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Efficient variants of the CMRH method for solving a sequence of multi-shifted non-Hermitian linear systems simultaneously

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ABSTRACT

Multi-shifted linear systems with non-Hermitian coefficient matrices arise in numerical solutions of time-dependent partial/fractional differential equations (PDEs/FDEs), in control theory, PageRank problems, and other research fields. We derive efficient variants of the restarted Changing Minimal Residual method based on the cost-effective Hessenberg procedure (CMRH) for this problem class. Then, we introduce a flexible variant of the algorithm that allows to use variable preconditioning at each iteration to further accelerate the convergence of shifted CMRH. We analyse the performance of the new class of methods in the numerical solution of PDEs and FDEs, also against other multi-shifted Krylov subspace methods.

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1. Introduction

In this paper we introduce efficient iterative methods for the simultaneous solution of a sequence of, say t , shifted non-Hermitian linear systems of the form

$$(A - \sigma_i I) \mathbf{x}^{(i)} = \mathbf{b}, \quad i = 1, 2, \dots, t, \quad (1.1)$$

where $A \in \mathbb{C}^{n \times n}$ is a large, sparse and nonsingular matrix, $\sigma_i \in \mathbb{C}$ are t shifts given at once, I is the $n \times n$ identity matrix, $\mathbf{x}^{(i)}$ and $\mathbf{b}$ are solutions and right-hand side vectors of the t linear systems, respectively. Problem (1.1) arises

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in implicit numerical solutions of partial differential (PDEs) [1,2] and fractional differential equations (FDEs) [3,4], in control theory [5,6], large-scale eigenvalue computations [7], quantum chromodynamics (QCD) applications [8] and in other computational science problems [9–11].

Krylov subspace methods are an efficient alternative to sparse direct methods for solving a sequence of multi-shifted linear systems, owing to the shift-invariance property

$$\mathcal{K}_m(A, \mathbf{b}) = \mathcal{K}_m(A - \sigma_i I, \mathbf{b}), \quad i = 1, 2, \dots, t, \quad (1.2)$$

where we denote by $\mathcal{K}_m(A, \mathbf{b}) := \text{span}\{\mathbf{b}, A\mathbf{b}, \dots, A^{m-1}\mathbf{b}\}$ the Krylov subspace of dimension m generated by A and $\mathbf{b}$ (see [6,12,13]). By a suitable choice of the initial vectors $\mathbf{x}_0^{(i)}$, for example take $\mathbf{x}_0^{(i)} = 0$, the solution of systems (1.1) requires a single Krylov basis [12,13]. This approach has shown to effectively reduce storage and algorithmic costs in the analysis of realistic QCD, PageRank and multi-frequency elastic wave propagation problems [9–11].

Over the last two decades, several shift-invariant Krylov subspace algorithms have been proposed for solving multi-shifted linear systems with general non-Hermitian coefficient matrices. Shifted extensions of the restarted generalized minimum residual (GMRES) method [14–19], the restarted full orthogonalization (FOM) method [20–22] and the restarted Hessenberg method [23] are some relevant examples built upon the well-known Arnoldi procedure. On the other hand, shifted versions of the quasi-minimal residual (QMR) method and its transpose-free variant (TFQMR) [24], the induced dimension reduction (IDR(s)) [25,26] and its QMR form [27], the biconjugate gradient (BiCG) method and its stabilized and generalized product-type extensions (BiCGStab, BiCGStab(ℓ) and GPBiCG) [12,13,28], the biconjugate residual (BiCR) method and its stabilized form (BiCRSTAB) [29] are built upon short-term vector recurrences such as the Bi-Lanczos [30, pp. 229–233] and the A-biorthogonalization [31, pp. 40–42] procedures. In [32,33], recycling variants of BiCG and BiCGSTAB have been applied to the solution of multi-shifted non-Hermitian linear systems arising in model reduction applications.

In this paper we consider the Changing Minimal Residual method based on the Hessenberg procedure [34, pp. 377–382] (shortly, CMRH¹) introduced in [37,38]. The method is based on long-term vector recurrences, like Arnoldi. However, each basis vector $\mathbf{l}_i$ has $i - 1$ components equal to zero and only one component equal to one; each matrix–vector product involved in the computation of $\mathbf{l}_i$ costs less than the N_z operations required by the Arnoldi procedure, where N_z is the number of nonzero entries of A . Therefore, the method can be cost-effective especially when large Krylov subspaces are generated [23,35–37,39]. It has been shown that CMRH and GMRES [40] convergence curves are often comparable [37,38,41]. On problems where GMRES exhibits superlinear convergence, so often does CMRH; when GMRES stagnates, CMRH does so as well. We point the reader to [41,42] for further discussions, and to [43–45] for some recent developments on the theoretical and algorithmic aspects of the CMRH method [36,44,46], including efficient parallel implementations [37].

We propose an extension of (restarted) CMRH for solving multi-shifted linear systems which preserves the shift-invariance property of Krylov subspaces by forcing the shifted residuals to be collinear to the *seed* system residual at every cycle, at moderate extra storage and arithmetic operations. It is well known that the use of a preconditioner is essential to accelerate the convergence of Krylov subspace solvers. Many conventional preconditioning techniques are not suitable for solving shifted linear systems as they do not ensure that property (1.2) holds for the preconditioned systems [6,12,23,26]. We present an inner–outer iterative scheme based on nested Krylov subspace methods, where the inner solver is a multi-shifted Krylov method such as shifted FOM, shifted IDR(s), shifted QMRIDR(s) or shifted BiCGSTAB(ℓ) methods that acts as a preconditioner for an outer flexible CMRH (FCMRH) solver [43].

The rest of the current paper is organized as follows. In Section 2, we briefly review the (restarted) CMRH method and we extend it to the solution of multi-shifted linear systems. In Section 3, we derive a restarted shifted CMRH method that preserves the shift-invariance property of Krylov subspaces by forcing the shifted residuals to be collinear to the *seed* system residual at every cycle. Implementation details and algorithmic complexity of the new method are discussed. In Section 4, we propose a cost-effective nested Krylov subspace method based on shifted CMRH for solving multi-shifted linear systems. Section 5 presents numerical evidence of the potential of the new family of methods to solve efficiently shifted linear systems arising from QCD and from the solutions of PDEs/FDEs. In Section 6, the paper closes with some final remarks.

2. The CMRH method for shifted linear systems

In this section, we briefly review the restarted CMRH method for solving general non-Hermitian linear systems $A\mathbf{x} = \mathbf{b}$; then, we extend it to the solution of problem (1.1).

¹ A short note described the relation between the ELMRES method [35,36] and Sadok's CMRH method is available at http://ncsu.edu/hpc/Documents/Publications/gary_howell/contents.html#codes.

2.1. The CMRH method

The CMRH algorithm for non-Hermitian systems applies the Hessenberg procedure with pivoting,² to compute a basis of the Krylov subspace $\mathcal{K}_m(A, \mathbf{r}_0)$. Starting from an initial vector $\mathbf{l}_1 = \mathbf{r}_0/\alpha$, where $\alpha = (\mathbf{r}_0)_1$ is the first entry of $\mathbf{r}_0$, m steps of the Hessenberg procedure yield a basis $\{\mathbf{l}_1, \mathbf{l}_2, \dots, \mathbf{l}_m\}$ and a matrix decomposition of the form

$$A\mathbf{l}_m = L_{m+1}\check{H}_m, \quad (2.1)$$

where $L_m = (\mathbf{l}_1, \mathbf{l}_2, \dots, \mathbf{l}_m)$ is an $n \times m$ unit lower trapezoidal matrix and $\check{H}_m \in \mathbb{C}^{(m+1) \times m}$ is upper Hessenberg. The CMRH approximation after m steps writes as $\mathbf{x}_m = \mathbf{x}_0 + \mathbf{z}_m$, where $\mathbf{z}_m \in \mathcal{K}_m(A, \mathbf{r}_0)$ solves the following constrained minimization problem

$$\min_{\mathbf{u} \in \mathbb{C}^{m+1}, \mathbf{z} \in \mathcal{K}_m(A, \mathbf{r}_0)} \|\mathbf{u}\|_2, \quad \text{subject to } A\mathbf{z} = \mathbf{r}_0 + L_{m+1}\mathbf{u}. \quad (2.2)$$

Since the columns of L_{m+1} are not orthogonal, vector $\mathbf{z}_m$ cannot be computed by minimizing directly the residual norm $\|\mathbf{u}\|_2$ in Eq. (2.2). Instead, CMRH computes $\mathbf{z}_m$ by minimizing the quasi-residual norm

$$\min_{\mathbf{z} \in \mathcal{K}_m(A, \mathbf{r}_0)} \|L_{m+1}^\dagger(A\mathbf{z} - \mathbf{r}_0)\|_2, \quad (2.3)$$

similarly to the well-known QMR method [30, pp. 236–241]. In Eq. (2.3), we denote by $L_{m+1}^\dagger$ the pseudo-inverse of L_{m+1} ; however, note that any left inverse of L_{m+1} would work here [41]. Problem (2.3) can be interpreted as a standard residual minimization using a semi-norm [37,38]. By writing $\mathbf{z} = L_m\mathbf{y} \in \mathcal{K}_m(A, \mathbf{r}_0)$, Eq. (2.3) is implemented in CMRH as the following small least squares problem

$$\begin{aligned} \min_{\mathbf{y} \in \mathbb{C}^m} \|L_{m+1}^\dagger(\mathbf{r}_0 - A\mathbf{l}_m\mathbf{y})\|_2 &= \min_{\mathbf{y} \in \mathbb{C}^m} \|L_{m+1}^\dagger(\alpha L_{m+1}\mathbf{e}_1^{(k+1)} - L_{m+1}\check{H}_m\mathbf{y})\|_2 \\ &= \min_{\mathbf{y} \in \mathbb{C}^m} \|\alpha\mathbf{e}_1^{(k+1)} - \check{H}_m\mathbf{y}\|_2. \end{aligned} \quad (2.4)$$

A detailed theoretical analysis of the method can be found in [37,38]. In particular, the result below compares the residual norms computed after m iterations of the CMRH and the GMRES methods:

Theorem 2.1 ([37, Theorem 4] and [41, Theorem 1]). Let $\mathbf{r}_m^G$ and $\mathbf{r}_m^C$ be the GMRES and CMRH residuals at the m th iteration beginning with the same initial residual $\mathbf{r}_0$ (e.g., $\mathbf{r}_0 = \mathbf{b}$), respectively. Then

$$\|\mathbf{r}_m^G\|_2 \leq \|\mathbf{r}_m^C\|_2 \leq \kappa(L_{m+1})\|\mathbf{r}_m^G\|_2,$$

where $\kappa(L_{m+1}) = \|L_{m+1}\|_2\|L_{m+1}^\dagger\|_2$ is the condition number of L_{m+1} .

Duintjer Tebbens and Meurant have proved that any non-increasing residual norm history is possible for the CMRH method with any set of nonzero eigenvalues of the system matrix [42]. Therefore, the distribution of the eigenvalues alone may not play any role in the convergence. However, similarly to other Krylov methods, for many problems and applications a tightly clustered spectrum around a single point away from the origin is favourable to achieve fast convergence, whereas widely spread eigenvalues and/or clusters close to zero are often bad. Being based on long-term vector recurrences, like GMRES also CMRH may need to be restarted to control the growing costs of the Hessenberg procedure. To date, much fewer results are available on the convergence of the restarted CMRH algorithm (referred to as CMRH(m)).

2.2. The CMRH method for shifted systems

The starting point to develop a shift-invariant extension of the CMRH method for solving a sequence of multi-shifted linear systems is the shifted Hessenberg relation

$$(A - \sigma_i I)L_m = L_{m+1}\check{H}_m(\sigma_i), \quad \check{H}_m(\sigma_i) := \check{H}_m(\sigma_{seed}) - \sigma_i \begin{bmatrix} I_m \\ \mathbf{0} \end{bmatrix} \in \mathbb{C}^{(m+1) \times m}, \quad (2.5)$$

where I_m is the identity matrix of order m , and $L_m, \check{H}_m(\sigma_{seed})$ are factors of the matrix decomposition (2.1) independent of σ_i . By no lack of generality we can assume that the shift of seed system is zero, i.e. $\sigma_{seed} = 0$; otherwise, if $\sigma_{seed} \neq 0$, we can rewrite Eq. (1.1) for $A := A - \sigma_{seed}I$ and $\sigma_i := \sigma_i - \sigma_{seed}$.

By using relation (2.5), the following shift-dependent CMRH quasi-minimization problem equivalent to Eq. (2.4) is derived

$$\min_{\mathbf{y} \in \mathbb{C}^m} \|L_{m+1}^\dagger \mathbf{r}_m^{(i)}\|_2 = \min_{\mathbf{y} \in \mathbb{C}^m} \|\alpha\mathbf{e}_1 - \check{H}_m(\sigma_i)\mathbf{y}\|_2. \quad (2.6)$$

² According to Refs. [23,35,36] it cannot be proved that the Hessenberg procedure with pivoting strategy is backward stable in finite precision arithmetic. However, in most of our experiments the backward error is very small.

The small-size least squares problem (2.6) can be solved in $\mathcal{O}(m^2)$ operations for each shift σ_i . Therefore, the most time-consuming part of the algorithm remains the construction of the Krylov basis L_m , but this has to be performed only once. Since the initial residuals must be shift independent, $\mathbf{x}_0 = \mathbf{0}$ should be used as initial vector for all shifted systems. Then, the whole sequence (1.1) can be solved simultaneously without additional matrix–vector products in terms of the seed system.

3. The restarted shifted CMRH method

In this section, we present the restarted version of the shifted CMRH algorithm, and a convergence analysis. We conclude the section with a complexity study of the new method compared to the restarted shifted GMRES solver.

3.1. The restarted shifted CMRH method

Shifted CMRH developed in Section 2.2 may suffer from memory problems in the case long vector recurrences are generated by the Hessenberg procedure, similarly to its unshifted counterpart. To alleviate such costs, it may be necessary to restart the algorithm after every, say m , Hessenberg steps. Upon restarting, the residual vectors $\mathbf{r}_m^{(i)}$ obtained from the quasi-minimum residual condition are not collinear in general, and therefore the shift-invariance property (1.2) may not be maintained. We impose on the *add* systems the collinearity condition used by Frommer and Glässner in the restarted shifted GMRES method [14], namely

$$\mathbf{r}_m^{(i)} = \gamma_m^{(i)} \mathbf{r}_m, \quad \gamma_m^{(i)} \in \mathbb{C}, \quad (3.1)$$

where $\mathbf{r}_m := \mathbf{r}_m^{(\sigma_{seed})}$ is the residual vector of *seed* system, to ensure that property (1.2) continues to hold at restart. For *seed* system, however, the same quasi-minimum residual condition enforced on the residual vector by the restarted shifted CMRH method is used. The following minimization problem is solved for the seed system

$$\mathbf{y}_m = \arg \min_{\mathbf{y} \in \mathbb{R}^m} \|\alpha \mathbf{e}_1 - \check{H}_m \mathbf{y}\|_2,$$

where $\check{H}_m := \check{H}_m(\sigma_{seed})$ from Eq. (2.5) and $\mathbf{y}_m := \mathbf{y}_m^{(\sigma_{seed})}$. The residual vector $\mathbf{r}_m$ appearing in Eq. (3.1) can be written as

$$\mathbf{r}_m = L_{m+1} \mathbf{u}_{m+1}, \quad \mathbf{u}_{m+1} := \alpha \mathbf{e}_1 - \check{H}_m \mathbf{y}_m \in \mathbb{R}^{m+1}.$$

Then, from the collinearity condition (3.1), it follows for the *add* systems

$$\begin{aligned} \mathbf{r}_m^{(i)} = \gamma_m^{(i)} \mathbf{r}_m &\Leftrightarrow \mathbf{b} - A(\sigma_i)(\mathbf{x}_0^{(i)} + L_m \mathbf{y}_m^{(i)}) = \gamma_m^{(i)} L_{m+1} \mathbf{u}_{m+1} \\ &\Leftrightarrow \mathbf{r}_0^{(i)} - A(\sigma_i) L_m \mathbf{y}_m^{(i)} = L_{m+1} \mathbf{u}_{m+1} \gamma_m^{(i)} \\ &\Leftrightarrow \gamma_0^{(i)} \mathbf{r}_0 - L_{m+1} \check{H}_m(\sigma_i) \mathbf{y}_m^{(i)} = L_{m+1} \mathbf{u}_{m+1} \gamma_m^{(i)} \\ &\Leftrightarrow L_{m+1} (\check{H}_m(\sigma_i) \mathbf{y}_m^{(i)} + \mathbf{u}_{m+1} \gamma_m^{(i)}) = \gamma_0^{(i)} \mathbf{r}_0 \\ &\Leftrightarrow \check{H}_m(\sigma_i) \mathbf{y}_m^{(i)} + \mathbf{u}_{m+1} \gamma_m^{(i)} = \gamma_0^{(i)} \alpha \mathbf{e}_1 \end{aligned}$$

using the matrix representation of the Hessenberg procedure; see [14,47] for details.

From the above relation, $\mathbf{y}_m^{(i)}$ and $\gamma_m^{(i)}$ can be read as solutions of the $(m+1) \times (m+1)$ linear systems

$$\begin{bmatrix} \check{H}_m(\sigma_i) & | & \mathbf{u}_{m+1} \end{bmatrix} \begin{bmatrix} \mathbf{y}_m^{(i)} \\ \gamma_m^{(i)} \end{bmatrix} = \gamma_0^{(i)} \alpha \mathbf{e}_1, \quad (3.2)$$

for $i = 1, 2, \dots, t_s$. Systems (3.2) are upper Hessenberg, and are solved efficiently using Givens rotations. The complete restarted shifted CMRH method is summarized in Algorithm 1.

The following convergence result can be given for the restarted shifted CMRH method.

Theorem 3.1. *If the coefficient matrix A is positive definite, i.e., $(A\mathbf{x}, \mathbf{x}) > 0, \forall \mathbf{x} \neq \mathbf{0}$, and $\sigma_i < 0$ for all i , and if the restarted CMRH method converges for the seed system, then the restarted shifted CMRH method also converges for the add systems for every restart frequency m . Moreover, we have*

$$\|\mathbf{r}_{j,m}^{(i)}\|_2 \leq |\gamma_0^{(i)}| \cdot \|\mathbf{r}_{j,m}\|_2 \quad (3.3)$$

for all j , where $\mathbf{r}_{j,m}^{(i)}$ and $\mathbf{r}_{j,m}$ represent the j th residual vectors for the *add* and the *seed* systems in a generic cycle, respectively.

Proof. Let ζ be any zero of the CMRH residual polynomial [45] after m iterations, φ_m . Since $\varphi_m(0) = 1$, it is $\zeta \neq 0$ and we can write

$$\varphi_m(t) = \left(1 - \frac{t}{\zeta}\right) \tau_{m-1}(t),$$

Algorithm 1 The restarted shifted CMRH method with pivoting

Input: the coefficient matrix A (or a user-defined function that applies A to a vector); the right-hand side vector $\mathbf{b}$; the set of shifts $\{\sigma_i\}_{i=1,\dots,t}$; the dimension m of the Krylov subspace; the maximum number of outer iterations, maxit .

Output: the set of solution vectors $\mathbf{x}^{(i)}$ of the sequence of multi-shifted linear systems.

- 1: Choose the restart dimension m and the initial guess $\mathbf{x}_0, \mathbf{r}_0$ such that $\mathbf{r}_0^{(i)} = \gamma_0^{(i)} \mathbf{r}_0$, e.g. $\mathbf{x}_0 = \mathbf{x}_0^{(i)} = \mathbf{0}$ (also implies that $\gamma_0^{(i)} = 1$)
- 2: Set $\mathbf{q} = [1, 2, \dots, n]^T$ and determine j_0 such that $|(\mathbf{r}_0)_{j_0}| = \|\mathbf{r}_0\|_\infty$
- 3: Set $\alpha = (\mathbf{r}_0)_{j_0}$, $\mathbf{l}_1 = \mathbf{r}_0/\alpha$ and $(\mathbf{q})_1 \leftrightarrow (\mathbf{q})_{j_0}$, where $\leftrightarrow$ is used to swap contents.
- 4: **for** $j = 1, 2, \dots, m$, **do**
- 5: Compute $\mathbf{u} = A\mathbf{l}_j$
- 6: **for** $k = 1, 2, \dots, j$, **do**
- 7: $\check{h}_{k,j} = (\mathbf{u})_{(\mathbf{q})_k}$
- 8: $\mathbf{u} = \mathbf{u} - \check{h}_{k,j}\mathbf{l}_k$
- 9: **end for**
- 10: **if** $j < n$ and $\mathbf{u} \neq \mathbf{0}$ **then**
- 11: Determine $j_0 \in \{j+1, \dots, n\}$ such that $|(\mathbf{u})_{(\mathbf{q})_{j_0}}| = \|(\mathbf{u})_{(\mathbf{q})_{j+1:(\mathbf{q})_n}\|_\infty$
- 12: $\check{h}_{j+1,j} = (\mathbf{u})_{(\mathbf{q})_{j_0}}$, $\mathbf{l}_{j+1} = \mathbf{u}/\check{h}_{j+1,j}$; $(\mathbf{q})_{j+1} \leftrightarrow (\mathbf{q})_{j_0}$
- 13: **else**
- 14: $\check{h}_{j+1,j} = 0$; **Stop**
- 15: **end if**
- 16: **end for**
- 17: Define the $(m+1) \times m$ Hessenberg matrix $\hat{H}_m = \{\check{h}_{k,j}\}_{1 \leq k \leq m+1, 1 \leq j \leq m}$ and collect the matrix $L_m = [\mathbf{l}_1, \mathbf{l}_2, \dots, \mathbf{l}_m]$
- 18: Compute $\mathbf{y}_m = \arg \min_{\mathbf{y} \in \mathbb{C}^m} \|\alpha \mathbf{e}_1 - \hat{H}_m \mathbf{y}\|_2$ and set $\mathbf{u}_{m+1} = \alpha \mathbf{e}_1 - \hat{H}_m \mathbf{y}_m$
- 19: $\mathbf{x}_m = \mathbf{x}_0 + L_m \mathbf{y}_m$, $\mathbf{r}_m = \mathbf{r}_0 - AL_m \mathbf{y}_m = L_{m+1} \mathbf{u}_{m+1}$
- 20: **for** $i = 1, 2, \dots, t_s$ **do**
- 21: Solve $[\check{H}_m(\sigma_i) \mid \mathbf{u}_{m+1}] \begin{bmatrix} \mathbf{y}_m^{(i)} \\ \gamma_m^{(i)} \end{bmatrix} = \gamma_0^{(i)} \alpha \mathbf{e}_1$
- 22: $\mathbf{x}_m^{(i)} = \mathbf{x}_0^{(i)} + L_m \mathbf{y}_m^{(i)}$, $\mathbf{r}_m^{(i)} = \mathbf{r}_0^{(i)} - AL_m \mathbf{y}_m^{(i)} = \gamma_m^{(i)} \mathbf{r}_m$
- 23: **end for**
- 24: Restart: if converged then stop; otherwise update $\mathbf{x}_0 := \mathbf{x}_m$, $\mathbf{x}_0^{(i)} := \mathbf{x}_m^{(i)}$, $\mathbf{r}_0 := \mathbf{r}_m$, $\mathbf{r}_0^{(i)} := \mathbf{r}_m^{(i)}$, $\gamma_0^{(i)} := \gamma_m^{(i)}$ and goto step 2–3.

with τ_{m-1} a polynomial of degree $m-1$ such that $\tau_{m-1}(0) = 1$. Denote $\mathbf{w} = \tau_{m-1}(A)\mathbf{r}_0$ and $\mathbf{r} = A\mathbf{w}$. Then

$$\|\varphi_m(A)\mathbf{r}_0\|_2 = \left\| \mathbf{w} - \frac{1}{\zeta} \mathbf{r} \right\|_2.$$

For $\gamma \in \mathbb{C}$, the functional $\|\mathbf{w} - \gamma \mathbf{r}\|_2$ is minimized for

$$\gamma^* = \frac{(\mathbf{r}, \mathbf{w})}{(\mathbf{r}, \mathbf{r})}.$$

Assuming that $\|\varphi_m(A)\mathbf{r}_0\|_2$ has been minimized, the norm $\|L_{m+1}^\dagger \mathbf{r}_m\|_2$ is also minimal due to the inequality $\|L_{m+1}^\dagger \mathbf{r}_m\|_2 \leq \|L_{m+1}^\dagger\|_2 \|\varphi_m(A)\mathbf{r}_0\|_2$. We conclude that

$$\frac{1}{\zeta} = \gamma^* = \frac{(\mathbf{r}, \mathbf{w})}{(\mathbf{r}, \mathbf{r})} = \frac{(\mathbf{r}, A^{-1}\mathbf{r})}{(\mathbf{r}, \mathbf{r})}$$

and $(\mathbf{r}, A^{-1}\mathbf{r})/(\mathbf{r}, \mathbf{r}) = (A^{-H}\mathbf{r}/\|\mathbf{r}\|_2, \mathbf{r}/\|\mathbf{r}\|_2) \in F(A^{-H})$. Here we denote by $F(A)$ the field of values $F(A) = \{(A\mathbf{x}, \mathbf{x})/\|\mathbf{x}\|_2^2 \mid \mathbf{x} \in \mathbb{C}^n, \|\mathbf{x}\|_2 = 1\} \subset \mathbb{C}$.

On the other hand, since A is positive definite and $(A\mathbf{x}, \mathbf{x}) = (A^{-H}\mathbf{y}, \mathbf{y})$ for $\mathbf{y} = A\mathbf{x}$, $F(A^{-H})$ is also contained in the right half-plane like $F(A)$. In conclusion, it holds $\text{Re}\left(\frac{1}{\zeta}\right) > 0$ and thus $\text{Re}(\zeta) > 0$. Since $\sigma_i < 0$, it is $\varphi(\sigma_i) \neq 0$. Similarly to [14, Lemma 2.4] for the restarted shifted GMRES method, this condition ensures that Eq. (3.2) has a unique solution. It follows that the restarted shifted CMRH method converges for both *seed* and *add* systems for each restart frequency m . Finally, Eq. (3.3) can be proved following a similar argument to [14, Theorem 3.3]. $\square$

Table 1

Computational cost of a generic cycle of the shifted versions of GMRES, SGMRES and CMRH.

Index	Shifted GMRES	Shifted SGMRES	Shifted CMRH
$\aleph_1$	$2mNz + (2m^2 + 5m + 3)n$	$2mNz + (2m^2 + 5m + 3)n$	$2mNz + (m + 2)n + m(m + 1)(n - \frac{m-1}{3})$
$\aleph_2$	FLOPs with an Hessenberg matrix H_m^C	FLOPs with an upper triangular matrix R_m	FLOPs with an Hessenberg matrix H_m^C
$\aleph_3$	$t_s(2mn)$	$t_s(2mn)$	$t_s(2mn)$
$\aleph_4$	FLOPs with $[H_m^C(\sigma_i) \mathbf{u}_{m+1}]$	FLOPs with $R_m - \sigma_i[V_m^H \mathbf{r}_{0,1}, I_{m-1}]$	FLOPs with $[H_m^C(\sigma_i) \mathbf{u}_{m+1}]$

 $\aleph_1$ represents the cost of iterates for *seed* system; $\aleph_2$ means the cost of least-squares solve for *seed* system; $\aleph_3$ represents the cost of necessary vector updates; $\aleph_4$ means the cost of least-squares solve for $t_s - 1$ add systems ($i = 1, \dots, t_s - 1$).

Remark: In fact, it is useful to mention that the $\mathcal{O}(m^2)$ operations are needed for coping with the problems in $\aleph_2$ and $\aleph_4$ of those above three solvers, respectively. However, to solve an upper-triangular least-squares problem (or linear system) is still slightly cheaper than to solve an upper-Hessenberg least-squares problem (or linear system).

Remark 1. Analogously to the restarted shifted GMRES method, since $\gamma_0^{(i)} = 1$ from $\mathbf{x}_0 = \mathbf{x}_0^{(i)} = \mathbf{0}$, according to Eq. (3.3) the *add* systems may converge more rapidly than the *seed* system. If not, the shift switching technique³[47,48] can be applied.

Remark 2. In Theorem 3.1, restarted CMRH is supposed to be convergent on the positive definite *seed* system. Unfortunately, there exist very few results in the literature on the convergence of restarted CMRH, even in the positive definite case; the topic is largely unexplored [36,37,41,42,49]. According to our computational experience, restarted shifted CMRH often enjoys similar convergence behaviour to the more costly restarted shifted GMRES method; in our experiments (see Section 5), in some cases it could even handle certain shifted systems where the latter failed.

3.2. Computational cost of the restarted shifted CMRH method

Following the idea introduced in our recent work [19,23], in Table 1 we present a comparative complexity analysis between shifted CMRH(m), shifted GMRES(m) and shifted SGMRES(m) [19] at equal restarting frequency m . The main difference in terms of floating-point operations (FLOPs) between shifted SGMRES(m) and shifted GMRES(m) is due to the cost of applying the Givens rotations in the least-squares solution for *seed* system. Shifted SGMRES(m) often requires less FLOPs than shifted GMRES(m) [19]. On the other hand, shifted CMRH(m) may require less FLOPs than both shifted SGMRES(m) and shifted GMRES(m) that are based on the more costly Arnoldi procedure.

4. Inner-outer variants of CMRH for shifted systems

It is celebrated that preconditioning is an essential ingredient to accelerate the convergence of Krylov subspace methods, including their shifted variants. Without further assumptions on the preconditioners $M(\sigma_i)$ applied to the t linear systems (1.1), the shift-invariant property (1.2) may not be preserved for the preconditioned Krylov subspaces [6,12,26]. One would like to find a matrix M , independent of σ_i , satisfying

$$\mathcal{K}_m(AM^{-1}, \mathbf{b}) = \mathcal{K}_m((A - \sigma_i I)M(\sigma_i)^{-1}, \mathbf{b}), \quad (4.1)$$

so that property (1.2) would hold true in the preconditioned case as well. It is not hard to find that Eq. (4.1) is satisfied if the preconditioned shifted matrix can be written as a shifted preconditioned matrix, that is

$$(A - \sigma_i I)M(\sigma_i)^{-1} = AM^{-1} - \eta_i I. \quad (4.2)$$

Although M is not needed to compute a basis of $\mathcal{K}_m((A - \sigma_i I)M(\sigma_i)^{-1}, \mathbf{b})$, it must be known explicitly to compute the solutions $\mathbf{x}^{(i)}$ of the unpreconditioned system from the knowledge of the solution $\mathbf{y}^{(i)}$ of the right-preconditioned system; see e.g., [50] for details.

Inspired by [9,50], in this work we use flexible preconditioning to solve sequence (1.1). Flexible preconditioning means that a different preconditioner can be applied at every iteration j of an iterative Krylov method, see e.g. [51–53] and our recent work [43,54]. If different preconditioners P_j , $P_j(\sigma)$ are used at every iteration j , a relation similar to Eq. (4.2), namely

$$(A - \sigma_i I)P_j(\sigma_i)^{-1} = \alpha_j(\sigma_i)AP_j^{-1} - \beta_j(\sigma_i)I, \quad (4.3)$$

must hold to ensure the shift invariance property of the preconditioned Krylov subspace given by Eq. (4.1). In Eq. (4.3), α_j and β_j are parameters dependent on the shifts σ_i . At each iteration j , the preconditioner is applied to a vector $\mathbf{v}_j$ in the form

$$(A - \sigma_i I)P_j(\sigma_i)^{-1} \mathbf{v}_j = \alpha_j(\sigma_i)AP_j^{-1} \mathbf{v}_j - \beta_j(\sigma_i) \mathbf{v}_j. \quad (4.4)$$

³ In general, the *seed* system may converge faster than the *add* systems. In this case, for efficient computation, it needs to change the *seed* system into one of the rest systems, this strategy is called the seed switching technique.

Next, we determine conditions on the coefficients α_j 's and β_j 's to ensure that Eqs. (4.3) and (4.4) hold. Preconditioning is applied by using an inner solver in a multi-shift Krylov method, and the preconditioned vectors

$$\mathbf{z}_j = P_j^{-1} \mathbf{v}_j, \quad \mathbf{z}_j^{(i)} = P_j(\sigma_i)^{-1} \mathbf{v}_j,$$

are computed via a truncated multi-shifted Krylov subspace solver. Therefore, the corresponding (inner) residuals are given by

$$\mathbf{r}_j = \mathbf{v}_j - A\mathbf{z}_j = \mathbf{v}_j - AP_j^{-1} \mathbf{v}_j, \quad (4.5)$$

$$\mathbf{r}_j^{(i)} = \mathbf{v}_j - (A - \sigma_i I)\mathbf{z}_j^{(i)} = \mathbf{v}_j - (A - \sigma_i I)P_j(\sigma_i)^{-1} \mathbf{v}_j. \quad (4.6)$$

We require the residuals (4.5)–(4.6) of the inner method to be collinear, i.e.

$$\exists \gamma_j^{(i)} \in \mathbb{C} : \quad \gamma_j^{(i)} \mathbf{r}_j = \mathbf{r}_j^{(i)}. \quad (4.7)$$

Note that the collinearity factors $\gamma_j^{(i)}$ change at each iteration j , for every shift σ_i . Eq. (4.7) is satisfied automatically by methods such as shifted FOM [20–22], shifted BiCGStab [12,13], shifted BiCRStab [29], shifted IDR(s) [25,26] and by the restarted shifted Hessenberg method [23]. From the conclusion in [26], α_j 's and β_j 's can be determined using Eq. (4.4) and the collinearity relation (4.7). The residuals are collinear if

$$\alpha_j = \gamma_j^{(i)}, \quad \beta_j = \alpha_j - 1 = \gamma_j^{(i)} - 1$$

at every (outer) iteration $1 \leq j \leq m$. One can show that the following relation,

$$(A - \sigma_i I)\mathbf{z}_j^{(i)} = \gamma_j^{(i)} A\mathbf{z}_j - (\gamma_j^{(i)} - 1)\mathbf{v}_j, \quad (4.8)$$

holds or, in terms of the flexible preconditioners P_j and $P_j(\sigma_i)$,

$$(A - \sigma_i I)P_j(\sigma_i)^{-1} \mathbf{v}_j = \left(\gamma_j^{(i)} AP_j^{-1} - (\gamma_j^{(i)} - 1)I \right) \mathbf{v}_j, \quad 1 \leq j \leq m.$$

It remarks that α_j 's and β_j 's do depend on σ_i , since the collinearity factors $\gamma_j^{(i)}$ change for each shift.

Based on the strategy proposed by Baumann and van Gijzen in [26], we now present a new nested multi-shifted Krylov solver in which the shifted Hessenberg (msHessen) method [23] is used as an inner preconditioner and flexible CMRH (FCMRH) is used as the outer Krylov iteration. We note that shifted FOM and flexible shifted GMRES [51] are related to the shifted Hessenberg and the flexible shifted CMRH methods, respectively. The Hessenberg relation given by Eq. (2.1) can be extended as follows,

$$AZ_m = L_{m+1} \check{H}_m, \quad (A - \sigma_i I)Z_m^{(\sigma_i)} = L_{m+1} \check{H}_m(\sigma_i),$$

where at iteration $1 \leq j \leq m$ flexible preconditioning is applied in the form $\mathbf{z}_j = P_j^{-1} \mathbf{v}_j$, $\mathbf{z}_j^{(\sigma_i)} = P_j^{-1}(\sigma_i) \mathbf{v}_j$, with $Z_m = [\mathbf{z}_1, \dots, \mathbf{z}_m]$ and $Z_m^{(\sigma_i)} = [\mathbf{z}_1^{(\sigma_i)}, \dots, \mathbf{z}_m^{(\sigma_i)}]$. It follows that both the Hessenberg process and the strategy proposed in [26] yield the modified Hessenberg matrix

$$\check{H}_m(\sigma_i) = (\check{H}_m - L_m) \Gamma_m^{(i)} + L_m,$$

where L_m is the $m \times m$ identity matrix with an extra column of zeros appended. The consecutive collinearity factors of the inner method then appear on a diagonal matrix $\Gamma_m^{(i)}$ defined as

$$\Gamma_m^{(i)} \equiv \begin{pmatrix} \gamma_1^{(i)} & & & \\ & \gamma_2^{(i)} & & \\ & & \ddots & \\ & & & \gamma_m^{(i)} \end{pmatrix} \in \mathbb{C}^{m \times m}. \quad (4.9)$$

After m outer iterations of the flexible shifted CMRH method, the solution to

$$\mathbf{z}_j^{(\sigma_i)} = \arg \min_{\mathbf{z} \in \mathbb{C}^j} \|(\check{H}_j - L_j) \Gamma_j^{(i)} + L_j \mathbf{z} - \alpha \mathbf{e}_1\|_2, \quad \mathbf{y}_j^{(\sigma_i)} = Z_j^{(\sigma_i)} \mathbf{z}_j^{(\sigma_i)} \quad (4.10)$$

yields approximate solutions to Eq. (1.1) in the search spaces $Z_j^{(\sigma_i)} \in \mathbb{C}^{2n \times j}$ that minimize the 2-norm of the *quasi-residual* of the i th shifted linear system, cf. Section 3 and [26,43, Section 3.4]. In Eq. (4.10), the Hessenberg matrix $\check{H}_j$ corresponds to the seed system, and $\Gamma_j^{(i)}$ is related to Eq. (4.9). Note that the shifted Hessenberg procedure yields collinear residuals by default [23]. We summarize the new nested Krylov subspace (dubbed Hessen-FCMRH) method for solving shifted linear systems in Algorithm 2.

The proposed Hessen-FCMRH method is related to the FOM-FGMRES method introduced in [26]. On the other hand, according to our recent work [23] msHessen can be cheaper than msFOM in terms of elapsed CPU time when it is used as the inner solver. Our numerical results presented in the next section confirm that shifted CMRH often requires less

Algorithm 2 The FCMRH method with pivoting and msHessen preconditioner

Input: the coefficient matrix A (or a user-defined function that applies A to a vector); the right-hand side vector $\mathbf{b}$; the set of shifts $\{\sigma_i\}_{i=1,\dots,t}$; the number of inner iterations, m_i ; the maximum number of outer iterations, m_o .

Output: the set of solution vectors $\mathbf{x}^{(i)}$ of the sequence of multi-shifted linear systems.

```

1: Choose the initial guess  $\mathbf{x}_0 = \mathbf{x}_0^{(\sigma_i)} = \mathbf{0}$ , then  $\mathbf{r}_0 = \mathbf{b}$ 
2: Set  $\mathbf{q} = [1, 2, \dots, n]^T$  and determine  $j_0$  such that  $|(\mathbf{r}_0)_{j_0}| = \|\mathbf{r}_0\|_\infty$ 
3: Set  $\beta = (\mathbf{r}_0)_{j_0}$ ,  $\mathbf{l}_1 = \mathbf{r}_0/\beta$  and  $(\mathbf{q})_1 \leftrightarrow (\mathbf{q})_{j_0}$ , where  $\leftrightarrow$  is used to swap contents.
4: for  $j = 1, 2, \dots, m_i$ , do
5:   Preconditioning:  $\mathbf{z}_j^{(\sigma_i)} = \text{msHessen}(A - \sigma_i I, \mathbf{l}_j, m_i)$ 
6:   Compute  $\gamma_j^{(\sigma_i)}$  according to the similar formula in [26, Eq. (3.9)]
7:   Compute  $\mathbf{u} = A\mathbf{z}_j^{(0)}$  (hint:  $\sigma_i = 0$ )
8:   for  $k = 1, 2, \dots, j$ , do
9:      $\check{h}_{k,j} = (\mathbf{u})_{(\mathbf{q})_k}$ 
10:     $\mathbf{u} = \mathbf{u} - \check{h}_{k,j}\mathbf{l}_k$ 
11:   end for
12:   if  $j < n$  and  $\mathbf{u} \neq \mathbf{0}$  then
13:     Determine  $j_0 \in \{j+1, \dots, n\}$  such that  $|(\mathbf{u})_{(\mathbf{q})_{j_0}}| = \|(\mathbf{u})_{(\mathbf{q})_{j+1}:(\mathbf{q})_n}\|_\infty$ 
14:      $\check{h}_{j+1,j} = (\mathbf{u})_{(\mathbf{q})_{j_0}}$ ,  $\mathbf{l}_{j+1} = \mathbf{u}/\check{h}_{j+1,j}$ ;  $(\mathbf{q})_{j+1} \leftrightarrow (\mathbf{q})_{j_0}$ 
15:   else
16:      $\check{h}_{j+1,j} = 0$ ; Stop
17:   end if
18:   // Loop over shifted systems:
19:   for  $i = 1, 2, \dots, t$ , do
20:     Define the matrix  $Z_j^{(\sigma_i)} = [\mathbf{z}_1^{(\sigma_i)}, \mathbf{z}_2^{(\sigma_i)}, \dots, \mathbf{z}_j^{(\sigma_i)}]$ 
21:     Set up  $\check{H}_j(\sigma_i)$  according to Eq. (4.9)
22:     Solve  $\mathbf{y}_j^{(\sigma_i)} = \arg \min_{\mathbf{y} \in \mathbb{C}^j} \|\beta \mathbf{e}_1 - \check{H}_j(\sigma_i)\mathbf{y}\|$  with  $\mathbf{e}_1 = [1, 0, \dots, 0]^T \in \mathbb{R}^{j+1}$ 
23:      $\mathbf{x}_j^{(\sigma_i)} = \mathbf{x}_0^{(\sigma_i)} + Z_j^{(\sigma_i)}\mathbf{y}_j^{(\sigma_i)}$ 
24:   end for
25: end for

```

operations than shifted GMRES. Thus, the proposed Hessen-FCMRH can be a cost effective nested Krylov solver for multi-shifted linear systems. However, note that the framework presented above may accommodate the use of other shifted Krylov subspace methods as inner preconditioners at Line 5 of Algorithm 2, for example shifted BiCGStab(ℓ), shifted IDR(s), shifted BiCRStab and shifted GPBiCG could be employed. Similarly to the FCMRH method for unshifted systems, extra memory is required to store the $Z_j^{(\sigma_i)}$'s matrices which span the solution space for each shifted problem [51,52]. The memory requirements increase to about $\mathcal{O}(2ntm_o)$ for $Z_{m_o}^{(\sigma_i)}$, and each iteration of the nested multi-shifted Krylov solver needs to evaluate $m_i m_o$ matrix-vector products (the leading cost), where m_o and m_i are the numbers of outer and inner iterations, respectively. This extra cost is the price to pay for using flexible preconditioning⁴ [43,51], and it applies for each shift.

5. Numerical experiments

In this section, we show the numerical behaviour of the restarted shifted CMRH method, shortly referred to as sCMRH(m), for solving some realistic shifted linear systems arising in real-world engineering modelling, also compared to the restarted shifted GMRES (sGMRES(m)), restarted shifted Simpler GMRES (sSGMRES(m)) and shifted QMRIDR(s) (sQMRIDR(s)) methods. Additionally, some experiments are reported with the framework of nested Krylov subspace solvers based on the CMRH and Hessenberg methods described in Section 4, and compared to the framework proposed in [26].

Our experiments are performed in double precision floating point arithmetic in MATLAB R2016a on a Windows 7 (64 bit) PC equipped with an Intel(R) Core(TM) i5-2400 CPU running at 3.10 GHz and with 10 GB of RAM. Unless stated otherwise, the right-hand side $\mathbf{b}$ is the vector with all 1's. The iterative solution is started from $\mathbf{x}_0^{(i)} = \mathbf{0}$ and is stopped at

⁴ One application of flexible preconditioning requires to evaluate m_i matrix-vector products and about $\mathcal{O}(tm_i^2)$ operations to solve t Hessenberg least-square problems of size m_i .

Table 2

Set and characteristics of the test problems used for Experiment 5.1.

Index	Matrix	Size	Field	$\text{nnz}(A)$
Σ_1	Poisson3Da	13,514	Computational fluid dynamics	352,762
Σ_2	epb1	14,734	Thermal problem	95,053
Σ_3	waveguide3D	21,036	Electromagnetics problem	303,468
Σ_4	kim1	38,415	2D/3D problem	933,195
Σ_5	Poisson3Db	85,623	Computational fluid dynamics	2,374,949
Σ_6	vfem	93,476	Electromagnetics problem	1,434,636
Σ_7	matrix-new_3	125,329	Semiconductor device problem	893,984
Σ_8	FEM_3D_thermal2	147,900	Thermal problem	3,489,300

Table 3Convergence results with different shifted Krylov subspace solvers for Experiment 5.1, using $m = 40$. Symbol † (or $\cdot^+$) means convergence failure (in terms of true residuals).

Index	sGMRES(m)		sCMRH(m)		sQMRIDR(1)		sQMRIDR(2)		sGMRES(m)	
	MVPs	CPU	MVPs	CPU	MVPs	CPU	MVPs	CPU	MVPs	CPU
Σ_1	320	0.665	360	0.358	250	0.464	225	0.510	240 ⁺	0.712
Σ_2	1160	1.339	1769	0.963	1367	1.694	989	1.559	1050 ⁺	2.444
Σ_3	480	2.644	560	2.065	437	2.640	392	3.275	†	†
Σ_4	2000	20.390	1640	11.268	†	†	2231	36.052	†	†
Σ_5	600	6.741	680	6.211	561	9.309	427	9.527	484 ⁺	9.524
Σ_6	240	4.461	280	3.367	413	10.241	224	9.189	†	†
Σ_7	120	0.789	120	0.476	287	3.423	152	3.215	†	†
Σ_8	520	12.124	560	6.764	793	17.560	503	16.932	†	†

iteration k when $\|\mathbf{r}_k^{(i)}\|_2 / \|\mathbf{b}\|_2 < 10^{-8}$ for $i = 1, 2, \dots, t_s$ for all linear systems, or after at most Max_{mvp} iterations. We do not compute the residuals of the additional shifted systems because of the collinearity condition.

5.1. General academic problems

The first set of eight linear systems are extracted from the SuiteSparse Matrix Collection [55]. The main characteristics of the test problems are listed in Table 2. We use shifts $\sigma_j = -j/10000$ ($j = 1, 2, 3, 4, 5$) for problems $\Sigma_1, \Sigma_4, \Sigma_5, \Sigma_6, \Sigma_8$, shifts $\sigma_j = -(8+j)/200000$ for Σ_2 , shifts $\sigma_j = -(179+j)/20000$ for Σ_3 , and $\sigma_j = -j/20000$ for Σ_7 . The first linear system $(A - \sigma_1 I)\mathbf{x}^{(1)} = \mathbf{b}$ is the *seed* system. We set the restart value m equal to 40 (this value is used throughout Sections 5.1–5.3) to ensure that all the multi-shifted linear systems converge successfully [9,15,16,26], and the maximum number of matrix–vector products Max_{mvp} equal to 6000.

In Table 3 we show number of matrix–vector products (abbreviated as MVPs) and elapsed CPU solution time in seconds (CPU) required by sCMRH(m), sGMRES(m), sQMRIDR(s) ($s = 1, 2$) and sGMRES(m) to converge to prescribed accuracy. All methods converge within the maximum number of iterations, except sQMRIDR(1) for Problem Π_4 and sGMRES(m) for Problem Π_ℓ , $\ell = 3, 4, 6, 7, 8$. In our runs, sCMRH(m) is the fastest solver although it often needs more MVPs, confirming the complexity analysis presented in Section 3.2. The timing performance of sQMRIDR(s) is penalized by the extra inner products and vector updates required at each iteration; note, however, that sQMRIDR(2) generally requires less matrix–vector products to converge. On this set of problems, sGMRES(m) is less robust than the other solvers.

The relative residual histories plotted in Fig. 1 for different shifts confirm the conclusion reported in [14] that sGMRES(m) converges more rapidly on the *add* systems than on the *seed* system, and that its convergence history is comparable to sCMRH(m). Overall, the sCMRH(m) method is very competitive on this set of matrices.

5.2. Quantum chromodynamics applications

Next, we report on experiments on seven $49,152 \times 49,152$ complex shifted linear systems arising from the discretization of the Dirac operator in quark simulations at different physical temperatures in lattice QCD applications. The seven test problems are named as conf5_4-8x8-05, conf5_4-8x8-10, conf5_4-8x8-15, conf5_4-8x8-20, conf6_0-8x8-20, conf6_0-8x8-30, conf6_0-8x8-80 in the SuiteSparse Matrix Collection [55]. Hereafter, they will be denoted as problems Π_i for $i = 1, 2, \dots, 7$. We select shifts equal to $\sigma_j \in \mathcal{I} = \{-0.001, -0.002, -0.003, -0.04, -0.05, -0.06, -0.07\}$ and we use $(A - \sigma_1 I)\mathbf{x}^{(1)} = \mathbf{b}$ as the *seed* system. The maximum number of matrix–vector products is set equal to 5000.

In Table 4, we report on elapsed CPU time and MVPs required by different iterative methods to reduce the initial residuals by eight orders of magnitude. Except for Problems Π_5 and Π_6 , sCMRH(m) is more cost-effective than sGMRES(m). In general sQMRIDR(s) requires less iterations but more CPU time to converge. One exception is Problem Π_6 , where sQMRIDR(1) is the fastest solver. In our experiments, sAd-SGMRES(m) is not a competitive choice in terms of both MVPs and elapsed CPU time.

Fig. 1. Relative residual histories of different iterative solvers for test problem Σ_1 in Table 3.

Table 4
Convergence results with different shifted Krylov subspace solvers for Experiment 5.2, using $m = 40$.

Index	sGMRES(m)		sCMRH(m)		sQMRIDR(1)		sQMRIDR(2)		sAd-sGMRES(m)	
	MVPs	CPU	MVPs	CPU	MVPs	CPU	MVPs	CPU	MVPs	CPU
Π_1	1120	15.007	1480	14.974	845	15.557	732	20.549	3459 ⁺	82.897
Π_2	880	11.388	1120	11.236	746	13.835	675	19.456	†	†
Π_3	720	9.173	880	8.815	709	13.345	633	19.018	†	†
Π_4	640	8.265	800	7.986	757	13.973	687	20.283	†	†
Π_5	640	8.255	840	8.279	589	11.473	477	14.797	†	†
Π_6	840	10.762	1160	11.712	539	10.257	456	13.468	†	†
Π_7	680	8.656	840	8.321	582	11.171	477	14.109	1743 ⁺	44.703

The convergence histories and the final accuracies of sGMRES(m) and sCMRH(m) are once again comparable based on the relative residual histories plotted in Fig. 2. The approximate solutions computed by sCMRH(m) are slightly more accurate than for the other solvers, whereas the final residual norms of sGMRES(m) are smaller than those of sQMRIDR(s). We conclude that sCMRH(m) can be an interesting alternative to other shifted Krylov subspace methods for this set of problems.

5.3. Time fractional differential equations

Fractional differential equations (FDEs) are widespread mathematical models in the study of physical, biological, geological and financial systems, to name only a few fields. Due to the increasing dimension and complexity of these systems, in recent years considerable attention has been devoted to the development of efficient numerical methods for

Fig. 2. Relative residual histories of different iterative solvers for test problem Π_2 in Table 4.

the approximate solution of FDEs in many areas, see e.g. [56,57]. Here we consider a benchmark problem coming from the 3D time-fractional convection–diffusion–reaction equation defined as

$$\begin{cases} \frac{\partial^\gamma u}{\partial t^\gamma} = \epsilon \Delta u - \vec{\beta} \cdot \nabla u + ru, & (x, y, z) \in \Omega = (0, 1)^3, \quad t \in [0, T], \\ u(x, y, z, t) = 0, & (x, y, z) \in \partial\Omega, \quad t \in [0, T], \\ u(x, y, z, 0) = x(1-x)y(1-y)z(1-z), & (x, y, z) \in \bar{\Omega}. \end{cases} \quad (5.1)$$

Problem (5.1) is a modification of the third example presented in Ref. [27], with diffusion constant $\epsilon = 1$, reaction constant $r = 400$ and convection parameter $\vec{\beta} = (0/\sqrt{5}, 250/\sqrt{5}, 500/\sqrt{5})^T$. Upon the finite difference discretization of Eqs. (5.1) on an uniformly spaced domain using naturally ordered grid points, a system of FDEs of the form

$$\frac{d^\gamma \mathbf{u}}{dt^\gamma} = A\mathbf{u}(t), \quad \mathbf{u}(0) = \mathbf{u}_0. \quad (5.2)$$

is obtained, where $\mathbf{u}$ denotes the vector of unknown approximate solutions at the grid points. Using a grid size $h = 0.025$, the order of the matrix A is about 60,000. It is well-known [2–4] that, for $0 < \gamma < 1$, the true solution of this problem can be expressed as

$$\mathbf{u}(t) = e_{\gamma,1}(t; A)\mathbf{u}_0, \quad \text{and} \quad e_{\gamma,1}(t; A) = t^{1-\gamma}E_{\gamma,1}(t^\gamma A) = E_{\gamma,1}(t^\gamma A), \quad (5.3)$$

where $E_{\gamma,1}(z)$ is the Mittag-Leffler (ML) function [4,57]

$$E_{\gamma,1}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\gamma k + 1)}, \quad \gamma > 0, \quad z \in \mathbb{C}.$$

Table 5Convergence results with different shifted Krylov subspace solvers for Experiment 5.3, using $m = 40$. Symbol † means convergence failure.

(γ, ν)	sGMRES(m)		sCMRH(m)		sQMRIDR(1)		sQMRIDR(2)		sAd-SGMRES(m)	
	MVPs	CPU	MVPs	CPU	MVPs	CPU	MVPs	CPU	MVPs	CPU
(0.2, 6)	800	3.421	1000	2.990	299	6.225	182	6.081	†	†
(0.4, 8)	800	3.553	1000	3.051	299	8.061	182	7.809	†	†
(0.6, 10)	800	3.560	1000	3.130	299	9.651	182	9.542	†	†
(0.8, 10)	800	3.547	1000	3.136	299	9.755	182	9.633	†	†
(0.9, 12)	800	3.589	1000	3.204	299	11.302	185	11.317	†	†

Table 6Convergence results with different shifted Krylov solvers for Experiment 5.3, using $m = 40$, $\gamma = 0.8$ and $\nu = 10$.

(h, r)	sGMRES(m)		sCMRH(m)		sQMRIDR(1)		sQMRIDR(2)		sAd-SGMRES(m)	
	MVPs	CPU	MVPs	CPU	MVPs	CPU	MVPs	CPU	MVPs	CPU
$(\frac{1}{50}, 400)$	†	†	1360	8.41	283	22.52	200	24.44	2653 ⁺	197.72
$(\frac{1}{50}, 500)$	†	†	1400	8.63	293	23.58	215	25.94	†	†
$(\frac{1}{80}, 400)$	†	†	1640	61.57	358	153.55	275	162.09	†	†
$(\frac{1}{80}, 500)$	†	†	3000	114.90	359	155.35	278	162.61	†	†
$(\frac{1}{100}, 400)$	†	†	1680	138.81	397	355.76	329	391.61	†	†
$(\frac{1}{100}, 500)$	†	†	2680	228.47	402	359.26	333	395.71	†	†

In light of Eq. (5.3), the numerical solution $\mathbf{u}(t)$ can be computed as the product of the matrix ML function $E_{\gamma,1}(t^\gamma A)$ times $\mathbf{u}_0$. This operation accounts for the major computational cost of the solution of Eq. (5.2). Recently, the numerical evaluation of the action of the matrix function on a vector, namely $E_{\gamma,1}(t^\gamma A)\mathbf{u}_0$, is receiving much consideration as shown by the spread of literature on this topic [2–4]. One approach is based on the Carathéodory–Fejér approximation of $E_{\gamma,1}(t^\gamma A)\mathbf{u}_0$ [58], that has the following representation

$$E_{\gamma,1}(A)\mathbf{u}_0 = f_\nu(A)\mathbf{u}_0 = \sum_{j=1}^v w_j(z_j I - A)^{-1}\mathbf{u}_0, \quad (5.4)$$

where w_j and z_j are quadrature weights and nodes, respectively. Implementing Eq. (5.4) requires the solution of a sequence of shifted linear systems of the form $(-A + z_j I)\mathbf{x}^j = \mathbf{u}_0$, $z_j \in \mathbb{C}$.

In Table 5 we compare different shifted Krylov subspace methods for solving five groups of real shifted linear systems with same seed system $-A\mathbf{x} = \mathbf{u}_0$ but a different number of shifts arising from this application. For this reason, the number of matrix–vector products required by different solvers to converge changes only slightly in Table 5. In our runs, sCMRH(m) exhibits the fastest convergence in terms of elapsed CPU time, although it requires more MVPs. As in previous experiments, the performance of sQMRIDR(s) is penalized by the $s+2$, possibly complex, n -length extra vectors that need to be stored and updated for each new shift. Unfortunately, the sAd-SGMRES(m) method fails to converge in our runs.

For a more comprehensive performance evaluation of different algorithms, in Table 6 we report on elapsed CPU time and MVPs required to solve the six shifted linear systems with different grid size and reaction parameters. Large values of convection coefficients β and reaction parameter r in Eq. (4.1) always result in highly nonsymmetric, ill-conditioned finite difference matrix A [27]. In these experiment we set $Max_{mvp} = 6000$. We can see from Table 6 that in our runs only sCMRH(m) and sQMRIDR(s) are able to solve all the shifted linear systems. The reason might be that the sGMRES(m) and sAd-SGMRES(m) methods are more sensitive than the other two shifted iterative solvers to the high nonsymmetry and indefiniteness of the coefficient matrix. In addition, although sQMRIDR(s) always requires less number of MVPs than the other two shifted iterative solvers, it is still more expensive in terms of elapsed CPU time due to the extra vector operations. Based on these results, we conclude that the proposed sCMRH(m) method is an efficient algorithm to solve shifted linear systems arising in the discretization of FDEs.

5.4. Experiments on flexible preconditioning for shifted systems

We illustrate the performance of the methods presented in Section 4, namely Hessen–FCMRH, Hessen–FGMRES and FOM–FCMRH against FOM–FGMRES [26] for solving some ill-conditioned shifted linear systems arising from realistic difficult problems, such as evaluating the action of the matrix function on a vector with large matrix norm [58,59] and the QCD simulation. In these runs, we select $A\mathbf{x} = \mathbf{b}$ as the seed system. Timings can be different from the experiments of the previous two sections as we use the norm of the true residual vector (which can help us to investigate how inner iterations actually affect the outer iterations) to monitor the (complete) convergence of the outer method (i.e., FCMRH and FGMRES).

In Group I, we solve some shifted linear systems arising from the computation of the Carathéodory–Fejér approximation $\exp(\tau L)\mathbf{u}_0$ in reactive transport simulations through heterogeneous porous media modelled by the advection–diffusion–reaction equation defined on a two-dimensional $[0, 2]^2$ square domain. The experimental setting is the same

Table 7

Number of inner and outer iterations and CPU solution time for experiments with different nested Krylov methods to solve Group I problems.

(h, τ)	IT_in	Hessen-FCMRH		Hessen-FGMRES		FOM-FCMRH		FOM-FGMRES	
		IT_out	CPU	IT_out	CPU	IT_out	CPU	IT_out	CPU
$(\frac{1}{100}, 0.04)$	110	2	0.364	3	0.543	4	1.147	4	1.219
	100	2	0.316	4	0.667	6	1.520	10	2.613
	90	2	0.291	3	0.445	27	6.570	15	3.163
$(\frac{1}{120}, 0.04)$	160	5	2.208	4	1.789	5	3.347	6	4.398
	150	6	2.341	6	2.422	29	20.155	8	4.919
	140	21	8.023	16	5.912	22	13.721	12	6.882
$(\frac{1}{140}, 0.03)$	160	4	2.127	5	2.828	4	3.433	3	2.641
	150	6	3.027	6	3.190	4	3.204	4	3.266
	140	6	2.913	8	3.863	7	4.932	10	7.126

Table 8

Number of inner and outer iterations and CPU solution time for experiments with different nested Krylov methods to solve Group II problems.

Index	IT_in	Hessen-FCMRH		Hessen-FGMRES		FOM-FCMRH		FOM-FGMRES	
		IT_out	CPU	IT_out	CPU	IT_out	CPU	IT_out	CPU
$\mathcal{E}_1$	80	2	1.281	3	1.989	3	2.626	3	2.679
	70	4	2.294	5	2.938	4	2.998	4	3.044
	60	18	11.442	7	3.766	6	3.826	5	3.030
$\mathcal{E}_2$	90	3	4.344	3	4.368	4	7.843	4	7.847
	80	5	6.639	5	6.658	6	10.633	4	6.947
	70	11	13.958	8	9.778	26	48.284	7	10.856
$\mathcal{E}_3$	100	2	3.123	3	4.732	5	11.094	4	8.739
	90	5	7.106	5	7.187	16	33.751	8	15.893
	80	7	8.948	9	12.011	12	21.645	7	11.992
$\mathcal{E}_4$	140	2	29.866	4	60.604	13	559.623	6	252.897
	130	6	82.819	7	98.412	18	700.114	4	149.293
	120	4	49.197	9	115.089	28	965.549	4	129.557

as the one proposed in [59, Example 2], except for different values of the shift τ . We use MATLAB codes available at <https://numerical-analysis.uibk.ac.at/exp-int-software> to generate matrices L of different sizes equal to 9801×9801 , $14,161 \times 14,161$, and $19,321 \times 19,321$, corresponding to grid sizes $h = 1/100, 1/120, 1/140$. In the matrix ML function evaluation, we use $\nu = 14$ poles. Numerical experiments with various nested Krylov subspace solvers are shown in Table 7.

In Group II, we use the same test problems of Section 5.3 with the following setup values: $\gamma = 0.9$ and $\beta = (0/\sqrt{5}, 250/\sqrt{5}, 500/\sqrt{5})^T$ with $h = 0.025$ and $h = 0.02$ for test problems $\mathcal{E}_1$ and $\mathcal{E}_2$. The sizes of these two systems are $59,319 \times 59,319$ and $117,649 \times 117,649$, respectively. On the other hand, we set $\gamma = 0.8$ and $\beta = (500/\sqrt{5}, 250/\sqrt{5}, 500/\sqrt{5})^T$ with $h = 0.02$ and $h = 0.0125$ for test problems $\mathcal{E}_3$ and $\mathcal{E}_4$. The sizes of these two test problems are $117,649 \times 117,649$ and $493,039 \times 493,039$, respectively. The other settings are set equal to the values used in Section 5.3. The results are illustrated in Table 8.

In Table 7, we show elapsed CPU time and number of inner and outer iterations (denoted as IT_in and IT_out, respectively) required by the four nested Krylov methods to solve the seven shifted linear systems within prescribed tolerance and maximum number of iterations. We adopt these notations throughout the subsection. Our nested solver Hessen-FCMRH is the most efficient one in terms of elapsed CPU time at equal number of inner steps, with the exception of $(1/120, 0.04)$ and IT_in = 140. The result is supported by the conclusions presented in [23] and by our previous analysis. Note that not only Hessen-FCMRH is faster than Hessen-FGMRES, but also FOM-FCMRH is more efficient than FOM-FGMRES in terms of elapsed time at similar number of outer iterations. We conclude that nested iterative solvers based on the Hessenberg procedure can be computationally efficient to solve multi-shifted linear systems.

Similar conclusions are derived from the convergence results of the seven shifted linear systems of Group II illustrated in Table 8. Nested Hessen-FCMRH is a robust method in terms of solution time at equal number of inner steps, except only problem $\mathcal{E}_1$ with IT_in = 60 and problem $\mathcal{E}_2$ with IT_in = 70. For most problems, Hessen-FCMRH and Hessen-FGMRES converge faster than FOM-FGMRES and FOM-FCMRH. In addition, we can see that FOM-FCMRH is still faster than FOM-FGMRES in terms of elapsed time at similar number of outer iterations. Under similar conditions, Hessen-FCMRH is also faster than Hessen-FGMRES thanks to the cost-effective Hessenberg procedure. The proposed Hessen-FCMRH method is remarkably robust for handling shifted linear systems, in terms of the elapsed CPU time.

Finally, we consider the last two test problems, denoted as MLMF and QCDx. MLMF arises from Eq. (4.1) setting $\gamma = 0.9$, $r = 500$, $\beta = (500/\sqrt{5}, 250/\sqrt{5}, 500/\sqrt{5})^T$ and $h = 0.02$. Experiments with nested iterative schemes with a different number of inner iterations (i.e., IT_in) are shown in Table 9. Our Hessen-FCMRH method with IT_out = 2 and IT_in = 100 exhibits the best overall performance in terms of CPU time. Nested schemes based on the Arnoldi procedure always require more time to converge, except the case of IT_in = 90. Often in our runs, the larger the number of inner

Table 9

Number of inner and outer iterations and CPU solution time for experiments with different nested Krylov methods to solve problem MLMF.

Solver	IT _{in} = 120		IT _{in} = 110		IT _{in} = 100		IT _{in} = 90	
	IT _{out}	CPU	IT _{out}	CPU	IT _{out}	CPU	IT _{out}	CPU
Hessen-FCMRH	2	4.18	2	3.83	2	3.44	6	9.45
Hessen-FGMRES	2	4.20	3	5.82	3	5.23	6	9.49
FOM-FCMRH	2	5.89	3	7.86	5	11.83	18	43.73
FOM-FGMRES	2	6.01	3	7.95	5	11.89	8	16.76

Table 10

Number of inner and outer iterations and CPU solution time for experiments with different nested Krylov methods to solve problem QCDx.

Solver	IT _{in} = 150		IT _{in} = 140		IT _{in} = 130		IT _{in} = 120	
	IT _{out}	CPU	IT _{out}	CPU	IT _{out}	CPU	IT _{out}	CPU
Hessen-FCMRH	7	22.73	7	20.67	8	21.39	8	18.95
Hessen-FGMRES	6	19.43	6	17.52	7	18.47	8	19.04
FOM-FCMRH	5	25.64	5	23.04	6	24.96	7	25.62
FOM-FGMRES	5	25.97	6	28.46	6	25.61	7	25.73

iterations, the smaller the number of outer steps, and vice versa for the solution time. The results show that the proposed Hessen-FCMRH method can be regarded as a robust choice for this problem.

Here problem QCDx is denoted as problem Π_2 in Section 5.2. Experiments with nested iterations using a different number of inner iterations IT_{in} are listed in Table 10. Our Hessen-FGMRES method with IT_{in} = 140 has the best overall performance among the four solvers in terms of elapsed CPU time. Again, nested solvers based on the Arnoldi procedure tend to require more CPU time than those based on the Hessenberg procedure. The larger the number of inner iterations, the smaller the number of outer steps, while elapsed CPU time costs do not always follow the same trend. Also in this case we conclude that the Hessen-FGMRES method can be considered as a robust choice for this test problem. The Hessen-FCMRH method is also an interesting alternative.

6. Conclusions

The paper presents two contributions to the development of shifted Krylov subspace methods built upon the Hessenberg process for the efficient solution of shifted linear systems. Firstly, we explore the algorithmic relation between the GMRES(m) and CMRH(m) methods. The reduced memory and algorithmic complexity of CMRH(m) motivated us to generalize this algorithm for solving shifted linear systems. The experiments reported in this paper show the effectiveness of the shifted CMRH(m) method against sGMRES(m), sAd-sGMRES(m) and sQMRIDR(s) ($s = 1, 2$) in terms of elapsed CPU time. Then, a new nested iterative framework of shifted linear systems is proposed based on the Hessenberg procedure. More precisely, we proposed three nested iterative solvers: Hessen-FCMRH, Hessen-FGMRES and FOM-FCMRH for shifted linear systems. The first two often converge significantly faster than FOM-FGMRES introduced in [26]. In particular, numerical experiments involving time integration of 3D fractional/partial differential equations are reported to illustrate the advantages of the proposed nested iterative solvers. We showed that these algorithms can be very effective to use in numerical schemes that require to evaluate the action of the matrix function on a vector (see e.g. [3,4]) for three-dimensional time-dependent (fractional) convection–diffusion–reaction equations. This point can be regarded as the second contribution of our manuscript.

In our experiments, the number of inner iterations was often large, potentially leading to high computational and memory requirements on realistic applications. As an outlook for the future, we plan to test shifted Krylov subspace solvers based on short-term vector recurrences, such as shifted BiCGSTAB(ℓ), shifted BiCRSTAB, shifted IDR(s), shifted GPBiCG, shifted TFQMR and shifted QMRIDR(s) as inner solvers in the nested iterative framework for shifted linear systems, see e.g. [26]. Meanwhile, the restarting technique can often remedy memory problems related to long-term recurrence Krylov subspace methods, e.g., FOM, GMRES, and CMRH. Thus, we are also interested to develop restarted shifted versions of FOM, GMRES, Hessenberg, and CMRH as inner solvers in our future research.

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