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

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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.

Key words: Krylov subspace methods; Shifted linear systems; Hessenberg procedure; GMRES; Shifted CMRH methods; FDEs.

AMS Classification: 65F12; 65L05; 65N22.

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

\[
(A - \sigma_i I)x^{(i)} = b, \quad i = 1, 2, \ldots, t, \tag{1.1}
\]

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, \( x^{(i)} \) and \( b \) are solutions and right-hand side vectors of the \( t \) linear systems, respectively. Problem (1.1) arises 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

\[
\mathcal{K}_m(A, b) = \mathcal{K}_m(A - \sigma_i I, b), \quad i = 1, 2, \ldots, t, \tag{1.2}
\]

where we denote by \( \mathcal{K}_m(A, b) := \text{span}\{b, Ab, \ldots, A^{m-1}b\} \) the Krylov subspace of dimension \( m \) generated by \( A \) and \( b \) (see [6, 12, 13]). By a suitable choice of the initial vectors \( x_0^{(i)} \), for example take \( x_0^{(i)} = 0 \), 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 [39–44], the restarted full orthogonalization (FOM) method [18–20] and the restarted Hessenberg method [21] 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) [14], the induced dimension reduction (IDR(s)) [15, 16] and its QMR form [17], the biconjugate gradient (BiCG) method and its stabilized and generalized product-type extensions (BiCGStab, BiCGStab(\( \ell \)) and GPBiCG) [12, 13, 25], the biconjugate residual (BiCR) method and its stabilized form (BiCRSTAB) [24] are built upon short-term vector recurrences such as the Bi-Lanczos [22, pp. 229-233] and the \( A \)-biorthogonalization [23, pp. 40-42] procedures.
In [26,27], 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 [28, pp. 377-382] (shortly, CMRH\(^1\)) introduced in [29,30]. The method is based on long-term vector recurrences, like Arnoldi. However, each basis vector \( l_i \) has \( i - 1 \) components equal to zero and only one component equal to one; each matrix-vector product involved in the computation of \( l_i \) 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 [21, 29,31–33]. It has been shown that CMRH and GMRES convergence curves are often comparable [29,30,45]. On problems where GMRES exhibits superlinear convergence, so often does CMRH; when GMRES stagnates, CMRH does so as well. We point the reader to [45, 48] for further discussions, and to [34–36] for some recent developments on the theoretical and algorithmic aspects of the CMRH method [31, 35, 37], including efficient parallel implementations [29].

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 [6,12,16,21]. 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(\( \ell \)) methods that acts as a preconditioner for an outer flexible CMRH (FCMRH) solver [34].

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.

\(^1\)A short note described the relation between the ELMRES method [31,32] and Sadok’s CMRH method is available at http://ncsu.edu/hpc/Documents/Publications/gary_howell/contents.html#codes.
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 $Ax = b$; then, we extend it to the solution of problem (1.1).

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 $K_m(A, r_0)$. Starting from an initial vector $l_1 = r_0/\alpha$, where $\alpha = (r_0)_1$ is the first entry of $r_0$, $m$ steps of the Hessenberg procedure yield a basis $\{l_1, l_2, \ldots, l_m\}$ and a matrix decomposition of the form

$$AL_m = L_{m+1}\tilde{H}_m,$$  \hspace{1cm} (2.1)

where $L_m = (l_1, l_2, \ldots, l_m)$ is an $n \times m$ unit lower trapezoidal matrix and $\tilde{H}_m \in \mathbb{C}^{(m+1) \times m}$ is upper Hessenberg. The CMRH approximation after $m$ steps writes as $x_m = x_0 + z_m$, where $z_m \in K_m(A, r_0)$ solves the following constrained minimization problem

$$\min_{u \in \mathbb{C}^{m+1}, \; z \in K_m(A, r_0)} \|u\|_2, \quad \text{subject to} \quad Az = r_0 + L_{m+1}u.$$  \hspace{1cm} (2.2)

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

$$\min_{z \in K_m(A, r_0)} \|L_m^\dagger(Alz - r_0)\|_2,$$  \hspace{1cm} (2.3)

similarly to the well-known QMR method [22, pp. 236-241]. In Eq. (2.3), we denote by $L_m^\dagger$ the pseudo-inverse of $L_{m+1}$; however, note that any left inverse of $L_{m+1}$ would work here [45]. Problem (2.3) can be interpreted as a standard residual minimization using a semi-norm [29,30]. By writing $z = L_my \in K_m(A, r_0)$, Eq. (2.3) is implemented in CMRH as the following small least squares problem

$$\min_{y \in \mathbb{C}^m} \|L_{m+1}^\dagger(r_0 - AL_my)\|_2 = \min_{y \in \mathbb{C}^m} \|L_{m+1}^\dagger(\alpha L_{m+1}e_1^{(k+1)} - L_{m+1}\tilde{H}_my)\|_2$$

$$= \min_{y \in \mathbb{C}^m} \|\alpha e_1^{(k+1)} - \tilde{H}_my\|_2.$$  \hspace{1cm} (2.4)

A detailed theoretical analysis of the method can be found in [29,30]. In particular, the result below compares the residual norms computed after $m$ iterations of the CMRH and the GMRES methods:

\(^2\)According to Refs. [21,31,32], 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.
Theorem 2.1. ([29, Theorem 4] and [45, Theorem 1]) Let $r_G^m$ and $r_c^m$ be the GMRES and CMRH residuals at the $m$th iteration beginning with the same initial residual $r_0$ (e.g., $r_0 = b$), respectively. Then

$$||r_G^m||_2 \leq ||r_c^m||_2 \leq \kappa(L_{m+1})||r_G^m||_2,$$

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

Duinjjer 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 [48]. 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

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

where $I_m$ is the identity matrix of order $m$, and $L_m$, $\hat{H}_m(\sigma_{seed})$ are factors of the matrix decomposition (2.1) independent of $\sigma_i$. 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

$$\min_{y \in \mathbb{C}^n} ||L_{m+1}^\dagger r_m^{(i)}||_2 = \min_{y \in \mathbb{C}^n} ||\alpha e_1 - \hat{H}_m(\sigma_i)y||_2.$$

The small-size least squares problem (2.6) can be solved in $O(m^2)$ operations for each shift $\sigma_i$. 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, $x_0 = 0$ 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 [39], namely

$$\gamma_m^{(i)} \mathbf{r}_m = \gamma_m^{(i)} \mathbf{r}_m,$$

(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

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

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

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

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

$$\mathbf{r}_m^{(i)} = \gamma_m^{(i)} \mathbf{r}_m \quad \Leftrightarrow \quad \mathbf{b} - A(\sigma_i)(\mathbf{x}_0^{(i)} + L_m \mathbf{y}_m^{(i)}) = \gamma_m^{(i)} L_{m+1} \mathbf{u}_{m+1}$$

$$\mathbf{r}_0^{(i)} - A(\sigma_i) L_m \mathbf{y}_m^{(i)} = L_{m+1} \mathbf{u}_{m+1} \gamma_m^{(i)}$$

$$\gamma_0^{(i)} \mathbf{r}_0 - L_{m+1} \tilde{H}_m(\sigma_i) \mathbf{y}_m^{(i)} = L_{m+1} \mathbf{u}_{m+1} \gamma_m^{(i)}$$

$$L_{m+1} (\tilde{H}_m(\sigma_i) \mathbf{y}_m^{(i)} + \mathbf{u}_{m+1} \gamma_m^{(i)}) = \gamma_0^{(i)} \mathbf{r}_0$$

$$\Leftrightarrow \quad \tilde{H}_m(\sigma_i) \mathbf{y}_m^{(i)} + \mathbf{u}_{m+1} \gamma_m^{(i)} = \gamma_0^{(i)} \alpha \mathbf{e}_1$$

using the matrix representation of the Hessenberg procedure; see [39] 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

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

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

**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 \( \{\sigma_i\}_{i=1, \ldots, t_s} \); 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 \( \mathbf{x}_0, \mathbf{x}_0^{(i)} \) such that \( r_0^{(i)} = \gamma_0^{(i)} \mathbf{r}_0 \), e.g. \( \mathbf{x}_0 = \mathbf{x}_0^{(i)} = \mathbf{0} \) (also implies that \( \gamma_0^{(i)} = 1 \))
2: Set \( q = [1, 2, \ldots, n]^T \) and determine \( j_0 \) such that \( \|(r_0)_{j_0}\| = \|\mathbf{r}_0\|_\infty \)
3: Set \( \alpha = (r_0)_{j_0}, l_1 = r_0/\alpha \) and \( (q)_1 \leftrightarrow (q)_{j_0} \), where \( \leftrightarrow \) is used to swap contents.
4: for \( j = 1, 2, \ldots, m, \) do
5: \hspace{1em} Compute \( \mathbf{u} = AL_j \)
6: \hspace{1em} for \( k = 1, 2, \ldots, j, \) do
7: \hspace{2em} \( \hat{h}_{k,j} = (u)_{(q)_{k}} \)
8: \hspace{2em} \( \mathbf{u} = \mathbf{u} - \hat{h}_{k,j}l_k \)
9: \hspace{1em} end for
10: \hspace{1em} if \( j < n \) and \( \mathbf{u} \neq \mathbf{0} \) then
11: \hspace{2em} Determine \( j_0 \in \{j + 1, \ldots, n\} \) such that \( \|(u)_{(q)_{j_0}}\| = \|(u)_{(q)_{j+1}}(q)_{n}\|_\infty \)
12: \hspace{2em} \( \hat{h}_{j+1,j} = (u)_{(q)_{j_0}}, l_{j+1} = u/\hat{h}_{j+1,j}; (q)_{j+1} \leftrightarrow (q)_{j_0} \)
13: \hspace{1em} else
14: \hspace{2em} \( \hat{h}_{j+1,j} = 0 \); Stop
15: \hspace{1em} end if
16: end for
17: Define the \((m + 1) \times m\) Hessenberg matrix \( \hat{H}_m = \{\hat{h}_{k,j}\}_{1 \leq k \leq m+1, 1 \leq j \leq m} \) and collect the matrix \( L_m = [l_1, l_2, \ldots, l_m] \)
18: Compute \( y_m = \arg \min_{y \in \mathbb{C}^m} \|\alpha \mathbf{e}_1 - \hat{H}_m \mathbf{y}\|_2 \) and set \( u_{m+1} = \alpha \mathbf{e}_1 - \hat{H}_m y_m \)
19: \( \mathbf{x}_m = \mathbf{x}_0 + L_m y_m, r_m = r_0 - A L_m y_m = L_{m+1} u_{m+1} \)
20: for \( i = 1, 2, \ldots, t_s \) do
21: \hspace{1em} Solve \( [\hat{H}_m(\sigma_i) \mid u_{m+1}] [y_m(i)] = \gamma_0^{(i)} \alpha \mathbf{e}_1 \)
22: \hspace{1em} \( \mathbf{x}_m^{(i)} = \mathbf{x}_0^{(i)} + L_m y_m^{(i)}, r_m^{(i)} = r_0^{(i)} - A L_m y_m^{(i)} = \gamma_m^{(i)} r_m \)
23: end for
24: Restart: if converged then stop; otherwise update \( \mathbf{x}_0 := \mathbf{x}_m, \mathbf{x}_0^{(i)} := \mathbf{x}_m^{(i)}, r_0 := r_m, r_0^{(i)} := r_m^{(i)}, \gamma_0^{(i)} := \gamma_m^{(i)} \) and goto step 2-3.

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., \( (\mathbf{A} \mathbf{x}, \mathbf{x}) > 0, \forall \mathbf{x} \neq \mathbf{0} \), 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
\[
\| \mathbf{r}_{j,m}^{(i)} \|_2 \leq |\gamma_0^{(i)}| \cdot \| \mathbf{r}_{j,m} \|_2
\]  
(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 \( \zeta \) be any zero of the CMRH residual polynomial \([36]\) after \( m \) iterations, \( \varphi_m \). Since \( \varphi_m(0) = 1 \), it is \( \zeta \neq 0 \) and we can write
\[
\varphi_m(t) = \left(1 - \frac{t}{\zeta} \right) \tau_{m-1}(t),
\]
with \( \tau_{m-1} \) 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 \( F(A) = \{(Ax, x) | x \in \mathbb{C}^n, \|x\|_2 = 1\} \subset \mathbb{C} \).

On the other hand, since \( A \) is positive definite and \( (Ax, x) = (A^{-H}y, y) \) for \( y = Ax, F(A^{-H}) \) 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 [39, 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 [39, Theorem 3.3].

**Remark 1.** Analogously to the restarted shifted GMRES method, since \( \gamma_0^{(i)} = 1 \) from \( \mathbf{x}_0 = \mathbf{x}_0^{(i)} = 0 \), according to Eq. (3.3) the add systems may converge more rapidly than the seed system. If not, the shift switching technique\(^3\) [50] can be applied.

\(^3\)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.
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 [29,31,45,46,48]. 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 [21,44], in Table 1 we present a comparative complexity analysis between shifted CMRH($m$), shifted GMRES($m$) and shifted SGMRES($m$) [44] 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($m$) [44]. 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 [6,12,16]. One would like to find a matrix $M$, independent of $\sigma_i$, satisfying

$$K_m(AM^{-1}, b) = K_m((A - \sigma_i I)M(\sigma_i)^{-1}, b),$$

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

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

Although $M$ is not needed to compute a basis of $K_m((A - \sigma_i I)M(\sigma_i)^{-1}, b)$, it must be known explicitly to compute the solutions $x^{(i)}$ of the unpreconditioned system from the knowledge of the solution $y^{(i)}$ of the right-preconditioned system; see e.g., [51] for details.

Inspired by [9,51], 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. [52–54] and our recent work [34,55].
Table 1: Computational cost of a generic cycle of the shifted versions of GMRES, SGMRES and CMRH

| Index | Shifted GMRES                                      | Shifted SGMRES                                      | Shifted CMRH                                      |
|-------|----------------------------------------------------|----------------------------------------------------|--------------------------------------------------|
| ℵ₁    | \[2mNz + (2m^2 + 5m + 3)n\]                       | \[2mNz + (2m^2 + 5m + 3)n\]                       | \[2mNz + (m + 2)n + m(m + 1)(n - \frac{m-1}{3})\] |
| ℵ₂    | FLOPs with an Hessenberg matrix \[\tilde{H}_m^G\] | FLOPs with an upper triangular matrix \[R_m\]       | FLOPs with an Hessenberg matrix \[\tilde{H}_m^c\] |
| ℵ₃    | \[t_s(2mn)\]                                      | \[t_s(2mn)\]                                      | \[t_s(2mn)\]                                    |
| ℵ₄    | FLOPs with \[\tilde{H}_m^G(\sigma_i) \mid u_{m+1}\] | FLOPs with \[R_m - \sigma_i[V_m^Hr_{0,1}, I_{m-1}]\] | FLOPs with \[\tilde{H}_m^c(\sigma_i) \mid u_{m+1}\] |

\(\text{ℵ₁}\) represents the cost of iterates for seed system;
\(\text{ℵ₂}\) means the cost of least-squares solve for seed system;
\(\text{ℵ₃}\) represents the cost of necessary vector updates;
\(\text{ℵ₄}\) means the cost of least-squares solve for \(t_s - 1\) add systems \((i = 1, \ldots, t_s - 1)\).

**Remark:** In fact, it is useful to mention that the \(O(m^2)\) operations are needed for coping with the problems in \(\text{ℵ₂}\) and \(\text{ℵ₄}\) 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).
If different preconditioners $P_j, P_j(\sigma)$ are used at every iteration $j$, a relation similar to Eq. (4.2), namely

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

must hold to ensure the shift invariance property of the preconditioned Krylov subspace given by Eq. (4.1). In Eq. (4.3), $\alpha_j$ and $\beta_j$ are parameters dependent on the shifts $\sigma_i$. At each iteration $j$, the preconditioner is applied to a vector $v_j$ in the form

$$(A - \sigma_i I)P_j(\sigma_i)^{-1}v_j = \alpha_j(\sigma_i)AP_j^{-1}v_j - \beta_j(\sigma_i)v_j.$$  

Next, we determine conditions on the coefficients $\alpha_j$’s and $\beta_j$’s to ensure that Eq. (4.3) and Eq. (4.4) hold. Preconditioning is applied by using an inner solver in a multi-shift Krylov method, and the preconditioned vectors

$$z_j = P_j^{-1}v_j, \quad z_j^{(i)} = P_j(\sigma_i)^{-1}v_j,$$

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

$$r_j = v_j - Az_j = v_j - AP_j^{-1}v_j,$$

$$r_j^{(i)} = v_j - (A - \sigma_i I)z_j^{(i)} = v_j - (A - \sigma_i I)P_j(\sigma_i)^{-1}v_j.$$  

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

$$\exists \gamma_j^{(i)} \in \mathbb{C}: \quad \gamma_j^{(i)}r_j = r_j^{(i)}.$$  

Note that the collinearity factors $\gamma_j^{(i)}$ change at each iteration $j$, for every shift $\sigma_i$. Eq. (4.7) is satisfied automatically by methods such as shifted FOM [18–20], shifted BiCGStab [12, 13], shifted BiCRStab [24], shifted IDR(s) [15,16] and by the restarted shifted Hessenberg method [21]. From the conclusion in [16], $\alpha_j$’s and $\beta_j$’s can be determined using Eq. (4.4) and the collinearity relation (4.7). The residuals are collinear if

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

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

$$(A - \sigma_i I)z_j^{(i)} = \gamma_j^{(i)}Az_j - (\gamma_j^{(i)} - 1)v_j,$$

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

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

It remarks that $\alpha_j$’s and $\beta_j$’s do depend on $\sigma_i$, since the collinearity factors $\gamma_j^{(i)}$ change for each shift.
Based on the strategy proposed by Baumann and van Gijzen in [16], we now present a new nested multi-shifted Krylov solver in which the shifted Hessenberg (msHessen) method [21] 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 [52] 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,

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

where at iteration \(1 \leq j \leq m\) flexible preconditioning is applied in the form

\[
z_j^{(\sigma_i)} = P_j^{-1} v_j, \quad z_j^{(\sigma_i)} = P_j^{-1}(\sigma_i) v_j,
\]

with \(Z_m = [z_1, \ldots, z_m]\) and \(Z_m^{(\sigma_i)} = [z_1^{(\sigma_i)}, \ldots, z_m^{(\sigma_i)}]\). It follows that both the Hessenberg process and the strategy proposed in [16] yield the modified Hessenberg matrix

\[
\tilde{H}_m^{(\sigma_i)} = (\tilde{H}_m - I_m) \Gamma_m^{(\sigma_i)} + I_m,
\]

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 \(\Gamma_m^{(\sigma_i)}\) defined as

\[
\Gamma_m^{(\sigma_i)} \equiv \begin{pmatrix}
\gamma_1^{(\sigma_i)} \\
\gamma_2^{(\sigma_i)} \\
\vdots \\
\gamma_m^{(\sigma_i)}
\end{pmatrix} \in \mathbb{C}^{m \times m}.
\]

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

\[
z_j^{(\sigma_i)} = \arg \min_{z \in \mathbb{C}^j} \|((\tilde{H}_j - L_j) \Gamma_j^{(\sigma_i)} + L_j) z - \alpha e_1\|_2, \quad y_j^{(\sigma_i)} = Z_j^{(\sigma_i)} z_j^{(\sigma_i)}
\]

yields approximate solutions to Eq. (1.1) in the search spaces \(Z_j^{(\sigma_i)} \in \mathbb{C}^{2nj \times j}\) that minimize the 2-norm of the quasi-residual of the \(i\)-th shifted linear system, cf. Section 3 and [16,34, Section 3.4]. In Eq. (4.10), the Hessenberg matrix \(\tilde{H}_j\) corresponds to the seed system, and \(\Gamma_j^{(\sigma_i)}\) is related to Eq. (4.9). Note that the shifted Hessenberg procedure yields collinear residuals by default [21]. 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 [16]. On the other hand, according to our recent work [21] 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 operations than shifted GMRES. Thus, the proposed Hessen-FCMRH can be a cost effective nested Krylov solvers 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
Algorithm 2 The FCMRH method with pivoting and \texttt{msHessen} preconditioner

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

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

1. Choose the initial guess $x_0 = x^{(\sigma_0)}_0 = 0$, then $r_0 = b$
2. Set $q = [1, 2, \ldots, n]^T$ and determine $j_0$ such that $|(r_0)_j| = \|r_0\|_{\infty}$
3. Set $\beta = (r_0)_{j_0}$, $l_1 = r_0/\beta$ and $(q)_1 \leftrightarrow (q)_{j_0}$, where $\leftrightarrow$ is used to swap contents.
4. for $j = 1, 2, \ldots, m_i$, do
5. Preconditioning: $z^{(\sigma_i)}_j = \texttt{msHessen}(A - \sigma_i I, l_j, m_i)$
6. Compute $\gamma^{(\sigma_i)}_j$ according to the similar formula in \cite[Eq. (3.9)]{}
7. Compute $u = Az^{(0)}_j$ (hint: $\sigma_i = 0$)
8. for $k = 1, 2, \ldots, j$, do
9. $\hat{h}_{k,j} = (u)_{(q)_k}$
10. $u = u - \hat{h}_{k,j}l_k$
11. end for
12. if $j < n$ and $u \neq 0$ then
13. Determine $j_0 \in \{j + 1, \ldots, n\}$ such that $|(u)_{(q)_{j_0}}| = \|(u)_{(q)_{j_0+1:(q)_n}}\|_{\infty}$
14. $\hat{h}_{j+1,j} = (u)_{(q)_{j_0}}$, $l_{j+1} = u/\hat{h}_{j+1,j}$; $(q)_{j+1} \leftrightarrow (q)_{j_0}$
15. else
16. $\hat{h}_{j+1,j} = 0$; Stop
17. end if
18. // Loop over shifted systems:
19. for $i = 1, 2, \ldots, t$ do
20. Define the matrix $Z^{(\sigma_i)}_j = [z^{(\sigma_i)}_1, z^{(\sigma_i)}_2, \ldots, z^{(\sigma_i)}_j]$
21. Set up $\tilde{H}_j(\sigma_i)$ according to Eq. \cite[(4.9)]{}
22. Solve $y^{(\sigma_i)}_j = \arg \min_{y \in \mathbb{C}^j} \|\beta e_1 - \tilde{H}_j(\sigma_i) y\|$ with $e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^{j+1}$
23. $x^{(\sigma_i)}_j = x^{(\sigma_i)}_0 + Z^{(\sigma_i)}_j y^{(\sigma_i)}_j$
24. end for
25. end for
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 $Z_j^{(σ_i)}$ matrices which span the solution space for each shifted problem [52,53]. The memory requirements increase to about $O(2ntm_o)$ for $Z_m^{(σ_i)}$, and each iteration of the nested multi-shifted Krylov solver needs to evaluate $m_o m_i$ 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 preconditioning [34,52], 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 [16].

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 $b$ is the vector with all 1’s. The iterative solution is started from $x_0^{(i)} = 0$ and is stopped at iteration $k$ when $\|r_k^{(i)}\|_2/\|b\|_2 < 10^{-8}$ for $i = 1, 2, \ldots, t_s$ for all linear systems, or after at most $Max_{mvps}$ 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 [56]. The main characteristics of the test problems are listed in Table 2. We use shifts $σ_j = -j/10000$ ($j = 1, 2, 3, 4, 5$) for problems $Σ_1$, $Σ_4$, $Σ_5$, $Σ_6$, $Σ_8$, shifts $σ_j = -(8 + j)/200000$ for $Σ_2$, shifts $σ_j = -(179 + j)/20000$ for $Σ_3$, and $σ_j = -j/20000$ for $Σ_7$. The first linear system $(A - σ_1 I)x^{(1)} = b$ 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 [9,16,40,41], and the maximum number of matrix-vector products $Max_{mvps}$ 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 $sSGMRES(m)$ to converge to prescribed accuracy. All methods converge within the maximum number of iterations, except $sQMRIDR(1)$ for Problem Π4.

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

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

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14
Table 2: Set and characteristics of the test problems used for Experiment 5.1.

| Index | Matrix             | Size   | Field                          | nnz(A)  |
|-------|--------------------|--------|--------------------------------|---------|
| Σ1    | poisson3Da         | 13,514 | Computational fluid dynamics    | 352,762 |
| Σ2    | epb1               | 14,734 | Thermal problem                 | 95,053  |
| Σ3    | waveguide3D        | 21,036 | Electromagnetics problem        | 303,468 |
| Σ4    | kim1               | 38,415 | 2D/3D problem                   | 933,195 |
| Σ5    | poisson3Db         | 85,623 | Computational fluid dynamics    | 2,374,949 |
| Σ6    | vfem               | 93,476 | Electromagnetics problem        | 1,434,636 |
| Σ7    | matrix-new_3       | 125,329| Semiconductor device problem    | 893,984 |
| Σ8    | FEM_3D_thermal2    | 147,900| Thermal problem                 | 3,489,300 |

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

| Index | sGMRES(\( m \)) | sCMRH(\( m \)) | sQMRIDR(1) | sQMRIDR(2) | sSGMRES(\( m \)) |
|-------|-----------------|----------------|------------|------------|------------------|
| Σ1    | 320             | 0.665          | 360        | 0.358      | 250              | 0.464            | 225 | 0.510 | 240\(^{+}\) | 0.712 |
| Σ2    | 1160            | 1.339          | 1769       | 0.963      | 1367             | 1.694            | 989 | 1.559 | 1050\(^{+}\) | 2.444 |
| Σ3    | 480             | 2.644          | 560        | 2.065      | 437              | 2.640            | 392 | 3.275 | ‡         | ‡     |
| Σ4    | 2000            | 20.390         | 1640       | 11.268     | ‡                | ‡                | 2231| 36.052| ‡         | ‡     |
| Σ5    | 600             | 6.741          | 680        | 6.211      | 561              | 9.309            | 427 | 9.527 | 484\(^{+}\) | 9.524 |
| Σ6    | 240             | 4.461          | 280        | 3.367      | 413              | 10.241           | 224 | 9.189 | ‡         | ‡     |
| Σ7    | 120             | 0.789          | 120        | 0.476      | 287              | 3.423            | 152 | 3.215 | ‡         | ‡     |
| Σ8    | 520             | 12.124         | 560        | 6.764      | 793              | 17.560           | 503 | 16.932| ‡         | ‡     |

and \( sSGMRES(\( m \)) \) for Problem \( \Pi_{\ell}, \ell = 3, 4, 6, 7, 8 \). 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 \( sQMRIDR(s) \) are 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, \( sSGMRES(\( m \)) \) is less robust that the other solvers.

The relative residual histories plotted in Fig. 1 for different shifts confirm the conclusion reported in [39] 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 [56]. Hereafter, they will be denoted as problems \( \Pi_i \) for \( i = 1, 2, \ldots, 7 \). We select shifts equals to \( \sigma_j \in \mathcal{I} = -\{0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07\} \) and we use \((A - \sigma_1 I)x^{(1)} = b\) as the seed system. The maximum number of matrix-vector products
is set equal to 5000.

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(\(m\)) |
|-------|----------------|---------------|-------------|-------------|-----------------|
| \( \Pi_1 \) | 1120            | 15.007        | 1480        | 14.974      | 845             | 15.557          | 732           | 20.549        | 3459\(^+\)    | 82.897         |
| \( \Pi_2 \) | 880             | 11.388        | 1120        | 11.236      | 746             | 13.835          | 675           | 19.018        | \( \dagger \) | \( \dagger \) |
| \( \Pi_3 \) | 720             | 9.173         | 880         | 8.815       | 709             | 13.345          | 633           | 19.018        | \( \dagger \) | \( \dagger \) |
| \( \Pi_4 \) | 640             | 8.265         | 800         | 7.986       | 757             | 13.973          | 687           | 20.283        | \( \dagger \) | \( \dagger \) |
| \( \Pi_5 \) | 640             | 8.255         | 840         | 8.279       | 589             | 11.473          | 477           | 14.797        | \( \dagger \) | \( \dagger \) |
| \( \Pi_6 \) | 840             | 10.762        | 1160        | 11.712      | 539             | 10.257          | 456           | 13.468        | \( \dagger \) | \( \dagger \) |
| \( \Pi_7 \) | 680             | 8.656         | 840         | 8.321       | 582             | 11.171          | 477           | 14.109        | 1743\(^+\)    | 44.703         |

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 \( \Pi_5 \) and \( \Pi_6 \), \( s\text{CMRH}(m) \) is more cost-effective than \( s\text{GMRES}(m) \). In general \( s\text{QMRIDR}(s) \) requires less iterations but more CPU time to converge. One exception is Problem \( \Pi_6 \), where \( s\text{QMRIDR}(1) \) is the fastest solver. In our experiments, \( s\text{Ad-SGMRES}(m) \) is not a competitive choice in terms of both MVPs and elapsed CPU time.

The convergence histories and the final accuracies of \( s\text{GMRES}(m) \) and \( s\text{CMRH}(m) \) are once again comparable based on the relative residual histories plotted in Fig. 2. The approximate solutions computed by \( s\text{CMRH}(m) \) are slightly more accurate than for the other solvers, whereas the final residual norms of \( s\text{GMRES}(m) \) are smaller than those of \( s\text{QMRIDR}(s) \). We conclude that \( s\text{CMRH}(m) \) 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 the approximate solution of FDEs in many areas, see e.g. [57, 58]. Here we consider a benchmark problem coming from the 3D time-fractional convection-diffusion-reaction equation defined as

\[
\begin{align*}
\frac{\partial^\alpha u}{\partial t^\alpha} &= \epsilon \Delta u - \vec{\beta} \cdot \nabla u + ru, \\
\Delta u &= \epsilon \Delta u - \vec{\beta} \cdot \nabla u + ru, \\
\frac{\partial^\alpha u}{\partial t^\alpha} &= \epsilon \Delta u - \vec{\beta} \cdot \nabla u + ru, \\
\end{align*}
\]

\( (x, y, z) \in \Omega = (0, 1)^3, \ t \in [0, T], \)

\( u(x, y, z, t) = 0, \quad (x, y, z) \in \partial \Omega, \ t \in [0, T], \) \quad (5.1)

\( u(x, y, z, 0) = x(1 - x)y(1 - y)z(1 - z), \quad (x, y, z) \in \Omega. \)

Problem (5.1) is a modification of the third example presented in Ref. [17], with diffusion constant \( \epsilon = 1 \), reaction constant \( r = 400 \) and convection parameter \( \vec{\beta} = \)
Fig. 2: Relative residual histories of different iterative solvers for test problem $\Pi_2$ in Table 4.
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

$$\frac{d^\gamma u}{dt^\gamma} = Au(t), \quad u(0) = u_0. \quad (5.2)$$

is obtained, where $u$ 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

$$u(t) = e_{\gamma,1}(t; A)u_0, \quad \text{and} \quad e_{\gamma,1}(t; A) = t^{\gamma-1}E_{\gamma,1}(t^-A) = E_{\gamma,1}(t^\gamma A), \quad (5.3)$$

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

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

In light of Eq. (5.3), the numerical solution $u(t)$ can be computed as the product of the matrix ML function $E_{\gamma,1}(t^\gamma A)$ times $u_0$. 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 $E_{\gamma,1}(t^\gamma A)u_0$, 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 $E_{\gamma,1}(t^\gamma A)u_0$ [59], that has the following representation

$$E_{\gamma,1}(A)u_0 = f_\nu(A)u_0 = \sum_{j=1}^{\nu} w_j(z_j I - A)^{-1}u_0, \quad (5.4)$$

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 $(-A + z_j I)x^{(j)} = u_0$, $z_j \in \mathbb{C}$.

In Table 5 we compare different shifted Krylov subspace methods for solving five groups of real shifted linear systems with same seed system $-Ax = u_0$ 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($s$) are 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
Table 5: Convergence results with different shifted Krylov subspace solvers for Experiment 5.3, using \( m = 40 \). Symbol \( \dagger \) means convergence failure.

| \((\gamma, \nu)\) | \( \text{sGMRES}(m) \) | \( \text{sCMRH}(m) \) | \( \text{sQMRIDR}(1) \) | \( \text{sQMRIDR}(2) \) | \( \text{sAd-SGMRES}(m) \) |
|----------------|----------------|----------------|----------------|----------------|----------------|
| \((0.2, 6)\)  | 800 3.421 1000 2.990 | 299 6.225 182 6.081 \( \dagger \) \( \dagger \) |
| \((0.4, 8)\)  | 800 3.553 1000 3.051 | 299 8.061 182 7.809 \( \dagger \) \( \dagger \) |
| \((0.6, 10)\) | 800 3.560 1000 3.130 | 299 9.651 182 9.542 \( \dagger \) \( \dagger \) |
| \((0.8, 10)\) | 800 3.547 1000 3.136 | 299 9.755 182 9.633 \( \dagger \) \( \dagger \) |
| \((0.9, 12)\) | 800 3.589 1000 3.204 | 299 11.302 185 11.317 \( \dagger \) \( \dagger \) |

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

| \((h, r)\) | \( \text{sGMRES}(m) \) | \( \text{sCMRH}(m) \) | \( \text{sQMRIDR}(1) \) | \( \text{sQMRIDR}(2) \) | \( \text{sAd-SGMRES}(m) \) |
|-----------|----------------|----------------|----------------|----------------|----------------|
| \((\frac{1}{3}, 400)\) | \( \dagger \) \( \dagger \) 1360 8.41 | 283 22.52 200 24.44 2653\( ^\dagger \) 197.72 |
| \((\frac{1}{5}, 500)\) | \( \dagger \) \( \dagger \) 1400 8.63 | 293 23.58 215 25.94 \( \dagger \) \( \dagger \) |
| \((\frac{1}{9}, 400)\) | \( \dagger \) \( \dagger \) 1640 61.57 | 358 153.55 275 162.09 \( \dagger \) \( \dagger \) |
| \((\frac{1}{15}, 500)\) | \( \dagger \) \( \dagger \) 3000 114.90 | 359 155.35 278 162.61 \( \dagger \) \( \dagger \) |
| \((\frac{1}{20}, 400)\) | \( \dagger \) \( \dagger \) 1680 138.81 | 397 355.76 329 391.61 \( \dagger \) \( \dagger \) |
| \((\frac{1}{50}, 500)\) | \( \dagger \) \( \dagger \) 2680 228.47 | 402 359.26 333 395.71 \( \dagger \) \( \dagger \) |

\( \vec{\beta} \) and reaction parameter \( r \) in Eq. (4.1) always result in highly nonsymmetric, ill-conditioned finite difference matrix \( A \) [17]. In these experiment we set \( \text{Max\_mups} = 6000 \). We can see from Table 6 that in our runs only \( \text{sCMRH}(m) \) and \( \text{sQMRIDR}(s) \) are able to solve all the shifted linear systems. The reason might be that the \( \text{sGMRES}(m) \) and \( \text{sAd-SGMRES}(m) \) methods are more sensitive than the other two shifted iterative solvers to the high nonsymmetry and indefiniteness of the coefficient matrix. In addition, although \( \text{sQMRIDR}(s) \) always requires less number of \text{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 \( \text{sCMRH}(m) \) 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 \( \text{Hessen-FCMRH}, \text{Hessen-FGMRES} \) and \( \text{FOM-FCMRH} \) against \( \text{FOM-FGMRES} \) [16] 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 [59, 60] and the QCD simulation. In these runs, we select \( Ax = b \) 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 \( \exp(\tau L)u_0 \) 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 as the one proposed in [60, Example 2], except for different values of the shift \( \tau \). We use MATLAB codes available at \( \text{https://numerical-analysis.uibk.ac.at/exp-int-software} \) to generate matrices \( L \) of different sizes equal to \( 9,801 \times 9,801 \), \( 14,161 \times 14,161 \), 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.

Table 7: Number of inner and outer iterations and CPU solution time for experiments with different nested Krylov methods to solve Group I problems.

| \((h, \tau)\) | Hessen-FCMRH | Hessen-FGMRES | FOM-FCMRH | FOM-FGMRES |
|--------------|----------------|----------------|-------------|-------------|
| \((\frac{1}{100},0.04)\) | IT_in | IT_out | CPU | IT_out | CPU | IT_out | CPU |
| 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 | 6 | 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 |

In Group II, we use the same test problems of Section 5.3 with the following setup values: \( \gamma = 0.9 \) and \( \vec{\beta} = (0/\sqrt{5},250/\sqrt{5},500/\sqrt{5})^T \) with \( h = 0.025 \) and \( h = 0.02 \) for test problems \( \Xi_1 \) and \( \Xi_2 \). 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 \( \vec{\beta} = (500/\sqrt{5},250/\sqrt{5},500/\sqrt{5})^T \) with \( h = 0.02 \) and \( h = 0.0125 \) for test problems \( \Xi_3 \) and \( \Xi_4 \). 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 \( \text{IT_in} \) and \( \text{IT_out} \), 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
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 | IT\_out | CPU | IT\_in | IT\_out | CPU | IT\_in | IT\_out | CPU |
|-------|--------|---------|-----|--------|---------|-----|--------|---------|-----|
| Ξ₁    | 80     | 2       | 1.281 | 3      | 1.989   | 3   | 2.626  | 3       | 2.679 |
|       | 70     | 4       | 2.294 | 3      | 2.938   | 4   | 3.044  | 4       | 3.044 |
|       | 60     | 18      | 11.442| 7      | 3.766   | 6   | 3.826  | 5       | 3.030 |
| Ξ₂    | 90     | 3       | 4.344 | 3      | 4.368   | 4   | 7.847  | 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|
| Ξ₃    | 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|
| Ξ₄    | 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|

inner steps, with the exception of (1/120, 0.04) and IT\_in = 140. The result is supported by the conclusions presented in [21] 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 Ξ₁ with IT\_in = 60 and problem Ξ₂ 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 γ = 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 iterations, the smaller the number of outer steps, and vice versa for the solution time. The results show that the proposed
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      |

The Hessen-FCMRH method can be regarded as a robust choice for this problem.

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      |

Here problem QCDx is denoted as problem Π₂ 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 [16]. 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. [16]. 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.

Acknowledgement

The authors are greatly grateful to Prof. Gang Wu and Prof. Yan-Fei Jing for their constructive discussions and insightful comments. Especially, we would like to thank Dr. Mohammed Heyouni and Dr. Jens-Peter M. Zemke for making their MATLAB package of Ref. [35] and codes of the multi-shifted QMRIDR(s) method, respectively, available for us. This research is supported by NSFC (61772003, 11601323, and 11801463), the Fundamental Research Funds for the Central Universities (JBK1902028) and the Ministry of Education of Humanities and Social Science Layout Project (19JYA790094).

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