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HERMITIAN AND SKEW-HERMITIAN SPLITTING METHODS FOR NON-HERMITIAN POSITIVE DEFINITE LINEAR SYSTEMS*

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Abstract. We study efficient iterative methods for the large sparse non-Hermitian positive definite system of linear equations based on the Hermitian and skew-Hermitian splitting of the coefficient matrix. These methods include a Hermitian/skew-Hermitian splitting (HSS) iteration and its inexact variant, the inexact Hermitian/skew-Hermitian splitting (IHSS) iteration, which employs some Krylov subspace methods as its inner iteration processes at each step of the outer HSS iteration. Theoretical analyses show that the HSS method converges unconditionally to the unique solution of the system of linear equations. Moreover, we derive an upper bound of the contraction factor of the HSS iteration which is dependent solely on the spectrum of the Hermitian part and is independent of the eigenvectors of the matrices involved. Numerical examples are presented to illustrate the effectiveness of both HSS and IHSS iterations. In addition, a model problem of a three-dimensional convection-diffusion equation is used to illustrate the advantages of our methods.

Key words. non-Hermitian matrix, splitting, Hermitian matrix, skew-Hermitian matrix, iterative methods

AMS subject classifications. 65F10, 65F15, 65T10

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1. Introduction.

Many problems in scientific computing give rise to a system of linear equations

$$Ax = b, \quad A \in \mathbb{C}^{n\times n} \text{ nonsingular}, \quad \text{and } x, b \in \mathbb{C}^n, \tag{1.1}$$

with A a large sparse non-Hermitian and positive definite matrix.

Iterative methods for the system of linear equations (1.1) require efficient splittings of the coefficient matrix A. For example, the Jacobi and the Gauss–Seidel iterations [16] split the matrix A into its diagonal and off-diagonal (respectively, strictly lower and upper triangular) parts, and the generalized conjugate gradient (CG) method [7] and the generalized Lanczos method [27] split the matrix A into its Hermitian and skew-Hermitian parts; see also [11, 17, 26, 1] and [2], respectively. Because the matrix A naturally possesses a Hermitian/skew-Hermitian splitting (HSS) [7]

$$A = H + S, \tag{1.2}$$

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where

$$H = \frac{1}{2}(A + A^*) \quad \text{and} \quad S = \frac{1}{2}(A - A^*), \tag{1.3}$$

we will study in this paper efficient iterative methods based on this particular matrix splitting for solving the system of linear equations (1.1).

Now $A = H(I + H^{-1}S)$, and thus $A^{-1} = (I + H^{-1}S)^{-1}H^{-1}$. Thus, if we replace $(I + H^{-1}S)^{-1}$ by its first order approximation $I - H^{-1}S$, then $(I - H^{-1}S)H^{-1}$ could be employed as a preconditioner to the matrix A. Of course, the preconditioning effect is completely determined by the spectral distribution of the matrix $H^{-1}S$, and it is satisfactory if the Hermitian part H is dominant [1]. On the other hand, if the skew-Hermitian part S is dominant, we can use an alternative preconditioning strategy recently presented by Golub and Vanderstraeten in [15]. Their basic idea is to invert the shifted skew-Hermitian matrix $\alpha I + S$ and then employ $(I - (S + \alpha I)^{-1}(H - \alpha I))(S + \alpha I)^{-1}$ as a preconditioner to the matrix A. In fact, the preconditioning effect for this preconditioner depends not only on the spectrum but also on the eigenvectors of the matrix $(S + \alpha I)^{-1}(H - \alpha I)$, which is, however, closely related to the shift α. For a nearly optimal α, numerical experiments in [15] on a variety of problems from real-world applications have shown that the reductions in terms of iteration count largely compensate for the additional work per iteration when compared to standard preconditioners. We remark that, for both preconditioners, exact inverses of the matrices H and $\alpha I + S$ are quite expensive, and, therefore, some further approximations, e.g., the incomplete Cholesky (IC) factorization [21, 20] and the incomplete orthogonal-triangular (IQR) factorization [3], to these two matrices may be respectively adopted in actual applications. However, theoretical analysis about existence, stability, and accuracy of the resulting iterative method are considerably difficult.

Moreover, based on the HSS (1.2)–(1.3), in this paper we present a different approach to solve the system of linear equations (1.1), called the HSS iteration, and it is as follows.

The HSS iteration method. *Given an initial guess $x^{(0)}$, for $k = 0, 1, 2, \ldots$, until $\{x^{(k)}\}$ converges, compute*

$$\begin{cases} (\alpha I + H)x^{(k+\frac{1}{2})} &= (\alpha I - S)x^{(k)} + b, \\ (\alpha I + S)x^{(k+1)} &= (\alpha I - H)x^{(k+\frac{1}{2})} + b, \end{cases} \tag{1.4}$$

where α is a given positive constant.

Evidently, each iterate of the HSS iteration alternates between the Hermitian part H and the skew-Hermitian part S of the matrix A, analogously to the classical alternating direction implicit (ADI) iteration for solving partial differential equations; see Peaceman and Rachford [23] and Douglas and Rachford [8]. Results associated to the stationary iterative method with alternation can be also found in Benzi and Szyld [4]. Theoretical analysis shows that the HSS iteration (1.4) converges unconditionally to the unique solution of the system of linear equations (1.1). The upper bound of the contraction factor of the HSS iteration is dependent on the spectrum of the Hermitian part H but is independent of the spectrum of the skew-Hermitian part S as well as the eigenvectors of the matrices H, S, and A. In addition, the optimal value of the parameter α for the upper bound of the contraction factor of the HSS iteration can be determined by the lower and the upper eigenvalue bounds of the matrix H.

Note that we can reverse the roles of the matrices H and S in the above HSS iteration method so that we may first solve the system of linear equations with coef-

ficient matrix $\alpha I + S$ and then solve the system of linear equations with coefficient matrix $\alpha I + H$.

The two half-steps at each HSS iterate require exact solutions with the n-by-n matrices $\alpha I + H$ and $\alpha I + S$. However, this is very costly and impractical in actual implementations. To further improve the computing efficiency of the HSS iteration, we can employ, for example, the CG method to solve the system of linear equations with coefficient matrix $\alpha I + H$ and some Krylov subspace method to solve the system of linear equations with coefficient matrix $\alpha I + S$ to some prescribed accuracy at each step of the HSS iteration. Other possible choices of inner iteration solvers are classical relaxation methods, multigrid methods or multilevel methods, etc. This results in an inexact Hermitian/skew-Hermitian splitting (IHSS) iteration. The tolerances (or numbers of inner iteration steps) for inner iterative methods may be different and may be changed according to the outer iteration scheme. Therefore, the IHSS iteration is actually a nonstationary iterative method for solving the system of linear equations (1.1).

Model problem analysis for a three-dimensional convection-diffusion equation and numerical implementations show that both HSS and IHSS iterations are feasible and efficient for solving the non-Hermitian positive definite system of linear equations (1.1).

The organization of this paper is as follows. In section 2, we study the convergence properties and analyze the convergence rate of the HSS iteration. In section 3, we establish the IHSS iteration and study its convergence property. The three-dimensional convection-diffusion equation is employed as a model problem to give intuitive illustration for the convergence theory for the HSS iteration in section 4. Numerical experiments are presented in section 5 to show the effectiveness of our methods. And, finally, in section 6, we draw a brief conclusion and include some remarks. Moreover, the basic lemma used in the model problem analysis in section 4 and some illustrative remarks can be found in the appendix.

2. Convergence analysis of the HSS iteration. In this section, we study the convergence rate of the HSS iteration. We first note that the HSS iteration method can be generalized to the two-step splitting iteration framework, and the following lemma describes a general convergence criterion for a two-step splitting iteration.

LEMMA 2.1. *Let $A \in \mathbb{C}^{n\times n}$, $A = M_i - N_i$ $(i = 1, 2)$ be two splittings*[1] *of the matrix A, and let $x^{(0)} \in \mathbb{C}^n$ be a given initial vector. If $\{x^{(k)}\}$ is a two-step iteration sequence defined by*

$$\begin{cases} M_1 x^{(k+\frac{1}{2})} &= N_1 x^{(k)} + b, \\ M_2 x^{(k+1)} &= N_2 x^{(k+\frac{1}{2})} + b, \end{cases}$$

$k = 0, 1, 2, \ldots$, then

$$x^{(k+1)} = M_2^{-1} N_2 M_1^{-1} N_1 x^{(k)} + M_2^{-1}(I + N_2 M_1^{-1})b, \quad k = 0, 1, 2, \ldots .$$

Moreover, if the spectral radius $\rho(M_2^{-1} N_2 M_1^{-1} N_1)$ of the iteration matrix $M_2^{-1} N_2 M_1^{-1} N_1$ is less than 1, then the iterative sequence $\{x^{(k)}\}$ converges to the unique solution $x^* \in \mathbb{C}^n$ of the system of linear equations (1.1) for all initial vectors $x^{(0)} \in \mathbb{C}^n$.

For the convergence property of the HSS iteration, we apply the above results to obtain the following main theorem.

[1] Here and in what follows, $A = M - N$ is called a splitting of the matrix A if M is a nonsingular matrix.

THEOREM 2.2. *Let $A \in \mathbb{C}^{n\times n}$ be a positive definite matrix, let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ be its Hermitian and skew-Hermitian parts, and let α be a positive constant. Then the iteration matrix $M(\alpha)$ of the HSS iteration is given by*

$$M(\alpha) = (\alpha I + S)^{-1}(\alpha I - H)(\alpha I + H)^{-1}(\alpha I - S), \tag{2.1}$$

and its spectral radius $\rho(M(\alpha))$ is bounded by

$$\sigma(\alpha) \equiv \max_{\lambda_i \in \lambda(H)} \left| \frac{\alpha - \lambda_i}{\alpha + \lambda_i} \right|,$$

where $\lambda(H)$ is the spectral set of the matrix H. Therefore, it holds that

$$\rho(M(\alpha)) \le \sigma(\alpha) < 1 \quad \forall \alpha > 0;$$

i.e., the HSS iteration converges to the unique solution $x^* \in \mathbb{C}^n$ of the system of linear equations (1.1).

Proof. By putting

$$M_1 = \alpha I + H, \quad N_1 = \alpha I - S, \quad M_2 = \alpha I + S, \quad \text{and} \quad N_2 = \alpha I - H$$

in Lemma 2.1 and noting that $\alpha I + H$ and $\alpha I + S$ are nonsingular for any positive constant α, we obtain (2.1).

By the similarity invariance of the matrix spectrum, we have

$$\begin{aligned} \rho(M(\alpha)) &= \rho((\alpha I - H)(\alpha I + H)^{-1}(\alpha I - S)(\alpha I + S)^{-1}) \\ &\le \|(\alpha I - H)(\alpha I + H)^{-1}(\alpha I - S)(\alpha I + S)^{-1}\|_2 \\ &\le \|(\alpha I - H)(\alpha I + H)^{-1}\|_2 \|(\alpha I - S)(\alpha I + S)^{-1}\|_2. \end{aligned}$$

Letting $Q(\alpha) = (\alpha I - S)(\alpha I + S)^{-1}$ and noting that $S^* = -S$, we see that

$$\begin{aligned} Q(\alpha)^* Q(\alpha) &= (\alpha I - S)^{-1}(\alpha I + S)(\alpha I - S)(\alpha I + S)^{-1} \\ &= (\alpha I - S)^{-1}(\alpha I - S)(\alpha I + S)(\alpha I + S)^{-1} \ = \ I. \end{aligned}$$

That is, $Q(\alpha)$ is a unitary matrix. ($Q(\alpha)$ is also called the Cayley transform of S.) Therefore, $\|Q(\alpha)\|_2 = 1$. It then follows that

$$\rho(M(\alpha)) \le \|(\alpha I - H)(\alpha I + H)^{-1}\|_2 = \max_{\lambda_i \in \lambda(H)} \left| \frac{\alpha - \lambda_i}{\alpha + \lambda_i} \right|.$$

Since $\lambda_i > 0 (i = 1, 2, \ldots, n)$ and α is a positive constant, it is easy to see that $\rho(M(\alpha)) \le \sigma(\alpha) < 1$. ∎

Theorem 2.2 shows that the convergence speed of the HSS iteration is bounded by $\sigma(\alpha)$, which depends only on the spectrum of the Hermitian part H but does not depend on the spectrum of the skew-Hermitian part S, on the spectrum of the coefficient matrix A, or on the eigenvectors of the matrices H, S, and A.

Now, if we introduce a vector norm $|||x||| = \|(\alpha I + S)x\|_2$ (for all $x \in \mathbb{C}^n$) and represent the induced matrix norm by $|||X||| = \|(\alpha I + S)X(\alpha I + S)^{-1}\|_2$ (for all $X \in \mathbb{C}^{n\times n}$), then, from the proof of Theorem 2.2, we see that

$$|||M(\alpha)||| = \|(\alpha I - H)(\alpha I + H)^{-1}(\alpha I - S)(\alpha I + S)^{-1}\|_2 \le \sigma(\alpha),$$

and it follows that

$$|||x^{(k+1)} - x^*||| \leq \sigma(\alpha)|||x^{(k)} - x^*|||, \qquad k = 0, 1, 2, \ldots .$$

Therefore, $\sigma(\alpha)$ is also an upper bound of the contraction factor of the HSS iteration in the sense of the $|||\cdot|||$-norm.

We remark that if the minimum and the maximum eigenvalues of the Hermitian part H are known, then the optimal parameter α for $\sigma(\alpha)$ (or the upper bound of $\rho(M(\alpha))$ or $|||M(\alpha)|||$) can be obtained. This fact is precisely stated as the following corollary.

COROLLARY 2.3. *Let $A \in \mathbb{C}^{n\times n}$ be a positive definite matrix, let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ be its Hermitian and skew-Hermitian parts, and let $\gamma_{\min}$ and $\gamma_{\max}$ be the minimum and the maximum eigenvalues of the matrix H, respectively, and let α be a positive constant. Then*

$$\alpha^* \equiv \arg\min_{\alpha} \left\{ \max_{\gamma_{\min}\leq\lambda\leq\gamma_{\max}} \left| \frac{\alpha - \lambda}{\alpha + \lambda} \right| \right\} = \sqrt{\gamma_{\min}\gamma_{\max}},$$

and

$$\sigma(\alpha^*) = \frac{\sqrt{\gamma_{\max}} - \sqrt{\gamma_{\min}}}{\sqrt{\gamma_{\max}} + \sqrt{\gamma_{\min}}} = \frac{\sqrt{\kappa(H)} - 1}{\sqrt{\kappa(H)} + 1},$$

where $\kappa(H)$ is the spectral condition number of H.

Proof. Now,

$$\sigma(\alpha) = \max\left\{ \left| \frac{\alpha - \gamma_{\min}}{\alpha + \gamma_{\min}} \right|, \left| \frac{\alpha - \gamma_{\max}}{\alpha + \gamma_{\max}} \right| \right\}. \tag{2.2}$$

To compute an approximate optimal $\alpha > 0$ such that the convergence factor $\rho(M(\alpha))$ of the HSS iteration is minimized, we can minimize the upper bound $\sigma(\alpha)$ of $\rho(M(\alpha))$ instead. If α^* is such a minimum point, then it must satisfy $\alpha^* - \gamma_{\min} > 0$, $\alpha^* - \gamma_{\max} < 0$, and

$$\frac{\alpha^* - \gamma_{\min}}{\alpha^* + \gamma_{\min}} = \frac{\gamma_{\max} - \alpha^*}{\gamma_{\max} + \alpha^*}.$$

Therefore,

$$\alpha^* = \sqrt{\gamma_{\min}\gamma_{\max}},$$

and the result follows. ∎

We emphasize that, in Corollary 2.3, the optimal parameter α^* minimizes only the upper bound $\sigma(\alpha)$ of the spectral radius of the iteration matrix but does not minimize the spectral radius itself; for an illustration of this phenomenon, see, e.g., Table 2.

Corollary 2.3 shows that, when the so-called optimal parameter α^* is employed, the upper bound of the convergence rate of the HSS iteration is about the same as that of the CG method, 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 $HS = SH$, and, therefore, $\rho(M(\alpha)) = |||M(\alpha)||| = \sigma(\alpha)$. The optimal parameter α^* then minimizes all of these three quantities.

3. The IHSS iteration. The two half-steps at each step of the HSS iteration require finding solutions with the n-by-n matrices $\alpha I + H$ and $\alpha I + S$, which is, however, very costly and impractical in actual implementations. To overcome this disadvantage and further improve the efficiency of the HSS iteration, we can solve the two subproblems iteratively. More specifically, we may employ the CG method to solve the system of linear equations with coefficient matrix $\alpha I + H$, because $\alpha I + H$ is Hermitian positive definite, and some Krylov subspace method [7, 24, 18] to solve the system of linear equations with coefficient matrix $\alpha I + S$. This results in the following IHSS iteration for solving the system of linear equations (1.1).

The IHSS iteration method. *Given an initial guess $\bar{x}^{(0)}$, for $k = 0, 1, 2, \ldots$, until $\{\bar{x}^{(k)}\}$ converges, solve $\bar{x}^{(k+\frac{1}{2})}$ approximately from*

$$(\alpha I + H)\bar{x}^{(k+\frac{1}{2})} \approx (\alpha I - S)\bar{x}^{(k)} + b$$

by employing an inner iteration (e.g., the CG method) with $\bar{x}^{(k)}$ as the initial guess; then solve $\bar{x}^{(k+1)}$ approximately from

$$(\alpha I + S)\bar{x}^{(k+1)} \approx (\alpha I - H)\bar{x}^{(k+\frac{1}{2})} + b$$

by employing an inner iteration (e.g., some Krylov subspace method) with $\bar{x}^{(k+\frac{1}{2})}$ as the initial guess, where α is a given positive constant.

To simplify numerical implementation and convergence analysis, we may rewrite the above IHSS iteration method as the following equivalent scheme.

Given an initial guess $\bar{x}^{(0)}$, for $k = 0, 1, 2, \ldots$, until $\{\bar{x}^{(k)}\}$ converges,

1. *approximate the solution of $(\alpha I + H)\bar{z}^{(k)} = \bar{r}^{(k)}$ ($\bar{r}^{(k)} = b - A\bar{x}^{(k)}$) by iterating until $\bar{z}^{(k)}$ is such that the residual*

$$\bar{p}^{(k)} = \bar{r}^{(k)} - (\alpha I + H)\bar{z}^{(k)} \tag{3.1}$$

satisfies

$$\|\bar{p}^{(k)}\| \le \varepsilon_k \|\bar{r}^{(k)}\|,$$

and then compute $\bar{x}^{(k+\frac{1}{2})} = \bar{x}^{(k)} + \bar{z}^{(k)}$;

2. *approximate the solution of $(\alpha I + S)\bar{z}^{(k+\frac{1}{2})} = \bar{r}^{(k+\frac{1}{2})}$ ($\bar{r}^{(k+\frac{1}{2})} = b - A\bar{x}^{(k+\frac{1}{2})}$) by iterating until $\bar{z}^{(k+\frac{1}{2})}$ is such that the residual*

$$\bar{q}^{(k+\frac{1}{2})} = \bar{r}^{(k+\frac{1}{2})} - (\alpha I + S)\bar{z}^{(k+\frac{1}{2})} \tag{3.2}$$

satisfies

$$\|\bar{q}^{(k+\frac{1}{2})}\| \le \eta_k \|\bar{r}^{(k+\frac{1}{2})}\|,$$

and then compute $\bar{x}^{(k+1)} = \bar{x}^{(k+\frac{1}{2})} + \bar{z}^{(k+\frac{1}{2})}$. Here $\|\cdot\|$ is a norm of a vector.

In the following theorem, we analyze the above IHSS iteration method in slightly more general terms. In particular, we consider inexact iterations for the two-step splitting technique (cf. Lemma 2.1). To this end, we generalize the norm $|||\cdot|||$ to $|||\cdot|||_{M_2}$, which is defined by $|||x|||_{M_2} = \|M_2 x\|$ (for all $x \in \mathbb{C}^n$), which immediately induces the matrix norm $|||X|||_{M_2} = \|M_2 X M_2^{-1}\|$ (for all $X \in \mathbb{C}^{n\times n}$).

THEOREM 3.1. *Let $A \in \mathbb{C}^{n\times n}$ and $A = M_i - N_i$ $(i = 1, 2)$ be two splittings of the matrix A. If $\{\bar{x}^{(k)}\}$ is an iterative sequence defined as*

$$\bar{x}^{(k+\frac{1}{2})} = \bar{x}^{(k)} + \bar{z}^{(k)}, \quad \text{with} \quad M_1 \bar{z}^{(k)} = \bar{r}^{(k)} + \bar{p}^{(k)}, \tag{3.3}$$

satisfying $\frac{\|\bar{p}^{(k)}\|}{\|\bar{r}^{(k)}\|} \leq \varepsilon_k$, *where* $\bar{r}^{(k)} = b - A\bar{x}^{(k)}$, *and*

$$\bar{x}^{(k+1)} = \bar{x}^{(k+\frac{1}{2})} + \bar{z}^{(k+\frac{1}{2})}, \quad \textit{with} \quad M_2\bar{z}^{(k+\frac{1}{2})} = \bar{r}^{(k+\frac{1}{2})} + \bar{q}^{(k+\frac{1}{2})}, \tag{3.4}$$

satisfying $\frac{\|\bar{q}^{(k+\frac{1}{2})}\|}{\|\bar{r}^{(k+\frac{1}{2})}\|} \leq \eta_k$, *where* $\bar{r}^{(k+\frac{1}{2})} = b - A\bar{x}^{(k+\frac{1}{2})}$, *then* $\{\bar{x}^{(k)}\}$ *is of the form*

$$\begin{aligned} \bar{x}^{(k+1)} &= M_2^{-1}N_2M_1^{-1}N_1\bar{x}^{(k)} + M_2^{-1}(I + N_2M_1^{-1})b \\ &\quad + M_2^{-1}(N_2M_1^{-1}\bar{p}^{(k)} + \bar{q}^{(k+\frac{1}{2})}). \end{aligned} \tag{3.5}$$

Moreover, if $x^* \in \mathbb{C}^n$ *is the exact solution of the system of linear equations* (1.1), *then we have*

$$|||\bar{x}^{(k+1)} - x^*|||_{M_2} \leq \left(\bar{\sigma} + \bar{\mu}\bar{\theta}\varepsilon_k + \bar{\theta}(\bar{\rho} + \bar{\theta}\bar{\nu}\varepsilon_k)\eta_k\right)|||\bar{x}^{(k)} - x^*|||_{M_2}, \quad k = 0, 1, 2, \ldots, \tag{3.6}$$

where

$$\begin{aligned} \bar{\sigma} &= \|N_2M_1^{-1}N_1M_2^{-1}\|, \quad \bar{\rho} = \|M_2M_1^{-1}N_1M_2^{-1}\|, \quad \bar{\mu} = \|N_2M_1^{-1}\|, \\ \bar{\theta} &= \|AM_2^{-1}\|, \qquad\qquad \bar{\nu} = \|M_2M_1^{-1}\|. \end{aligned}$$

In particular, if

$$\bar{\sigma} + \bar{\mu}\bar{\theta}\varepsilon_{\max} + \bar{\theta}(\bar{\rho} + \bar{\theta}\bar{\nu}\varepsilon_{\max})\eta_{\max} < 1, \tag{3.7}$$

then the iterative sequence $\{\bar{x}^{(k)}\}$ *converges to* $x^* \in \mathbb{C}^n$, *where* $\varepsilon_{\max} = \max_k\{\varepsilon_k\}$ *and* $\eta_{\max} = \max_k\{\eta_k\}$.

Proof. From (3.3), we obtain

$$\begin{aligned} \bar{x}^{(k+\frac{1}{2})} &= \bar{x}^{(k)} + M_1^{-1}(\bar{r}^{(k)} + \bar{p}^{(k)}) \\ &= (I - M_1^{-1}A)\bar{x}^{(k)} + M_1^{-1}b + M_1^{-1}\bar{p}^{(k)} \\ &= M_1^{-1}N_1\bar{x}^{(k)} + M_1^{-1}b + M_1^{-1}\bar{p}^{(k)}. \end{aligned} \tag{3.8}$$

Similarly, from (3.4), we get

$$\begin{aligned} \bar{x}^{(k+1)} &= \bar{x}^{(k+\frac{1}{2})} + M_2^{-1}(\bar{r}^{(k+\frac{1}{2})} + \bar{q}^{(k+\frac{1}{2})}) \\ &= (I - M_2^{-1}A)\bar{x}^{(k+\frac{1}{2})} + M_2^{-1}b + M_2^{-1}\bar{q}^{(k+\frac{1}{2})} \\ &= M_2^{-1}N_2\bar{x}^{(k+\frac{1}{2})} + M_2^{-1}b + M_2^{-1}\bar{q}^{(k+\frac{1}{2})}. \end{aligned}$$

Therefore, we have

$$\begin{aligned} \bar{x}^{(k+1)} &= M_2^{-1}N_2(M_1^{-1}N_1\bar{x}^{(k)} + M_1^{-1}b + M_1^{-1}\bar{p}^{(k)}) \\ &\quad + M_2^{-1}b + M_2^{-1}\bar{q}^{(k+\frac{1}{2})} \\ &= M_2^{-1}N_2M_1^{-1}N_1\bar{x}^{(k)} + M_2^{-1}(I + N_2M_1^{-1})b \\ &\quad + M_2^{-1}(N_2M_1^{-1}\bar{p}^{(k)} + \bar{q}^{(k+\frac{1}{2})}), \end{aligned} \tag{3.9}$$

which is exactly (3.5).

Because $x^* \in \mathbb{C}^n$ is the exact solution of the system of linear equations (1.1), it must satisfy

$$x^* = M_1^{-1}N_1x^* + M_1^{-1}b \tag{3.10}$$

and

$$x^* = M_2^{-1}N_2M_1^{-1}N_1x^* + M_2^{-1}(I + N_2M_1^{-1})b. \tag{3.11}$$

By subtracting (3.10) from (3.8) and (3.11) from (3.9), respectively, we have

$$\bar{x}^{(k+\frac{1}{2})} - x^* = M_1^{-1}N_1(\bar{x}^{(k)} - x^*) + M_1^{-1}\bar{p}^{(k)} \tag{3.12}$$

and

$$\bar{x}^{(k+1)} - x^* = M_2^{-1}N_2M_1^{-1}N_1(\bar{x}^{(k)} - x^*) + M_2^{-1}(N_2M_1^{-1}\bar{p}^{(k)} + \bar{q}^{(k+\frac{1}{2})}). \tag{3.13}$$

Taking norms on both sides of the identities (3.12) and (3.13), we can obtain

$$\begin{aligned} |||\bar{x}^{(k+\frac{1}{2})} - x^*|||_{M_2} &\le |||M_1^{-1}N_1(\bar{x}^{(k)} - x^*)|||_{M_2} + |||M_1^{-1}\bar{p}^{(k)}|||_{M_2} \\ &\le |||M_1^{-1}N_1|||_{M_2}|||\bar{x}^{(k)} - x^*|||_{M_2} + |||M_1^{-1}\bar{p}^{(k)}|||_{M_2} \\ &\le \|M_2M_1^{-1}N_1M_2^{-1}\| \cdot |||\bar{x}^{(k)} - x^*|||_{M_2} \\ &\quad + \|M_2M_1^{-1}\| \cdot \|\bar{p}^{(k)}\| \end{aligned} \tag{3.14}$$

and

$$\begin{aligned} |||\bar{x}^{(k+1)} - x^*|||_{M_2} &\le |||M_2^{-1}N_2M_1^{-1}N_1|||_{M_2}|||\bar{x}^{(k)} - x^*|||_{M_2} \\ &\quad + |||M_2^{-1}(N_2M_1^{-1}\bar{p}^{(k)} + \bar{q}^{(k+\frac{1}{2})})|||_{M_2} \\ &= \|N_2M_1^{-1}N_1M_2^{-1}\| \cdot |||\bar{x}^{(k)} - x^*|||_{M_2} \\ &\quad + \|N_2M_1^{-1}\bar{p}^{(k)} + \bar{q}^{(k+\frac{1}{2})}\| \\ &\le \|N_2M_1^{-1}N_1M_2^{-1}\| \cdot |||\bar{x}^{(k)} - x^*|||_{M_2} \\ &\quad + \|N_2M_1^{-1}\| \cdot \|\bar{p}^{(k)}\| + \|\bar{q}^{(k+\frac{1}{2})}\|. \end{aligned} \tag{3.15}$$

Noticing that

$$\|\bar{r}^{(k)}\| = \|b - A\bar{x}^{(k)}\| = \|A(x^* - \bar{x}^{(k)})\| \le \|AM_2^{-1}\| \cdot |||x^* - \bar{x}^{(k)}|||_{M_2}$$

and

$$\|\bar{r}^{(k+\frac{1}{2})}\| = \|b - A\bar{x}^{(k+\frac{1}{2})}\| = \|A(x^* - \bar{x}^{(k+\frac{1}{2})})\| \le \|AM_2^{-1}\| \cdot |||x^* - \bar{x}^{(k+\frac{1}{2})}|||_{M_2},$$

by (3.12), (3.14), and the definitions of the sequences $\{\bar{p}^{(k)}\}$ and $\{\bar{q}^{(k+\frac{1}{2})}\}$, we have

$$\|\bar{p}^{(k)}\| \le \varepsilon_k\|\bar{r}^{(k)}\| \le \varepsilon_k\|AM_2^{-1}\| \cdot |||\bar{x}^{(k)} - x^*|||_{M_2} \tag{3.16}$$

and

$$\begin{aligned} \|\bar{q}^{(k+\frac{1}{2})}\| &\le \eta_k\|\bar{r}^{(k+\frac{1}{2})}\| \\ &\le \eta_k\|AM_2^{-1}\|(\|M_2M_1^{-1}N_1M_2^{-1}\| \cdot |||\bar{x}^{(k)} - x^*|||_{M_2} \\ &\quad + \|M_2M_1^{-1}\| \cdot \|\bar{p}^{(k)}\|) \\ &\le \eta_k\|AM_2^{-1}\|(\|M_2M_1^{-1}N_1M_2^{-1}\| \\ &\quad + \varepsilon_k\|M_2M_1^{-1}\| \cdot \|AM_2^{-1}\|)|||\bar{x}^{(k)} - x^*|||_{M_2}. \end{aligned} \tag{3.17}$$

Through substituting (3.16) and (3.17) into (3.15), we finally obtain

$$\begin{aligned} |||\bar{x}^{(k+1)} - x^*|||_{M_2} &\le \|N_2M_1^{-1}N_1M_2^{-1}\| \cdot |||\bar{x}^{(k)} - x^*|||_{M_2} \\ &\quad + \|N_2M_1^{-1}\| \cdot \varepsilon_k\|AM_2^{-1}\| \cdot |||\bar{x}^{(k)} - x^*|||_{M_2} \\ &\quad + \eta_k\|AM_2^{-1}\|(\|M_2M_1^{-1}N_1M_2^{-1}\| \\ &\quad + \varepsilon_k\|M_2M_1^{-1}\| \cdot \|AM_2^{-1}\|)|||\bar{x}^{(k)} - x^*|||_{M_2} \\ &\le \left(\bar{\sigma} + \bar{\mu}\bar{\theta}\varepsilon_k + \bar{\theta}(\bar{\rho} + \bar{\theta}\bar{\nu}\varepsilon_k)\eta_k\right)|||\bar{x}^{(k)} - x^*|||_{M_2}. \end{aligned}$$

□

We remark that, if the inner systems can be solved exactly in some applications, the corresponding quantities $\{\varepsilon_k\}$ and $\{\eta_k\}$, and hence $\varepsilon_{\max}$ and $\eta_{\max}$, are equal to zero. It then follows that the convergence rate of the IHSS iteration reduces to the same as that of the HSS iteration. In general, Theorem 3.1 shows that, in order to guarantee the convergence of the IHSS iteration, it is not necessary for $\{\varepsilon_k\}$ and $\{\eta_k\}$ to approach zero as k is increasing. All we need is that the condition (3.7) is satisfied.

By specializing Theorem 3.1 to the shifted Hermitian and skew-Hermitian splittings

$$\begin{aligned} A &= M_1 - N_1 \equiv (\alpha I + H) - (\alpha I - S) \\ &= M_2 - N_2 \equiv (\alpha I + S) - (\alpha I - H), \end{aligned}$$

we straightforwardly obtain the following convergence theorem about the IHSS iteration method.

THEOREM 3.2. *Let $A \in \mathbb{C}^{n\times n}$ be a positive definite matrix, let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ be its Hermitian and skew-Hermitian parts, and let α be a positive constant. If $\{\bar{x}^{(k)}\}$ is an iterative sequence generated by the IHSS iteration method (cf.* (3.1) *and* (3.2)*) and if $x^* \in \mathbb{C}^n$ is the exact solution of the system of linear equations* (1.1)*, then it holds that*

$$|||\bar{x}^{(k+1)} - x^*||| \le (\sigma(\alpha) + \theta\rho\eta_k)(1 + \theta\varepsilon_k)|||\bar{x}^{(k)} - x^*|||, \quad k = 0, 1, 2, \dots,$$

where

$$\rho = \|(\alpha I + S)(\alpha I + H)^{-1}\|_2, \quad \theta = \|A(\alpha I + S)^{-1}\|_2. \tag{3.18}$$

In particular, if $(\sigma(\alpha) + \theta\rho\eta_{\max})(1 + \theta\varepsilon_{\max}) < 1$, then the iterative sequence $\{\bar{x}^{(k)}\}$ converges to $x^* \in \mathbb{C}^n$, where $\varepsilon_{\max} = \max_k\{\varepsilon_k\}$ and $\eta_{\max} = \max_k\{\eta_k\}$.

According to Theorem 3.1, we want to choose tolerances so that the computational work of the two-step splitting iteration method is minimized. In fact, as we have remarked previously, the tolerances $\{\varepsilon_k\}$ and $\{\eta_k\}$ are not required to approach zero as k increases in order to get the convergence of the IHSS iteration but are required to approach zero in order to asymptotically recover the original convergence rate (cf. Theorem 2.2) of the HSS iteration.

The following theorem presents one possible way of choosing the tolerances $\{\varepsilon_k\}$ and $\{\eta_k\}$ such that the original convergence rate (cf. Lemma 2.1) of the two-step splitting iterative scheme can be asymptotically recovered.

THEOREM 3.3. *Let the assumptions in Theorem* 3.1 *be satisfied. Suppose that both $\{\tau_1(k)\}$ and $\{\tau_2(k)\}$ are nondecreasing and positive sequences satisfying $\tau_1(k) \ge 1$, $\tau_2(k) \ge 1$, and $\lim_{k\to\infty} \sup \tau_1(k) = \lim_{k\to\infty} \sup \tau_2(k) = +\infty$, and that both δ_1 and δ_2 are real constants in the interval $(0, 1)$ satisfying*

$$\varepsilon_k \le c_1\delta_1^{\tau_1(k)} \quad \text{and} \quad \eta_k \le c_2\delta_2^{\tau_2(k)}, \qquad k = 0, 1, 2, \dots, \tag{3.19}$$

where c_1 and c_2 are nonnegative constants. Then we have

$$|||\bar{x}^{(k+1)} - x^*|||_{M_2} \le \left(\sqrt{\bar{\sigma}} + \bar{\omega}\bar{\theta}\delta^{\tau(k)}\right)^2 |||\bar{x}^{(k)} - x^*|||_{M_2}, \quad k = 0, 1, 2, \dots,$$

where

$$\tau(k) = \min\{\tau_1(k), \tau_2(k)\}, \quad \delta = \max\{\delta_1, \delta_2\}, \tag{3.20}$$

and

$$\bar{\omega} = \max\left\{\sqrt{c_1 c_2 \bar{\nu}}, \quad \frac{1}{2\sqrt{\bar{\sigma}}}(c_1\bar{\mu} + c_2\bar{\rho})\right\}.$$

In particular, we have

$$\lim_{k\to\infty} \sup \frac{|||\bar{x}^{(k+1)} - x^*|||_{M_2}}{|||\bar{x}^{(k)} - x^*|||_{M_2}} = \bar{\sigma};$$

i.e., the convergence rate of the inexact two-step splitting iterative scheme is asymptotically the same as that of the exact two-step splitting iterative scheme.

Proof. From (3.6) and (3.19), we obtain, for $k = 0, 1, 2, \ldots$, that

$$\begin{aligned}
|||\bar{x}^{(k+1)} - x^*|||_{M_2} &\le \left(\bar{\sigma} + \bar{\mu}\bar{\theta}\varepsilon_k + \bar{\theta}(\bar{\rho} + \bar{\theta}\bar{\nu}\varepsilon_k)\eta_k\right)|||\bar{x}^{(k)} - x^*|||_{M_2} \\
&\le \left(\bar{\sigma} + \bar{\mu}\bar{\theta}c_1\delta_1^{\tau_1(k)} + \bar{\theta}(\bar{\rho} + \bar{\theta}\bar{\nu}c_1\delta_1^{\tau_1(k)})c_2\delta_2^{\tau_2(k)}\right)|||\bar{x}^{(k)} - x^*|||_{M_2} \\
&\le \left(\bar{\sigma} + \bar{\mu}\bar{\theta}c_1\delta^{\tau(k)} + \bar{\theta}(\bar{\rho} + \bar{\theta}\bar{\nu}c_1\delta^{\tau(k)})c_2\delta^{\tau(k)}\right)|||\bar{x}^{(k)} - x^*|||_{M_2} \\
&= \left(\bar{\sigma} + (c_1\bar{\mu} + c_2\bar{\rho})\bar{\theta}\delta^{\tau(k)} + c_1c_2\bar{\nu}\bar{\theta}^2\delta^{2\tau(k)}\right)|||\bar{x}^{(k)} - x^*|||_{M_2} \\
&\le \left(\bar{\sigma} + 2\bar{\omega}\sqrt{\bar{\sigma}}\bar{\theta}\delta^{\tau(k)} + \bar{\omega}^2\bar{\theta}^2\delta^{2\tau(k)}\right)|||\bar{x}^{(k)} - x^*|||_{M_2} \\
&= \left(\sqrt{\bar{\sigma}} + \bar{\omega}\bar{\theta}\delta^{\tau(k)}\right)^2|||\bar{x}^{(k)} - x^*|||_{M_2}.
\end{aligned}$$

The result follows straightforwardly. ∎

Theorems 3.2 and 3.3 immediately result in the following convergence result of the IHSS iteration method.

THEOREM 3.4. *Let the assumptions in Theorem* 3.2 *be satisfied. Suppose that both* $\{\tau_1(k)\}$ *and* $\{\tau_2(k)\}$ *are nondecreasing and positive sequences satisfying* $\tau_1(k) \ge 1$, $\tau_2(k) \ge 1$, *and* $\lim_{k\to\infty} \sup \tau_1(k) = \lim_{k\to\infty} \sup \tau_2(k) = +\infty$, *and that both* δ_1 *and* δ_2 *are real constants in the interval* $(0, 1)$ *satisfying* (3.19). *Then it holds that*

$$|||\bar{x}^{(k+1)} - x^*||| \le \left(\sqrt{\sigma(\alpha)} + \omega\theta\delta^{\tau(k)}\right)^2|||\bar{x}^{(k)} - x^*|||, \quad k = 0, 1, 2, \ldots,$$

where ρ *and* θ *are defined by* (3.18), $\tau(k)$ *and* δ *are defined by* (3.20), *and*

$$\omega = \max\left\{\sqrt{c_1 c_2 \rho}, \quad \frac{1}{2\sqrt{\sigma(\alpha)}}(c_1\sigma(\alpha) + c_2\rho)\right\}.$$

In particular, we have

$$\lim_{k\to\infty} \sup \frac{|||\bar{x}^{(k+1)} - x^*|||}{|||\bar{x}^{(k)} - x^*|||} = \sigma(\alpha);$$

i.e., the convergence rate of the IHSS iteration method is asymptotically the same as that of the HSS iteration method.

According to Theorem 3.4, we show that, if the tolerances $\{\varepsilon_k\}$ and $\{\eta_k\}$ are chosen as in (3.19), then the IHSS iteration converges to the unique solution $x^* \in \mathbb{C}^n$ of the system of linear equations (1.1), and the upper bound of the asymptotic convergence factor of the IHSS iteration tends to $\sigma(\alpha)$ of that of the HSS iteration (cf. Theorem 2.2). Moreover, we remark that we may replace (3.19) by other rules for which $\{\varepsilon_k\}$ and $\{\eta_k\}$ approach zero. See [14].

TABLE 1
Work to compute a sweep of the IHSS method.

Operation	Work
$\bar{r}^{(k)} = b - A\bar{x}^{(k)}$	$n + a$
$(\alpha I + H)\bar{z}^{(k+\frac{1}{2})} = \bar{r}^{(k)}$	$\chi_k(H)$
$\bar{x}^{(k+\frac{1}{2})} = \bar{x}^{(k)} + \bar{z}^{(k+\frac{1}{2})}$	n
$\bar{r}^{(k+\frac{1}{2})} = b - A\bar{x}^{(k+\frac{1}{2})}$	$n + a$
$(\alpha I + S)\bar{z}^{(k+1)} = \bar{r}^{(k+\frac{1}{2})}$	$\chi_k(S)$
$\bar{x}^{(k+1)} = \bar{x}^{(k+\frac{1}{2})} + \bar{z}^{(k+1)}$	n

Computational complexity. To analyze the computational complexity of the HSS and the IHSS iterations, we need to estimate their computer times (via operation counts) and computer memories. Assume that a is the number of operations required to compute Ay for a given vector $y \in \mathbb{C}^n$ and $\chi_k(H)$ and $\chi_k(S)$ are the numbers of operations required to solve inner systems (3.1) and (3.2) inexactly with the tolerances $\{\varepsilon_k\}$ and $\{\eta_k\}$, respectively. Then the work to compute a sweep of the IHSS iteration is estimated using the results of Table 1. Straightforward calculations show that the total work to compute each step of the IHSS iteration is $\mathcal{O}(4n + 2a + \chi_k(H) + \chi_k(S))$.

In addition, a simple calculation shows that the memory is required to store $\bar{x}^{(k)}$, b, $\bar{r}^{(k)}$, $\bar{z}^{(k)}$. For the inexact solvers for inner systems (3.1) and (3.2), we require only some auxiliary vectors; for instance, CG-type methods need about five vectors [24]. Moreover, it is not necessary to store H and S explicitly as matrices, as all we need are two subroutines that perform the matrix-vector multiplications with respect to these two matrices. Therefore, the total amount of computer memory required is $\mathcal{O}(n)$, which has the same order of magnitude as the number of unknowns.

4. Application to the model convection-diffusion equation. We consider the three-dimensional convection-diffusion equation

$$-(u_{xx} + u_{yy} + u_{zz}) + q(u_x + u_y + u_z) = f(x, y, z) \tag{4.1}$$

on the unit cube $\Omega = [0, 1] \times [0, 1] \times [0, 1]$, with constant coefficient q and subject to Dirichlet-type boundary conditions. When the seven-point finite difference discretization, for example, the centered differences to the diffusive terms, and the centered differences or the first order upwind approximations to the convective terms are applied to the above model convection-diffusion equation, we get the system of linear equations (1.1) with the coefficient matrix

$$A = T_x \otimes I \otimes I + I \otimes T_y \otimes I + I \otimes I \otimes T_z, \tag{4.2}$$

where the equidistant step-size $h = \frac{1}{n+1}$ is used in the discretization on all of the three directions and the natural lexicographic ordering is employed to the unknowns. In addition, $\otimes$ denotes the Kronecker product, and T_x, T_y, and T_z are tridiagonal matrices given by

$$T_x = \text{ tridiag}(t_2, t_1, t_3), \quad T_y = \text{ tridiag}(t_2, 0, t_3), \quad \text{and} \quad T_z = \text{ tridiag}(t_2, 0, t_3),$$

with

$$t_1 = 6, \quad t_2 = -1 - r, \quad t_3 = -1 + r$$

if the first order derivatives are approximated by the centered difference scheme and

$$t_1 = 6 + 6r, \quad t_2 = -1 - 2r, \quad t_3 = -1$$

if the first order derivatives are approximated by the upwind difference scheme. Here

$$r = \frac{qh}{2}$$

is the mesh Reynolds number. For details, we refer to [9, 10] and [12, 13].

From (4.2), we know that the Hermitian part H and the skew-Hermitian part S of the matrix A are

$$H = H_x \otimes I \otimes I + I \otimes H_y \otimes I + I \otimes I \otimes H_z \tag{4.3}$$

and

$$S = S_x \otimes I \otimes I + I \otimes S_y \otimes I + I \otimes I \otimes S_z, \tag{4.4}$$

where

$$H_x = \text{ tridiag}\left(\frac{t_2+t_3}{2}, t_1, \frac{t_2+t_3}{2}\right), \quad H_y = H_z = \text{ tridiag}\left(\frac{t_2+t_3}{2}, 0, \frac{t_2+t_3}{2}\right),$$

$$S_\xi = \text{ tridiag}\left(\frac{t_2-t_3}{2}, 0, -\frac{t_2-t_3}{2}\right), \quad \xi \in \{x, y, z\}.$$

From Lemma A.1, we know, for the centered difference scheme, that

$$\begin{aligned} &\min_{1\le j,k,l\le n} \lambda_{j,k,l}(H) = 6(1-\cos(\pi h)), && \max_{1\le j,k,l\le n} \lambda_{j,k,l}(H) = 6(1+\cos(\pi h)), \\ &\min_{1\le j,k,l\le n} |\lambda_{j,k,l}(S)| = 0, && \max_{1\le j,k,l\le n} |\lambda_{j,k,l}(S)| = 6r\cos(\pi h). \end{aligned}$$

Therefore, the quantities in Theorem 2.2 can be obtained by concrete computations.

THEOREM 4.1. *For the system of linear equations* (1.1) *with the coefficient matrix* (4.2) *arising from the centered difference scheme for the three-dimensional model convection-diffusion equation* (4.1) *with the homogeneous Dirichlet boundary condition, the iteration sequence* $\{x^{(k)}\}$ *generated by the HSS iteration from an initial guess* $x^{(0)} \in \mathbb{C}^n$ *converges to its unique solution* $x^* \in \mathbb{C}^n$ *and satisfies*

$$|||x^{(k+1)} - x^*||| \le \left[1 - \pi h + \frac{1}{2}\pi^2 h^2 + \mathcal{O}(h^3)\right] \cdot |||x^{(k)} - x^*|||, \qquad k = 0, 1, 2, \ldots .$$

We note that this bound is independent of q and the mesh Reynolds number. The results for the upwind difference scheme can be obtained in an analogous fashion. Since H and S in (4.3) and (4.4) can be diagonalized by sine transforms, the number of operations required at each HSS iteration is about $O(n^3 \log n)$. It follows that the total complexity of the HSS iteration is about $O(n^4 \log n)$ operations. Here n is the number of grid points in all three directions. Here the model problem is used as an example to illustrate the convergence rate of the HSS iteration. We remark that there may be other efficient methods for solving the model convection-diffusion equation (see [12, 13, 6]).

For a three-dimensional convection-diffusion system of linear equations arising from performing one step of cyclic reduction on an equidistant mesh, discretized by the centered and the upwind difference schemes, Greif and Varah [9, 10] considered two ordering strategies, analyzed block splittings of the coefficient matrices, and showed that the associated block Jacobi iterations converge for both the one-dimensional and the two-dimensional splittings with their spectral radii bounded by

$$1 - \left(\frac{10}{9}\pi^2 + \frac{1}{6}q^2\right)h^2 + O(h^3) \quad \text{and} \quad 1 - \left(2\pi^2 + \frac{9}{10}q^2\right)h^2 + O(h^3),$$

respectively. It is clear that these two bounds are larger than those of the HSS and the IHSS methods. Moreover, for the three-dimensional convection-diffusion model equation, the number of operations required for each step of the block Jacobi iteration is about $O(n^3)$ operations, and hence its total complexity is about $O(n^5)$ operations. We remark that their methods can provide an ordering for block Jacobi which can be used for preconditioning.

5. Numerical examples. In this section, we perform some numerical examples to demonstrate the effectiveness of both HSS and IHSS iterations.

5.1. Spectral radius. In this subsection, we first show in Figures 1 and 2 the spectral radius $\rho(M(\alpha))$ of the iteration matrix $M(\alpha)$ and its upper bound $\sigma(\alpha)$ for different α. Here the coefficient matrices A arise from the discretization of the differential equation

$$-u'' + qu' = 0$$

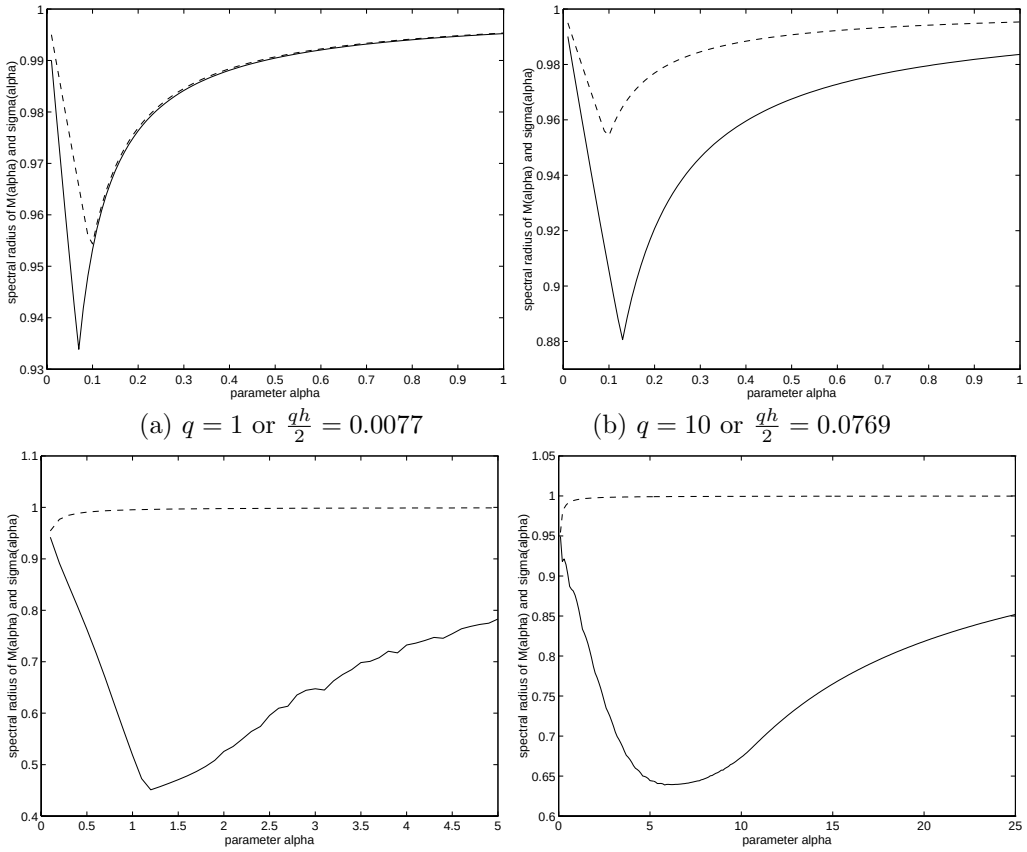
with the homogeneous boundary condition using the centered and the upwind difference schemes. In the tests, the size of the matrix A is 64-by-64. We see from the figures that both $\rho(M(\alpha))$ and $\sigma(\alpha)$ are always less than 1 for $\alpha > 0$. These results show that the HSS iteration always converges. Moreover, when q (or $qh/2$) is small, $\sigma(\alpha)$ is close to $\rho(M(\alpha))$, i.e., $\sigma(\alpha)$ is a good approximation to $\rho(M(\alpha))$. However, when q (or $qh/2$) is large (the skew-Hermitian part is dominant), $\sigma(\alpha)$ deviates from $\rho(M(\alpha))$ very much. From Figures 1 and 2, we see that the optimal parameter α_t,

$$\alpha_t \equiv \arg \min_{\alpha}\{\rho(M(\alpha))\},$$

is roughly equal to $qh/2$. To further investigate $\sigma(\alpha)$, we examine the parameter α in the HSS iteration in Figure 3. In the figure, we depict the spectral radii of the iteration matrices for different q (or $qh/2$) by using α^* in Corollary 2.3, $\tilde{\alpha} = qh/2$, and the optimal parameter α_t. It is clear that, when q (or $qh/2$) is small (i.e., the skew-Hermitian part is not dominant), α^* is close to α_t, and $M(\alpha^*)$ is a good estimate of $M(\alpha_t)$. However, when q (or $qh/2$) is large, α^* is not very useful; see Table 2. In contrast to α^*, we observe that $\tilde{\alpha}$ is close to α_t when q (or $qh/2$) is large. In the appendix, we give a remark to further explain why the spectral radius of $M(\tilde{\alpha})$ is less than $\sigma(\alpha^*)$ by using a 2-by-2 matrix example.

In Figure 4, we depict the eigenvalue distributions of the iteration matrices using α_t when $q = 1, 10, 100, 1000$. We see that the spectral radius of the iteration matrix for large q is less than that of the iteration matrix for small q.

5.2. Results for the HSS iteration. In this subsection, we test the HSS iteration by numerical experiments. All tests are started from the zero vector, performed



(a) $q = 1$ or $\frac{qh}{2} = 0.0077$ (b) $q = 10$ or $\frac{qh}{2} = 0.0769$

(c) $q = 100$ or $\frac{qh}{2} = 0.7692$ (d) $q = 1000$ or $\frac{qh}{2} = 7.6923$

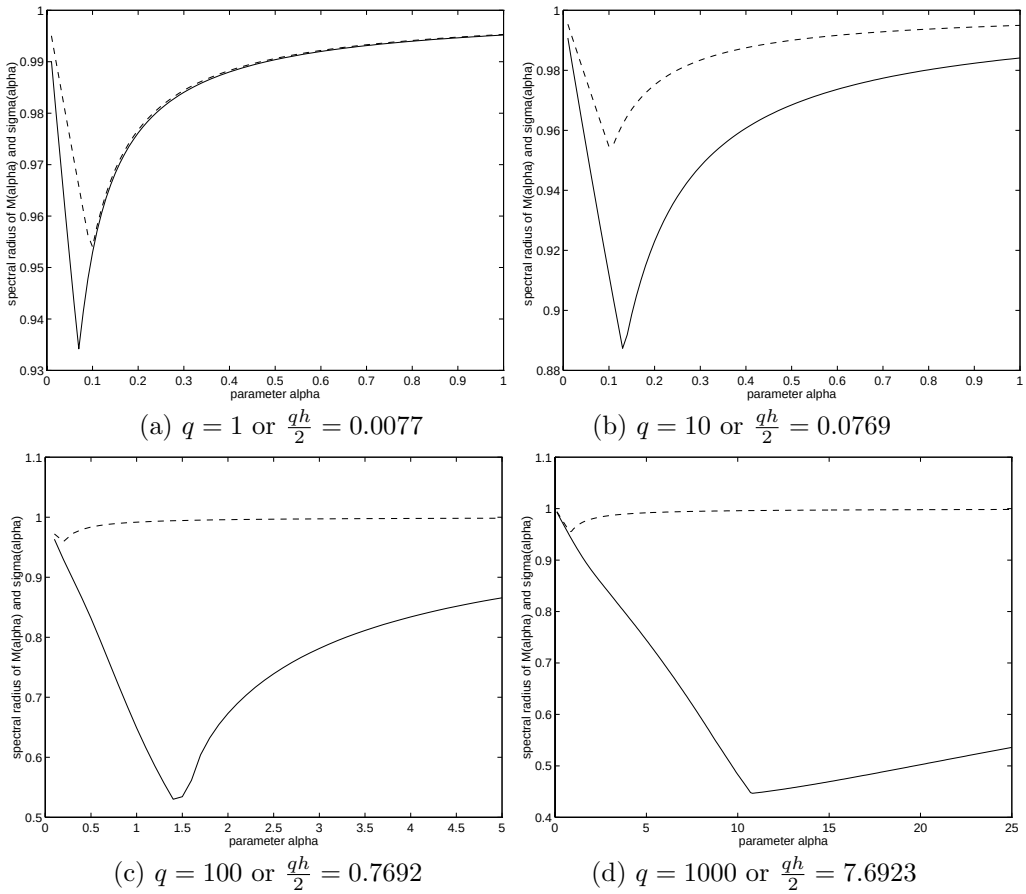
FIG. 1. *The spectral radius $\rho(M(\alpha))$ of the iteration matrices for different α: "——" and the upper bound $\sigma(\alpha)$ for different α: "- - - -" (centered difference scheme).*

TABLE 2
The spectral radii of the iteration matrices $M(\alpha^*)$, $M(\tilde{\alpha})$, and $M(\alpha_t)$ when $n = 64$.

Difference scheme	q	α^*	$\rho(M(\alpha^*))$	$\tilde{\alpha}$	$\rho(M(\tilde{\alpha}))$	α_t	$\rho(M(\alpha_t))$
centered	1	0.0966	0.9516	0.0077	0.9923	0.0700	0.9339
centered	10	0.0966	0.9086	0.0769	0.9264	0.1300	0.8807
centered	100	0.0966	0.9438	0.7692	0.6339	1.160	0.4487
centered	1000	0.0966	0.9511	7.6923	0.6445	5.800	0.6389
upwind	1	0.0974	0.9517	0.0077	0.9924	0.0700	0.9342
upwind	10	0.1041	0.9085	0.0769	0.9314	0.1300	0.8874
upwind	100	0.1710	0.9388	0.7692	0.7321	1.450	0.5237
upwind	1000	0.8399	0.9447	7.6923	0.6092	10.75	0.4466

in MATLAB with machine precision 10^{-16}, and terminated when the current iterate satisfies $\|r^{(k)}\|_2/\|r^{(0)}\|_2 < 10^{-6}$, where $r^{(k)}$ is the residual of the kth HSS iteration.

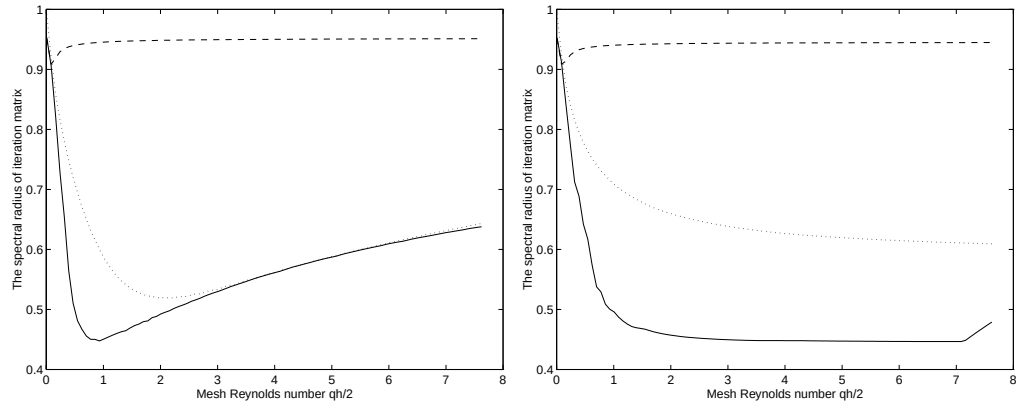
We solve the three-dimensional convection-diffusion equation (4.1) with the homogeneous Dirichlet boundary condition by the HSS iteration. The number n of grid points in all three directions is the same, and the n^3-by-n^3 linear systems with respect to the coefficient matrices $\alpha I + H$ and $\alpha I + S$ are solved efficiently by the sine and



(a) $q = 1$ or $\frac{qh}{2} = 0.0077$ (b) $q = 10$ or $\frac{qh}{2} = 0.0769$

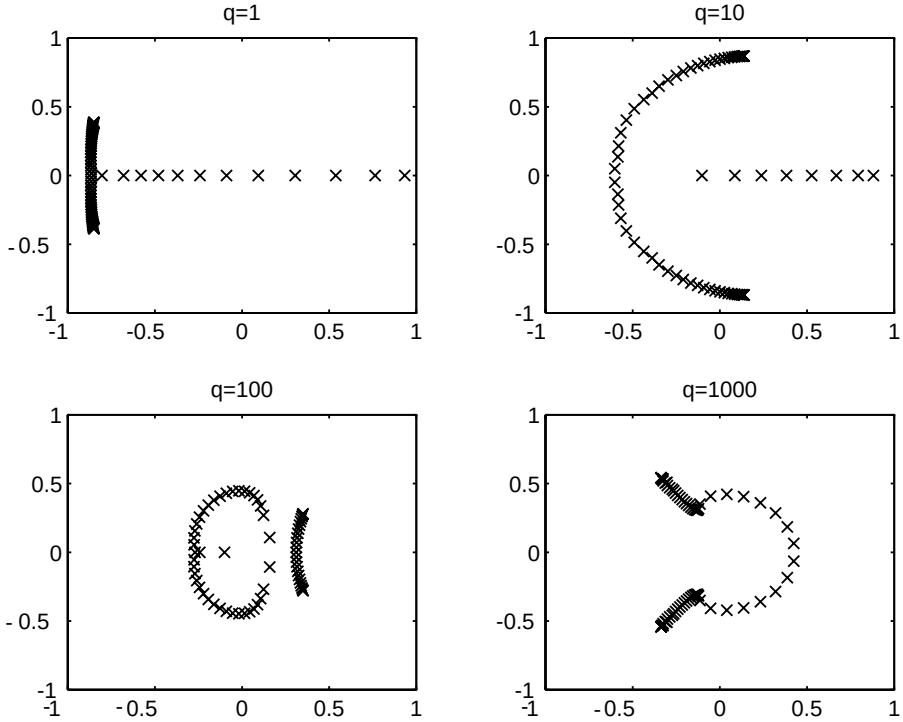
(c) $q = 100$ or $\frac{qh}{2} = 0.7692$ (d) $q = 1000$ or $\frac{qh}{2} = 7.6923$

FIG. 2. *The spectral radius $\rho(M(\alpha))$ of the iteration matrices for different α: "——" and the upper bound $\sigma(\alpha)$ for different α: "- - - -" (upwind difference scheme).*

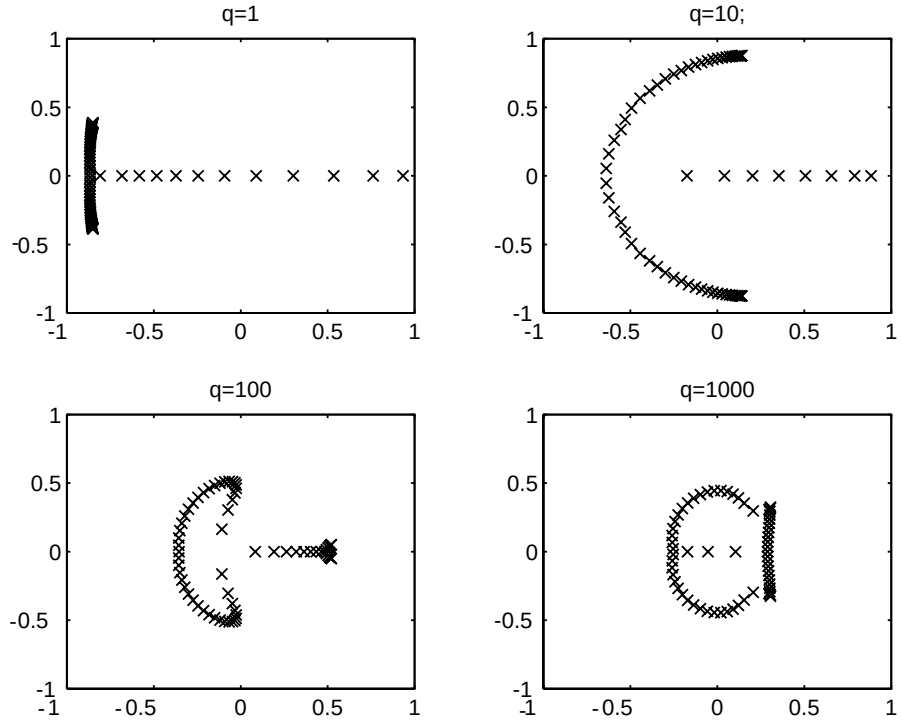


centered difference scheme upwind difference scheme

FIG. 3. *The spectral radius of the iteration matrices for different q: using α_t "——," α^* in Corollary 2.3 "- - - -," and $\tilde{\alpha} = qh/2$ "....."*



(a) centered difference scheme



(b) upwind difference scheme

FIG. 4. *The eigenvalue distributions of the iteration matrices when* $\alpha = \alpha_t$.

TABLE 3

Number of HSS iterations for the centered (left) and the upwind (right) difference schemes using α^* in Corollary 2.3.

	q			
n	1	10	100	1000
8	34	23	34	35
16	61	42	59	62
32	116	83	117	123
64	234	169	231	244

	q			
n	1	10	100	1000
8	33	22	27	28
16	59	42	52	53
32	114	82	102	109
64	226	158	205	228

TABLE 4

Number of HSS iterations for the centered (left) and the upwind (right) difference schemes using $\tilde{\alpha} = qh/2$.

	q			
n	1	10	100	1000
8	208	28	25	193
16	433	52	22	106
32	844	102	25	76
64	>1000	195	33	66

	q			
n	1	10	100	1000
8	220	40	22	20
16	446	63	26	22
32	852	115	33	25
64	>1000	208	48	33

TABLE 5

Number of HSS iterations for the centered (left) and the upwind (right) difference schemes using the optimal α_t.

	q			
n	1	10	100	1000
8	33	16	20	37
16	58	31	21	48
32	113	57	25	46
64	221	105	33	51

	q			
n	1	10	100	1000
8	33	22	15	15
16	59	35	18	18
32	114	63	26	23
64	204	109	40	33

the modified sine transforms, respectively (cf. Lemma A.1). In Table 3, we list the numerical results for the centered difference and the upwind difference schemes when $q = 1, 10, 100, 1000$. Evidently, when q is large, the cell Reynolds number is also large for each fixed n. Since the eigenvalues of H are known, the parameter α^* can be computed according to Corollary 2.3. We observe that the number of iterations is not only increasing linearly with n but also roughly independent of q as predicted from the convergence analysis in Corollary 2.3. We also test $\tilde{\alpha}$ and the optimal α given in Table 2. In Tables 4 and 5, we present their numbers of HSS iterations. We see from the tables that the number of iterations using the optimal α is less than that using α^* especially when q is large. Moreover, when q is large, the numbers of iterations using the optimal α and $\tilde{\alpha}$ are about the same.

5.3. Results for IHSS iterations. The second test is for the three-dimensional convection-diffusion equation

$$-(u_{xx} + u_{yy} + u_{zz}) + q \exp(x + y + z)(xu_x + yu_y + zu_z) = f(x, y, z)$$

on the unit cube $\Omega = [0, 1] \times [0, 1] \times [0, 1]$, with the homogeneous Dirichlet boundary conditions. For this problem, the n^3-by-n^3 linear systems with respect to the coefficient matrices $\alpha I + H$ and $\alpha I + S$ cannot be solved efficiently by the sine and the modified sine transforms. Therefore, we solve the linear systems with coefficient matrices $\alpha I + H$ iteratively by the preconditioned CG (PCG) method with the sine transform based preconditioner presented in [22], and we solve the linear systems

TABLE 6
Number of IHSS iterations for the centered difference scheme using α^* in Table 3.

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	38	37	36	25	21	21	28	28	28	35	39	35
16	72	65	60	45	45	38	55	55	54	59	59	59
32	171	160	142	91	86	84	105	104	103	114	114	114
64	462	339	298	249	210	172	205	202	202	237	233	233

TABLE 7
Number of IHSS iterations for the centered difference scheme using the optimal α_t in Table 5.

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	42	41	41	24	24	24	17	17	17	35	35	35
16	78	71	68	42	38	38	34	34	34	43	41	41
32	167	146	136	81	75	73	60	60	60	44	44	44
64	453	355	292	161	150	137	116	116	116	54	54	54

with the coefficient matrix $\alpha I + S$ iteratively by the preconditioned CG for normal equations (PCGNE) method with the modified sine transform based preconditioner given in [19]. This results in the IHSS iteration discussed in section 3. We choose CGNE as the inner solver because it is quite stable, convergent monotonically, and transpose-free. Therefore, as an inner iteration, it could produce an approximate solution satisfying a prescribed rough accuracy in a few iteration steps.

In our computations, the inner PCG and PCGNE iterates are terminated if the current residuals of the inner iterations satisfy

$$\frac{\|p^{(j)}\|_2}{\|r^{(k)}\|_2} \le \max\{0.1\delta^k, 1\times 10^{-7}\} \quad \text{and} \quad \frac{\|q^{(j)}\|_2}{\|r^{(k)}\|_2} \le \max\{0.1\delta^k, 1\times 10^{-6}\} \tag{5.1}$$

(cf. (3.19) and (3.20) in Theorem 3.3), where $p^{(j)}$ and $q^{(j)}$ are, respectively, the residuals of the jth inner PCG and iterates at the $(k+1)$st outer IHSS iterate, $r^{(k)}$ is the residual of the kth outer IHSS iterate, and δ is a control tolerance. In Tables 6–9, we list numerical results for the centered difference and the upwind difference schemes when $q = 1, 10, 100, 1000$. Since the eigenvalues of H cannot be explicitly obtained, the parameter α^* is not exactly known, and we employ the corresponding parameters used in HSS iterations in Tables 3 and 5 instead.

According to Tables 6–9, the number of IHSS iterations generally increases when δ increases. We see that these increases in IHSS iterations for small q are more significant than those for large q. We also observe that the number of IHSS iterations again increases linearly with n and roughly independent of q. In the tables, the number of iterations using the optimal α is again less than that using α^*, especially when q is large. Moreover, when the optimal α is used, the number of IHSS iterations is about the same for $q = 1, 10, 100, 1000$.

In Table 10, we list the average number of inner PCGNE iterations corresponding to the centered difference scheme. In this case, the Hermitian linear systems with the coefficient matrix $\alpha I + H$ can be solved efficiently by the sine transform. Therefore, we report only the average number of inner PCGNE iterations. In Tables 11 and 12, we report the average number of inner PCG and inner PCGNE iterations corresponding to the upwind difference scheme. It is obvious that, when the control parameter

TABLE 8
Number of IHSS iterations for the upwind difference scheme using α^* in Table 3.

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	33	33	32	24	23	23	27	26	26	28	28	28
16	78	68	68	46	42	42	63	61	60	70	70	69
32	171	155	129	103	87	82	131	127	127	166	164	164
64	460	348	306	263	180	164	248	248	246	370	367	366

TABLE 9
Number of IHSS iterations for the upwind difference scheme using the optimal α_t in Table 5.

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	42	35	35	24	24	22	30	30	30	29	29	29
16	80	70	70	44	44	44	48	48	48	59	59	59
32	165	144	131	83	82	80	85	85	85	95	95	95
64	316	258	239	179	143	141	137	137	137	143	143	143

TABLE 10
Average number of PCGNE iterations for the centered difference scheme using (a) *α^* in Table 3 and* (b) *the optimal α_t in Table 5.*

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	1.4	1.8	2.3	3.4	4.0	4.5	6.8	7.1	7.4	6.9	7.0	7.4
16	2.0	2.8	3.5	5.9	7.4	8.6	13.9	14.6	14.9	15.1	15.2	15.2
32	3.5	5.6	6.9	10.2	14.1	17.6	29.0	30.0	30.2	31.7	31.7	31.7
64	7.3	8.5	9.1	22.4	31.2	34.1	60.1	61.9	62.5	55.0	56.8	57.5

(a)

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	1.5	2.0	2.6	2.8	3.4	4.1	4.9	4.9	5.2	6.7	7.2	7.6
16	2.1	3.0	3.8	4.4	5.8	7.1	7.0	8.4	9.6	12.0	13.7	14.5
32	3.3	5.1	6.6	6.7	9.7	12.6	10.7	14.7	17.7	21.1	23.7	27.0
64	7.1	8.5	9.1	10.8	17.1	21.1	16.7	25.8	33.7	29.1	38.4	45.4

(b)

δ becomes small, the average number of inner PCG and inner PCGNE iterations becomes large. We observe from the tables that the average number of inner PCGNE iterations increases with q, but the average number of inner PCG iterations required is almost nonchanging. The reason is that the parameter q in the convection part does not affect the convergence rate of the Hermitian linear system but does affect the convergence rate of the shifted skew-Hermitian linear system. Moreover, the average number of inner PCGNE iterations using the optimal α_t is less than that of those using α^*, especially when q is large.

Moreover, we find that when δ decreases, the number of inner (PCG or PCGNE) iterations required increases in the numerical tests. In Figure 5, we show an example of this general phenomenon. This is mainly because the inner PCG and the inner PCGNE iterates are terminated if the current residuals of the inner iterations satisfy (5.1). When δ is small, more iterations are required to satisfy the stopping criterion.

Furthermore, instead of PCGNE, we solve the linear systems with the coefficient

TABLE 11

Average number of PCG iterations for the upwind difference scheme using (a) α^* *in Table* 3 *and* (b) *the optimal* α_t *in Table* 5.

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	1.5	2.3	3.1	1.3	1.9	2.5	1.4	2.0	2.7	1.4	2.1	2.8
16	2.8	4.3	5.3	2.1	3.1	4.3	2.5	4.0	5.1	2.6	4.4	5.3
32	5.4	6.6	7.0	3.8	5.6	6.4	4.6	6.3	7.0	5.3	6.7	7.2
64	7.9	8.3	8.5	7.1	7.7	8.1	7.0	8.1	8.4	7.6	8.4	8.6

(a)

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	1.3	1.6	2.1	1.0	1.5	1.6	1.0	1.6	2.0	1.0	1.6	1.9
16	1.6	2.3	2.6	1.3	1.9	2.3	1.4	2.0	2.4	1.5	2.2	2.5
32	3.0	3.5	3.6	2.2	3.1	3.4	2.2	3.1	3.4	2.3	3.2	3.5
64	4.3	4.6	4.7	3.8	4.3	4.6	3.4	4.3	4.5	3.5	4.3	4.6

(b)

TABLE 12

Average number of PCGNE iterations for the upwind difference scheme using (a) α^* *in Table* 3 *and* (b) *the optimal* α_t *in Table* 5.

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	1.4	1.7	2.1	2.7	3.2	3.8	4.6	4.9	5.5	4.7	5.2	6.0
16	2.0	2.8	3.8	4.9	6.3	7.7	10.4	12.5	13.9	11.6	13.8	14.6
32	3.4	5.4	6.5	9.8	13.0	16.0	24.6	28.6	29.8	28.4	29.9	30.5
64	7.3	8.6	9.2	21.9	27.6	32.3	55.8	59.9	61.2	62.5	63.2	63.5

(a)

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	1.5	1.9	2.3	2.9	3.4	4.0	3.1	3.9	4.4	3.6	4.2	4.9
16	2.1	2.9	3.9	3.9	5.4	6.7	5.5	7.4	8.8	6.1	7.9	9.9
32	3.3	5.0	6.5	5.9	9.2	11.9	9.1	13.2	16.8	10.8	15.3	19.8
64	5.1	7.1	8.0	11.3	16.1	20.9	15.3	24.0	31.0	19.7	30.5	38.3

(b)

matrix $\alpha I + S$ iteratively by the preconditioned GMRES method (PGMRES [25, 24]) with the modified sine transform based preconditioner given in [19]. Using the same stopping criterion as for the PCGNE, we report the average number of inner PGMRES iterations in Table 13. We see from Tables 10 and 13 that, when q is small, the average number of inner PCGNE iterations is slightly less than that of inner PGMRES iterations. However, when q is large, the average number of inner PGMRES iterations is less than that of inner PCGNE iterations.

6. Conclusion and remarks. For the non-Hermitian positive definite system of linear equations, we present a class of (inexact) splitting iteration methods based on the HSS of the coefficient matrix and the Krylov subspace iterations such as CG and CGNE, and we demonstrate that these methods converge unconditionally to the unique solution of the linear system. In fact, this work presents a general framework of iteration methods for solving this class of system of linear equations. There are several combinations in the framework of iterations. We can solve the Hermitian

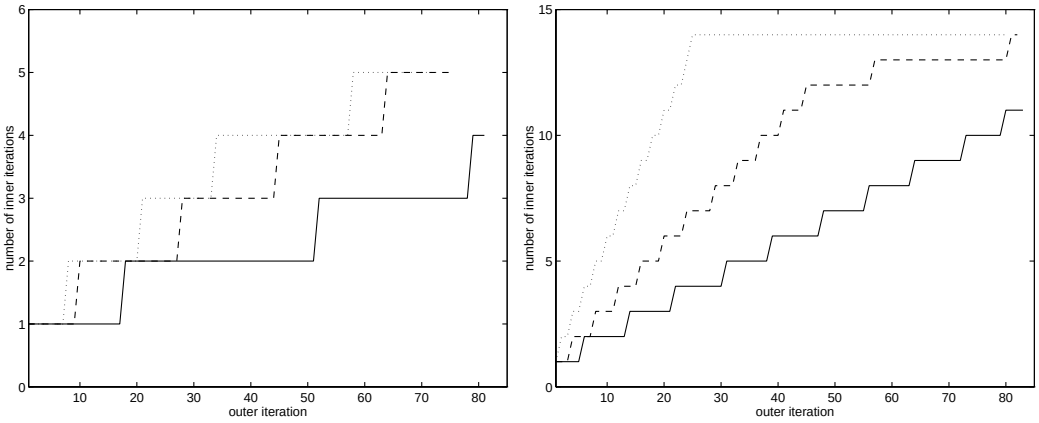


FIG. 5. *The number of inner iterations required for each outer iteration when* $n = 32$ *and* $q = 10$ *in the upwind difference scheme using the optimal* α_t*: (left) PCG inner iterations and (right) PCGNE inner iterations.* —– ($\delta = 0.9$), - - - - ($\delta = 0.8$), ... ($\delta = 0.7$).

TABLE 13

Average number of PGMRES iterations for the centered difference scheme using (a) α^* *in Table* 3 *and* (b) *the optimal* α_t *in Table* 5.

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	1.6	1.9	2.3	4.0	4.3	4.9	6.9	7.1	7.4	6.9	7.1	7.5
16	2.2	2.9	3.6	6.4	7.5	8.6	14.5	14.6	14.9	15.2	15.3	15.5
32	3.7	5.7	7.0	10.9	14.5	17.6	27.8	28.1	30.2	28.5	29.7	30.7
64	7.5	9.1	9.2	23.6	31.3	34.1	48.1	51.3	54.5	48.5	51.8	52.5

(a)

	$q=1$			$q=10$			$q=100$			$q=1000$		
	δ			δ			δ			δ		
n	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7	0.9	0.8	0.7
8	1.8	2.1	2.5	2.8	3.5	4.1	4.9	5.0	5.2	6.8	7.4	7.7
16	2.3	3.0	3.9	4.4	5.8	7.2	7.0	8.5	9.5	12.1	13.9	14.5
32	3.3	5.2	6.7	6.8	9.7	12.7	9.1	12.5	15.1	16.5	18.3	21.0
64	7.3	8.5	9.2	10.8	17.2	21.2	13.3	19.4	24.9	19.9	23.8	33.5

(b)

part exactly or inexactly and the skew-Hermitian part exactly or inexactly. The best choice depends on the structures of the Hermitian and the skew-Hermitian matrices. Convergence theories for the correspondingly resulted exact HSS or IHSS iterations can be established following an analogous analysis to this paper with slight technical modifications.

Moreover, instead of CG and CGNE, we can employ other efficient iterative methods of types of Krylov subspace [24, 7], multigrid, multilevel, classical relaxation, etc. to solve the systems of linear equations with coefficient matrices $\alpha I + H$ and $\alpha I + S$ involved at each step of the HSS iteration. In particular, we mention that, when GMRES is applied to the linear system with coefficient matrix $\alpha I + S$, it automatically reduces to a two-term recurrence process, and its convergence property is dependent only on the eigenvalues, but independent of the eigenvectors, of the matrix $\alpha I + S$.

Appendix. The basic lemma used in the model problem analysis in section 4 is shown in this section.

LEMMA A.1 (see [5, 19]). *The matrix H in (4.3) can be diagonalized by the matrix $F^{(1)} \otimes F^{(1)} \otimes F^{(1)}$. Here $F^{(1)} = ([F^{(1)}]_{j,k})$ is the sine transform matrix defined by*

$$[F^{(1)}]_{j,k} = \sqrt{\frac{2}{n+1}} \sin\left(\frac{jk\pi}{n+1}\right), \quad j,k = 1,2,\ldots,n.$$

The corresponding eigenvalues of H are given by

$$\lambda_{j,k,l}(H) = t_1 + (t_2 + t_3) \cdot \left[\cos\left(\frac{j\pi}{n+1}\right) + \cos\left(\frac{k\pi}{n+1}\right) + \cos\left(\frac{l\pi}{n+1}\right)\right], \quad j,k,l = 1,2,\ldots,n.$$

The matrix S in (4.4) can be diagonalized by the matrix $F^{(2)} \otimes F^{(2)} \otimes F^{(2)}$. Here $F^{(2)} = ([F^{(2)}]_{j,k})$ is the modified sine transform matrix defined by

$$[F^{(2)}]_{j,k} = \sqrt{\frac{2}{n+1}} i^{j+k+1} \sin\left(\frac{jk\pi}{n+1}\right), \quad j,k = 1,2,\ldots,n.$$

The corresponding eigenvalues of S are given by

$$\lambda_{j,k,l}(S) = i(t_2 - t_3) \cdot \left[\cos\left(\frac{j\pi}{n+1}\right) + \cos\left(\frac{k\pi}{n+1}\right) + \cos\left(\frac{l\pi}{n+1}\right)\right], \quad j,k,l = 1,2,\ldots,n.$$

Here i is used to represent the imaginary unit.

Remark. We consider the 2-by-2 matrix

$$A = \begin{pmatrix} 2 + 2\cos(\pi h) & -qh/2 \\ qh/2 & 2 - 2\cos(\pi h) \end{pmatrix}$$

as an example to illustrate the use of the iteration parameter $\alpha = \tilde{\alpha} = qh/2$. It is clear that

$$H = \begin{pmatrix} 2 + 2\cos(\pi h) & 0 \\ 0 & 2 - 2\cos(\pi h) \end{pmatrix} \quad \text{and} \quad S = \begin{pmatrix} 0 & -qh/2 \\ qh/2 & 0 \end{pmatrix}.$$

We note that $2+2\cos(\pi h)$ and $2-2\cos(\pi h)$ are the largest and the smallest eigenvalues, respectively, of the Hermitian part of the discretization matrix of the differential equation $-u'' + qu' = 0$. In this case, the iteration matrix $M(\alpha)$ of the HSS iteration is similar to the matrix

$$\begin{aligned} \widetilde{M}(\alpha) = & \begin{pmatrix} \alpha - 2 - 2\cos(\pi h) & 0 \\ 0 & \alpha - 2 + 2\cos(\pi h) \end{pmatrix} \\ & \times \begin{pmatrix} \alpha + 2 + 2\cos(\pi h) & 0 \\ 0 & \alpha + 2 - 2\cos(\pi h) \end{pmatrix}^{-1} \times \begin{pmatrix} \alpha & qh/2 \\ -qh/2 & \alpha \end{pmatrix} \\ & \times \begin{pmatrix} \alpha & -qh/2 \\ qh/2 & \alpha \end{pmatrix}^{-1}. \end{aligned}$$

When $\alpha = \tilde{\alpha} = qh/2$, we have

$$\begin{pmatrix} \alpha & qh/2 \\ -qh/2 & \alpha \end{pmatrix} \times \begin{pmatrix} \alpha & -qh/2 \\ qh/2 & \alpha \end{pmatrix}^{-1} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Then we compute the eigenvalues λ of $\widetilde{M}(\tilde{\alpha})$, and they are given by

$$\pm\sqrt{\frac{(2+2\cos(\pi h)-\frac{qh}{2})(-2+2\cos(\pi h)+\frac{qh}{2})}{(2+2\cos(\pi h)+\frac{qh}{2})(2-2\cos(\pi h)+\frac{qh}{2})}}.$$

By using the series expansion of the above expression in terms of h, we obtain

$$\lambda = \pm\sqrt{\frac{-\pi+\frac{q}{2}}{\pi+\frac{q}{2}}}\cdot\left(1-\frac{qh}{4}+\mathcal{O}(h^2)\right).$$

However, if we use α^* as the iteration parameter, the upper bound $\sigma(\alpha^*)$ of the spectral radius $\rho(M(\alpha^*))$ of the iteration matrix $M(\alpha^*)$ is given by

$$\frac{\sqrt{2+2\cos(\pi h)}-\sqrt{2-2\cos(\pi h)}}{\sqrt{2+2\cos(\pi h)}+\sqrt{2-2\cos(\pi h)}} = 1-\pi h+\mathcal{O}(h^2);$$

see Corollary 2.3. Hence, when $q > 4\pi$, $\rho(M(\tilde{\alpha}))$ is less than $\sigma(\alpha^*)$. From this example, we see that $\tilde{\alpha}$ is a good iteration parameter when q is large. Figure 3 indeed shows that $\tilde{\alpha}$ is close to α_t.

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