficient matrix $A \in \mathbf{C}^{n\times n}$, our theoretical analysis has shown that the Hermitian and skew-Hermitian splitting possesses a nice index property under the null space restriction $\mathrm{null}(A) = \mathrm{null}(\mathcal{H}(A))$ and, hence, leads to the semi-convergent HSS iteration method. This index property also leads to good preconditioning property of the correspondingly induced HSS preconditioner employed to accelerate the semi-convergence rates of the Krylov subspace methods such as GMRES. For future research, it is interesting from both theoretical and practical points of view to study the extensions of the algebraic properties of the Hermitian and skew-Hermitian splitting and the semi-convergence results of the HSS iteration method to their various variants and generalizations, e.g., the *normal and skew-Hermitian splitting* (**NSS**) and the NSS iteration method [1,8,9], the *positive-definite and skew-Hermitian splitting* (**PSS**) and the PSS iteration method [1,6], the *triangular and skew-Hermitian splitting* (**TSS**) and the TSS iteration method [1,6], the *block triangular and skew-Hermitian splitting* (**BTSS**) and the BTSS iteration method [1,6], and their preconditioned versions [1,5]; see [2,3,10,14,21].

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