Applied Numerical Mathematics 81 (2014) 105–118

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

Krylov subspace recycling for sequences of shifted linear systems ☆

Kirk M. Soodhalter [a,*], Daniel B. Szyld [b], Fei Xue [c]

[a] Industrial Mathematics Institute, Johannes Kepler University, Altenbergerstraße 69, A-4040 Linz, Austria
[b] Department of Mathematics, Temple University, 1805 N Broad Street, Philadelphia, PA 19122-6094, United States
[c] Department of Mathematics, University of Louisiana at Lafayette, Lafayette, LA 70504, United States

ARTICLE INFO

Article history:
Received 4 September 2013
Received in revised form 28 January 2014
Accepted 4 February 2014
Available online 15 March 2014

Keywords:
Krylov subspace methods
Subspace recycling
Shifted linear systems
QCD

ABSTRACT

We study the use of Krylov subspace recycling for the solution of a sequence of slowly-changing families of linear systems, where each family consists of shifted linear systems that differ in the coefficient matrix only by multiples of the identity. Our aim is to explore the simultaneous solution of each family of shifted systems within the framework of subspace recycling, using one augmented subspace to extract candidate solutions for all the shifted systems. The ideal method would use the same augmented subspace for all systems and have fixed storage requirements, independent of the number of shifted systems per family. We show that a method satisfying both requirements cannot exist in this framework.

As an alternative, we introduce two schemes. One constructs a separate deflation space for each shifted system but solves each family of shifted systems simultaneously. The other builds only one recycled subspace and constructs approximate corrections to the solutions of the shifted systems at each cycle of the iterative linear solver while only minimizing the base system residual. At convergence of the base system solution, we apply the method recursively to the remaining unconverged systems. We present numerical examples involving systems arising in lattice quantum chromodynamics.

1. Introduction

We consider the solution of a sequence of families of non-Hermitian linear systems. Let $\mathcal{F}$ denote a family of coefficient matrices differing by multiples of the identity. In other words,

$$\mathcal{F} = \left\{\mathbf{A} + \sigma^{(\ell)}\mathbf{I}\right\}_{\ell=1}^{L} \subset \mathbb{C}^{n\times n}, \tag{1}$$

where L is the number of matrices in the family, and we are solving the family of linear systems

$$\left(\mathbf{A} + \sigma^{(\ell)}\mathbf{I}\right)\mathbf{x}^{(\ell)} = \mathbf{b} \quad \text{for } \ell = 1, \ldots, L. \tag{2}$$

☆ This research was supported in part by the U.S. Department of Energy under grant DE-FG02-05ER25672 and the U.S. National Science Foundation under grant DMS-1115520.

* Corresponding author.
E-mail addresses: soodhalter@indmath.uni-linz.ac.at (K.M. Soodhalter), szyld@temple.edu (D.B. Szyld), fxue@louisiana.edu (F. Xue).

http://dx.doi.org/10.1016/j.apnum.2014.02.006
0168-9274/

We call the numbers $\{\sigma^{(\ell)}\}_{\ell=1}^{L} \subset \mathbb{C}$ *shifts*, $\mathbf{A}$ the *base matrix*, and $\mathbf{A}+\sigma\mathbf{I}$ a *shifted matrix*. Systems of the form (2) are called *shifted linear systems*. There are many applications which warrant the solution of a family of shifted linear systems with coefficient matrices belonging to $\mathcal{F}$, such as those arising in lattice quantum chromodynamics (QCD) (see, e.g., [13]) as well as other applications such as Tikhonov–Philips regularization (see, e.g., [14] and [12]), global methods of nonlinear analysis, and Newton trust region methods [5]. Krylov subspace methods have been proposed to simultaneously solve this family of systems [10,11,27].

Our goal is to explore simultaneously solving a family of shifted systems (or a sequence of families) over an augmented Krylov subspace, i.e., we explore how one would incorporate existing shifted system techniques into the subspace recycling framework [23]. Does a method exist which (a) simultaneously solves all systems in the family, using one subspace to extract candidate solutions, and (b) satisfies a fixed storage requirement,[1] independent of the number of shifts?

In this paper, we treat this question in the context of the recycled GMRES framework [23] combined with GMRES for shifted systems [11]. We demonstrate that the two mentioned requirements (a) and (b) cannot be achieved simultaneously. We present two methods: one which sacrifices fixed storage and the other which sacrifices the simultaneous solution of all shifted systems in each family, instead solving one system and simultaneously improving the approximations of the others at a very modest cost.

For simplicity (and to avoid excessive indices), our discussion will mostly center around solving the model problem,

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{3}$$

$$(\mathbf{A}+\sigma\mathbf{I})\mathbf{x}^{(\sigma)} = \mathbf{b}, \tag{4}$$

using Recycled GMRES in the presence of a k-dimensional initial recycled subspace $\mathcal{U}$. However, what we derive applies to a more general situation. Let $\mathcal{F}_i$ denote the ith family of linear systems, defined by

$$\mathcal{F}_i = \left\{\mathbf{A}_i + \sigma_i^{(\ell)}\mathbf{I}\right\}_{\ell=1}^{L_i} \subset \mathbb{C}^{n\times n},$$

where L_i denotes the number of linear systems to be solved at step i. In other words, at step i, for shifts $\{\sigma_i^{(\ell)}\}_{\ell=1}^{L_i}$ we are solving systems of the form

$$\left(\mathbf{A}_i + \sigma_i^{(\ell)}\mathbf{I}\right)\mathbf{x}_i^{(\ell)} = \mathbf{b}_i \quad \text{for } \ell = 1\ldots L_i.$$

This is the general problem our desired method is meant to address.

It should be noted that, for solving the model problem in the absence of the initial subspace $\mathcal{U}$, techniques already have been developed to solve a family of systems simultaneously, building deflation subspaces from harmonic Ritz vectors; see, e.g., [7]. We are exploring here the situation in which we have an initial deflation subspace $\mathcal{U}$, a case for which the techniques presented in [7] do not apply.

In the next section, we review some existing methods for solving (3) and (4), and we describe the framework of subspace recycling used in, e.g., [23]. In Section 3, we show that it is generally *not* possible to construct solutions for all shifted systems over the same augmented subspace in a way that is compatible with restarting while allowing for the simultaneous solution of all systems. In Section 4, we present a method which sacrifices the fixed storage requirement. This method is a direct extension of the one presented in [11]. We present a scheme in Section 5 which sacrifices the requirement that each family be solved simultaneously. This method produces improved approximations for the shifted system while solving the base system, using only one recycled subspace. This method is also derived from [11], but the approximations are not computed according to the same residual collinearity constraints as described in [11]. In Section 6, we present numerical results for a family of simple bidiagonal matrices and for some sequences of QCD matrices obtained from [8] and [18].

2. Preliminaries

In many Krylov subspace iterative methods, recall that we generate an orthonormal basis for the Krylov subspace

$$\mathcal{K}_j(\mathbf{A},\mathbf{u}) = \operatorname{span}\left\{\mathbf{u}, \mathbf{A}\mathbf{u}, \ldots, \mathbf{A}^{j-1}\mathbf{u}\right\}$$

with the Arnoldi process, where $\mathbf{u}$ is some starting vector. Let $\mathbf{V}_j \in \mathbb{C}^{n\times j}$ be the matrix with orthonormal columns generated by the Arnoldi process spanning $\mathcal{K}_j(\mathbf{A},\mathbf{u})$. Then we have the Arnoldi relation

$$\mathbf{A}\mathbf{V}_j = \mathbf{V}_{j+1}\overline{\mathbf{H}}_j \tag{5}$$

with $\overline{\mathbf{H}}_j \in \mathbb{C}^{(j+1)\times j}$; see, e.g., [25, Section 6.3] and [29]. Let $\mathbf{x}_0$ be an initial approximation and $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ be the initial residual. At iteration j, we compute $\mathbf{x}_j = \mathbf{x}_0 + \mathbf{t}_j$, where $\mathbf{t}_j \in \mathcal{K}_j(\mathbf{A},\mathbf{r}_0)$. In GMRES [26], we choose

[1] We note that "fixed storage" in this context means that, aside from storing an approximation for each additional shifted system, the method incurs no further memory cost per shift.

$$\mathbf{t}_j = \underset{\mathbf{t}\in\mathcal{K}_j(\mathbf{A},\mathbf{r}_0)}{\operatorname{argmin}} \left\|\mathbf{b}-\mathbf{A}(\mathbf{x}_0+\mathbf{t})\right\|,$$

and this is equivalent to solving the smaller minimization problem

$$\mathbf{y}_j = \underset{\mathbf{y}\in\mathbb{C}^j}{\operatorname{argmin}} \left\|\bar{\mathbf{H}}_j\mathbf{y} - \|\mathbf{r}_0\|\mathbf{e}_1^{(j+1)}\right\|, \tag{6}$$

where we use the notation $\mathbf{e}_\ell^{(k)}$ to denote the ℓth Cartesian basis vector in $\mathbb{C}^k$, and setting $\mathbf{x}_j = \mathbf{x}_0 + \mathbf{V}_j\mathbf{y}_j$. In restarted GMRES (GMRES(m)), we halt this process at step m, discard the matrix $\mathbf{V}_m$, and restart with the new initial residual $\mathbf{r}_0 \leftarrow \mathbf{b} - \mathbf{A}\mathbf{x}_m$. This process is repeated until we achieve convergence. Adaptions of restarted GMRES to solve (2) have been previously proposed; see, e.g., [11].

It should be noted that methods based on the nonsymmetric Lanczos process have also been adapted for solving (2). Extensions of methods, such as BiCGStab [10] and QMR, have been developed [13]. A recently proposed method called IDR [32], which has been shown to be a generalization of BiCGStab [30], has also been extended to solve (3) and (4) [17]. We will not deal with nonsymmetric Lanczos-based methods in this paper, but these alternatives are worth mentioning.

Many methods for solving (2) use the fact that for any shift σ, the Krylov subspace generated by $\mathbf{A}$ and $\mathbf{b}$ is invariant under the shift, i.e.,

$$\mathcal{K}_j(\mathbf{A},\mathbf{b}) = \mathcal{K}_j(\mathbf{A}+\sigma\mathbf{I},\widetilde{\mathbf{b}}),$$

as long as the starting vectors are collinear, i.e., $\widetilde{\mathbf{b}} = \beta\mathbf{b}$, with a shifted Arnoldi relation similar to (5)

$$(\mathbf{A}+\sigma\mathbf{I})\mathbf{V}_j = \mathbf{V}_{j+1}\bar{\mathbf{H}}_j^{(\sigma)}, \tag{7}$$

where

$$\bar{\mathbf{H}}_m^{(\sigma)} = \bar{\mathbf{H}}_m + \begin{bmatrix}\sigma\mathbf{I}_{m\times m}\\ \mathbf{0}_{1\times m}\end{bmatrix}.$$

Note that the shift-invariance no longer holds if general preconditioning is used. However, polynomial preconditioning [15,39] would be appropriate in this setting. There has been recent work on choosing optimal polynomial preconditioners in the setting of solving multiple shifted systems [2,20]. In this project, though, we focus on the unpreconditioned case, as in [11,22].

The shift-invariance property indicates that large savings in storage and time can be achieved by generating only one sequence of Krylov subspaces and solving all shifted systems in one Krylov subspace simultaneously. Suppose that the initial residuals of (3) and (4) are collinear. As we iterate, we simply apply the Petrov–Galerkin condition with the same subspaces for all residuals. However, once restarting is introduced, the situation becomes more complicated. The projected residuals may no longer be collinear and the Krylov subspaces at restart will not be equivalent. In [10], a general theorem is presented which describes conditions under which the residuals will be naturally collinear in this manner. In [11] it is observed that the GMRES residual projection does not have this property.

Frommer and Glässner [11] proposed a restarted GMRES method to solve (3)–(4). Suppose that the residuals for the shifted and base systems are collinear, i.e., $\mathbf{r}_0^{(\sigma)} = \beta_0\mathbf{r}_0$. Within a cycle, for the base system approximation, the residual is minimized using GMRES. The shifted system approximation is found by requiring the residual to be collinear to that of the base system, i.e.,

$$\mathbf{r}_m^{(\sigma)} = \beta_m\mathbf{r}_m. \tag{8}$$

After computing the GMRES solution for the base system, we can denote the GMRES least-squares residual $\mathbf{z}_{m+1} = \|\mathbf{r}_0\|\mathbf{e}_1^{(m+1)} - \bar{\mathbf{H}}_m\mathbf{y}_m$. It is shown in [11] that for (8) to hold, we must have

$$\bar{\mathbf{H}}_m^{(\sigma)}\mathbf{y}_m^{(\sigma)} + \mathbf{z}_{m+1}\beta_m = \beta_0\|\mathbf{r}_0\|\mathbf{e}_1^{(m+1)},$$

and $\mathbf{x}_m^{(\sigma)} = \mathbf{x}_0^{(\sigma)} + \mathbf{V}_m\mathbf{y}_m^{(\sigma)}$. Thus, we can compute both $\mathbf{y}_m^{(\sigma)}$ and β_m by solving the augmented linear system,

$$\begin{bmatrix}\bar{\mathbf{H}}_m^{(\sigma)} & \mathbf{z}_{m+1}\end{bmatrix}\begin{bmatrix}\mathbf{y}_m^{(\sigma)}\\ \beta_m\end{bmatrix} = \beta_0\|\mathbf{r}_0\|\mathbf{e}_1^{(m+1)}. \tag{9}$$

The collinear residual exists if and only if the residual polynomial $r_m(t)$, associated with $\mathbf{r}_m$ satisfies $r_m(-\sigma)\neq 0$; otherwise, the augmented system is singular [11, Lemmas 2.1 and 2.4]. For a positive-real matrix $\mathbf{A}$ (field of values being contained in the right half-plane), restarted GMRES for shifted linear systems computes solutions at every iteration for all shifts $\sigma^{(i)} > 0$ and, in addition, we have $\|\mathbf{r}_m\| \leqslant \|\mathbf{r}_m^{(\sigma_i)}\|$ for such shifts [11]. The shifts applied in the setting of QCD yield a family of coefficient matrices which are, in theory, real-positive [11].

We briefly review the Recycled GMRES method described in [23]. This algorithm represents the confluence of two approaches: those descending from the implicitly restarted Arnoldi method [19], such as Morgan's GMRES-DR [22], and those

descending from de Sturler's GCRO method [35]. GMRES-DR is a restarted GMRES algorithm, where at the end of each cycle, harmonic Ritz vectors are computed, and a subset of them are used to augment the Krylov subspace generated at the next cycle. The GCRO method allows the user to select the optimal correction over arbitrary subspaces. This concept is extended by de Sturler in [36], where a framework is provided for selecting the optimal subspace to retain from one cycle to the next so as to minimize the error produced by discarding useful information accumulated in the subspace for candidate solutions before restart. This algorithm is called GCROT, where OT stands for optimal truncation. A simplified version of the GCROT approach, based on restarted GMRES (called LGMRES) is presented in [3]. Parks et al. in [23] combine the ideas of [22] and [36] and extend them to a sequence of slowly-changing linear systems. They call their method GCRO-DR (Recycled GMRES).

Suppose we are solving (3), and we have a k-dimensional subspace $\mathcal{U}$ whose image under the action of $\mathbf{A}$ is $\mathcal{C} = \mathbf{A}\mathcal{U}$. Let $\mathbf{P}$ be the orthogonal projector onto $\mathcal{C}^{\perp}$. Furthermore, let $\mathbf{x}_0$ be such that $\mathbf{r}_0 \in \mathcal{C}^{\perp}$ (this is always cheaply available). We generate the Krylov subspace with respect to the projected operator $\mathbf{PA}$, $\mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$. At iteration m, the Recycled GMRES method generates the approximation

$$\mathbf{x}_m = \mathbf{x}_0 + \mathbf{s}_m + \mathbf{t}_m$$

where $\mathbf{s}_m \in \mathcal{U}$ and $\mathbf{t}_m \in \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$. The corrections $\mathbf{s}_m$ and $\mathbf{t}_m$ are chosen according to the minimum residual, Petrov–Galerkin condition over the augmented Krylov subspace, i.e.,

$$\mathbf{r}_m \perp \mathbf{A}\big(\mathcal{U} + \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)\big). \tag{10}$$

At the end of the cycle, an updated $\mathcal{U}$ is constructed, the Krylov subspace basis is discarded, and we restart. At convergence, $\mathcal{U}$ is saved, to be used when solving the next linear system.

In terms of implementation, Recycled GMRES can be described as a modification of the GMRES algorithm. Let $\mathbf{U} \in \mathbb{C}^{n\times k}$ have columns spanning $\mathcal{U}$, scaled such that $\mathbf{C} = \mathbf{AU}$ has orthonormal columns. Then we can explicitly construct $\mathbf{P} = \mathbf{I} - \mathbf{CC}^*$. At each iteration, applying $\mathbf{P}$ is equivalent to performing k steps of the Modified Gram–Schmidt process to orthogonalize the new Arnoldi vector against the columns of $\mathbf{C}$. The orthogonalization coefficients generated at step m are stored in the mth column of $\mathbf{B}_m = \mathbf{C}^*\mathbf{AV}_m$, and $\mathbf{B}_{m+1}$ is simply $\mathbf{B}_m$ with one new column appended. Let $\overline{\mathbf{H}}_m$ and $\mathbf{V}_m$ be defined as before, but for the projected Krylov subspace $\mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$. Enforcing (10) is equivalent to solving the GMRES minimization problem (6) for $\mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$ and setting

$$\mathbf{s}_m = -\mathbf{UB}_m\mathbf{y}_m \quad \text{and} \quad \mathbf{t}_m = \mathbf{V}_m\mathbf{y}_m,$$

so that

$$\mathbf{x}_m = \mathbf{x}_0 - \mathbf{UB}_m\mathbf{y}_m + \mathbf{V}_m\mathbf{y}_m = \mathbf{x}_0 + [\,\mathbf{U} \quad \mathbf{V}_m\,]\begin{bmatrix} -\mathbf{B}_m\mathbf{y}_m \\ \mathbf{y}_m \end{bmatrix}.$$

This is a consequence of the fact that the Recycled GMRES least squares problem, as stated in [23, Equation 2.13] can be satisfied exactly in the first k rows.

Convergence results for augmented Krylov subspace methods were shown in, e.g., [9,24], but not much work has been done in the context of Recycled GMRES. Some not-yet-published work has been presented by de Sturler that specifically addresses the convergence behavior of optimal methods in which we recycle using the above framework [37]. This work asserts that the improvement of convergence bounds from recycling a particular subspace can be quantified according to the quality of the recycled subspace as an invariant subspace of $\mathbf{A}$. A particular finding, backed up by empirical observation, is that an approximate invariant subspace of modest quality (as judged by the largest principal angle between $\mathbf{U}$ and $\mathbf{C}$) will still yield improvements in bounds on the residual norm.

It should be noted that for a single system, deflation and seeding of the Krylov subspace in the context lattice QCD have been previously considered; see, e.g., [1,34]. Furthermore, if we have no initial recycled space and compute harmonic Ritz vectors at each restart, Recycled GMRES is algebraically equivalent to Morgan's GMRES-DR [22]. In fact, Morgan's method was extended in [7] to the case of shifted systems.

Iterating orthogonally to an approximate invariant subspace to accelerate convergence of GMRES can be justified by the theoretical work in [28]. It was shown that the widely observed two-stage convergence behavior of GMRES, which has been termed *superlinear convergence*, is governed by how well the Krylov subspace approximates a certain eigenspace. Specifically, when the Krylov subspace contains a good approximation to the eigenspace (call this eigenspace $\mathcal{S}$) associated to eigenvalues hindering convergence, we will switch from the slow phase to the fast phase, and convergence will mimic that of GMRES on the projected operator $\mathbf{P}_{\mathcal{S}}^{\perp}\mathbf{A}$ where $\mathbf{P}_{\mathcal{S}}^{\perp}$ is the orthogonal projector onto the orthogonal complement of $\mathcal{S}$. This analysis complements previous discussions of this phenomenon, see e.g., [4,38].

3. Nonexistence of the ideal method

Subspace recycling has shown great potential to improve the convergence of restarted methods, in many cases, without dramatically increasing memory costs. Therefore, if we can incorporate GMRES for shifted linear systems into the recycling framework described in [23], we will have a storage-efficient method which will solve all shifted systems simultaneously.

In this context, it is most natural to consider extending GMRES for shifted systems [11] into the recycling framework. We denote such a method *Recycled GMRES for shifted systems*. We explore how such an algorithm would look and show that we generally cannot satisfy the fixed memory requirement while achieving simultaneous solution of all systems using a single augmented subspace.

Consider the simplified model problem, with linear systems (3)–(4), subspaces $\mathcal{U}$ and $\mathcal{C}$, and their respective matrix counterparts $\mathbf{U}$ and $\mathbf{C}$. The ideal method will solve (3) using Recycled GMRES while generating approximations for (4) of the form

$$\mathbf{x}_m^{(\sigma)} = \mathbf{x}_0^{(\sigma)} + \mathbf{s}_m^{(\sigma)} + \mathbf{t}_m^{(\sigma)} \tag{11}$$

with $\mathbf{s}_m^{(\sigma)} \in \mathcal{U}$ and $\mathbf{t}_m^{(\sigma)} \in \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$, such that we have residual collinearity. Such a method could be used for any number of shifts without increasing storage requirements.

We begin with a useful result about Krylov subspaces for projected operators.

Proposition 1. *Let* $\mathbf{C}$ *be a matrix with orthonormal columns spanning* $\mathcal{C}$. *Let* $\mathbf{P} = \mathbf{I} - \mathbf{C}\mathbf{C}^*$. *For any non-zero* $\mathbf{v}$, *if* $\mathbf{v} \in \mathcal{C}^\perp$, *i.e., if* $\mathbf{C}^*\mathbf{v} = \mathbf{0}$, *then*

$$\mathcal{K}_m(\mathbf{PA}, \mathbf{v}) = \mathcal{K}_m\big(\mathbf{P}(\mathbf{A} + \sigma\mathbf{I}), \mathbf{v}\big) \quad \text{for all } m \text{ and all } \sigma \in \mathbb{C}. \tag{12}$$

Proof. If $\sigma = 0$, there is nothing to prove. Consider then the case of $\sigma \neq 0$. Since $\mathbf{C}^*\mathbf{v} = \mathbf{0}$, we have

$$\big(\mathbf{I} - \mathbf{C}\mathbf{C}^*\big)(\mathbf{A} + \sigma\mathbf{I})\mathbf{v} = \big(\mathbf{I} - \mathbf{C}\mathbf{C}^*\big)\mathbf{A}\mathbf{v} + \sigma\big(\mathbf{I} - \mathbf{C}\mathbf{C}^*\big)\mathbf{v} = \big(\mathbf{I} - \mathbf{C}\mathbf{C}^*\big)\mathbf{A}\mathbf{v} + \sigma\mathbf{v}.$$

Therefore, when restricted to vectors orthogonal to $\mathcal{R}(\mathbf{C})$, we have that

$$\big(\mathbf{I} - \mathbf{C}\mathbf{C}^*\big)(\mathbf{A} + \sigma\mathbf{I}) = \big(\mathbf{I} - \mathbf{C}\mathbf{C}^*\big)\mathbf{A} + \sigma\mathbf{I}.$$

Furthermore, since any $\mathbf{u} \in \mathcal{R}(\mathbf{P}(\mathbf{A} + \sigma\mathbf{I}))$ is orthogonal to $\mathcal{R}(\mathbf{C})$, we have that for any $\mathbf{v} \perp \mathcal{R}(\mathbf{C})$,

$$\big[\big(\mathbf{I} - \mathbf{C}\mathbf{C}^*\big)(\mathbf{A} + \sigma\mathbf{I})\big]^j\mathbf{v} = \big[\big(\mathbf{I} - \mathbf{C}\mathbf{C}^*\big)\mathbf{A} + \sigma\mathbf{I}\big]^j\mathbf{v}.$$

Thus,

$$\mathcal{K}_m\big(\mathbf{P}(\mathbf{A} + \sigma\mathbf{I}), \mathbf{v}\big) = \mathcal{K}_m(\mathbf{PA} + \sigma\mathbf{I}, \mathbf{v}) = \mathcal{K}_m(\mathbf{PA}, \mathbf{v}),$$

where the last equality follows from the shift invariance property of Krylov subspaces. □

Thus, for $\mathbf{r}_0 \in \mathcal{C}^\perp$, the projected Krylov subspace is invariant under a constant shift of the matrix $\mathbf{A}$, and the shifted Arnoldi relation (7) holds as well.

In [23], it is shown that the augmented Krylov subspace satisfies an Arnoldi-like relation, namely

$$\mathbf{A}\widehat{\mathbf{V}}_m = \widehat{\mathbf{W}}_{m+1}\bar{\mathbf{G}}_m, \tag{13}$$

where

$$\widehat{\mathbf{V}}_m = [\,\mathbf{U} \quad \mathbf{V}_m\,], \qquad \widehat{\mathbf{W}}_{m+1} = [\,\mathbf{C} \quad \mathbf{V}_{m+1}\,], \quad \text{and} \quad \bar{\mathbf{G}}_m = \begin{bmatrix} \mathbf{I}_k & \mathbf{B}_m \\ \mathbf{0} & \bar{\mathbf{H}}_m \end{bmatrix}.$$

Even with Proposition 1, the relation (13) does not have a shifted analog, as in (7). Instead, we have

$$(\mathbf{A} + \sigma\mathbf{I})\widehat{\mathbf{V}}_m = \widehat{\mathbf{W}}_{m+1}\begin{bmatrix} \mathbf{I}_k & \mathbf{B}_m \\ \mathbf{0} & \bar{\mathbf{H}}_m \end{bmatrix} + \sigma\widehat{\mathbf{V}}_m.$$

If we have

$$\mathcal{R}(\widehat{\mathbf{V}}_m) \subset \mathcal{R}(\widehat{\mathbf{W}}_{m+1}), \tag{14}$$

the relation could be easily modified so that a relation similar to (7) holds, allowing the collinearity condition to be enforced. For example, if $\mathcal{U}$ is an invariant subspace, then (14) holds. However, this inclusion, in general, does not hold; the columns of $\mathbf{U}$ might span an approximate invariant subspace of $\mathbf{A}$, not a true invariant subspace. Similar observations are made in the context of Hermitian systems in [16].

There is at least one other scenario in which (14) does hold. Consider the situation in which we begin with no starting recycled space and compute harmonic Ritz vectors at the end of each cycle to pass to the next cycle. We run an m-step cycle of shifted GMRES, and at the end of that cycle, let the columns of $\mathbf{U}$ be k harmonic Ritz vectors, we compute $\mathbf{C}$ as before, and restart. Morgan [21] showed that for a harmonic Ritz pair $(\mathbf{g}, \theta)$, the eigenvector residual $\mathbf{A}\mathbf{g} - \theta\mathbf{g}$ is a multiple

of the GMRES residual $\mathbf{r}_m$. At the end of a cycle, if we compute k harmonic Ritz vectors and store them as the columns of $\widetilde{\mathbf{U}}$, then we know that

$$\mathcal{R}(\mathbf{A}\widetilde{\mathbf{U}} - \widetilde{\mathbf{U}}\mathbf{D}) = \operatorname{span}(\mathbf{r}_m), \tag{15}$$

where $\mathbf{D} = \operatorname{diag}(\theta_1, \ldots, \theta_k)$, the diagonal matrix containing the harmonic Ritz values associated to the columns of $\widetilde{\mathbf{U}}$. If we compute the QR-factorization of $\mathbf{A}\widetilde{\mathbf{U}} = \mathbf{C}\mathbf{R}$ and let $\mathbf{U} = \widetilde{\mathbf{U}}\mathbf{R}^{-1}$, then for $\mathbf{T} = \mathbf{R}\mathbf{D}\mathbf{R}^{-1}$ we have

$$\mathcal{R}(\mathbf{C} - \mathbf{U}\mathbf{T}) = \operatorname{span}(\mathbf{r}_m).$$

At the beginning of the next cycle, we take $\mathbf{v}_1 = \mathbf{r}_m/\|\mathbf{r}_m\|$ as the first Krylov vector; and in this case, the containment (14) holds. This is the same fact exploited in [7], where the authors observe that the augmented Krylov subspace is itself actually a larger Krylov subspace with a different starting vector. Thus, the shifted GMRES method can be applied directly to the Krylov subspace augmented with the harmonic Ritz vectors, as long as there was no deflation space at the beginning of the process.

What about in the general setting? This is important for when the coefficient matrix changes, and we use a recycled subspace from one system to accelerate the iteration of the next system. Let $\mathbf{E}$ be a matrix whose columns form a basis for the orthogonal complement of $\mathcal{C} \oplus \mathcal{K}_{m+1}(\mathbf{PA}, \mathbf{r}_0)$ in $\mathbb{C}^n$. We note that $\mathbf{E}$ needs not be computed; we use it here as a theoretical tool. We can write

$$\mathbf{U} = \mathbf{C}\mathbf{Y} + \mathbf{V}_{m+1}\mathbf{Z} + \mathbf{E}\mathbf{F}, \tag{16}$$

where $\mathbf{Y} \in \mathbb{C}^{k\times k}$, $\mathbf{Z} \in \mathbb{C}^{(m+1)\times k}$, and $\mathbf{F} \in \mathbb{C}^{(n-m-1-k)\times k}$. This yields the following *imperfect* Arnoldi-like relation for the shifted system,

$$(\mathbf{A} + \sigma\mathbf{I})\begin{bmatrix}\mathbf{U} & \mathbf{V}_m\end{bmatrix} = \begin{bmatrix}\mathbf{C} & \mathbf{V}_{m+1}\end{bmatrix}\begin{bmatrix}\mathbf{I}_k + \sigma\mathbf{Y} & \mathbf{B} \\ \sigma\mathbf{Z} & \bar{\mathbf{H}}_m^{(\sigma)}\end{bmatrix} + \sigma\begin{bmatrix}\mathbf{E}\mathbf{F} & \mathbf{0}\end{bmatrix}. \tag{17}$$

If we let

$$\widetilde{\mathbf{G}}_m^{(\sigma)} = \begin{bmatrix}\mathbf{I}_k + \sigma\mathbf{Y} & \mathbf{B} \\ \sigma\mathbf{Z} & \bar{\mathbf{H}}_m^{(\sigma)}\end{bmatrix},$$

together with (13), then the Arnoldi-like relation (17) can be rewritten as

$$(\mathbf{A} + \sigma\mathbf{I})\widehat{\mathbf{V}}_m = \widehat{\mathbf{W}}_{m+1}\widetilde{\mathbf{G}}_m^{(\sigma)} + \sigma\begin{bmatrix}\mathbf{E}\mathbf{F} & \mathbf{0}\end{bmatrix}.$$

We can write the correction $\mathbf{s}_m$ and $\mathbf{t}_m$ obtained by the Recycled GMRES minimization as,

$$\mathbf{s}_m = \mathbf{U}\mathbf{y}_m^{(1)} \quad \text{and} \quad \mathbf{t}_m = \mathbf{V}_m\mathbf{y}_m^{(2)}, \tag{18}$$

and stack $\mathbf{y}_m^{(1)}$ and $\mathbf{y}_m^{(2)}$ in the vector

$$\widehat{\mathbf{y}}_m = \begin{bmatrix}\mathbf{y}_m^{(1)} \\ \mathbf{y}_m^{(2)}\end{bmatrix}.$$

In [23], the Recycled GMRES minimization is written so that we are computing $\widehat{\mathbf{y}}_m$, satisfying

$$\begin{aligned}\mathbf{r}_m &= \mathbf{r}_0 - \widehat{\mathbf{W}}_{m+1}\bar{\mathbf{G}}_m\widehat{\mathbf{y}}_m \\ &= \|\mathbf{r}_0\|\widehat{\mathbf{W}}_{m+1}\mathbf{e}_{k+1}^{(m+1)} - \widehat{\mathbf{W}}_{m+1}\bar{\mathbf{G}}_m\widehat{\mathbf{y}}_m = \widehat{\mathbf{W}}_{m+1}\widehat{\mathbf{z}}_{m+1},\end{aligned}$$

where we used (13) and

$$\widehat{\mathbf{z}}_{m+1} = \|\mathbf{r}_0\|\mathbf{e}_{k+1}^{(m+1)} - \bar{\mathbf{G}}_m\widehat{\mathbf{y}}_m \tag{19}$$

is the Recycled GMRES least-squares residual. Now, for the shifted system, we would like to enforce the collinearity condition. If a collinear residual were to exist for the shifted system, then it would satisfy

$$\begin{aligned}&\mathbf{r}_m^{(\sigma)} = \beta_m\mathbf{r}_m \\ &\iff \quad \mathbf{b} - (\mathbf{A} + \sigma\mathbf{I})\big(\mathbf{x}_0^{(\sigma)} + \widehat{\mathbf{V}}_m\mathbf{y}_m^{(\sigma)}\big) = \beta_m\widehat{\mathbf{W}}_{m+1}\widehat{\mathbf{z}}_{m+1} \\ &\iff \quad \mathbf{r}_0^{(\sigma)} - (\mathbf{A} + \sigma\mathbf{I})\widehat{\mathbf{V}}_m\mathbf{y}_m^{(\sigma)} = \widehat{\mathbf{W}}_{m+1}\widehat{\mathbf{z}}_{m+1}\beta_m \\ &\iff \quad \beta_0\mathbf{r}_0 - \big(\widehat{\mathbf{W}}_{m+1}\widetilde{\mathbf{G}}_m^{(\sigma)} + \sigma\begin{bmatrix}\mathbf{E}\mathbf{F} & \mathbf{0}\end{bmatrix}\big)\widehat{\mathbf{y}}_m^{(\sigma)} = \widehat{\mathbf{W}}_{m+1}\widehat{\mathbf{z}}_{m+1}\beta_m \\ &\iff \quad \beta_0\mathbf{r}_0 = \widehat{\mathbf{W}}_{m+1}\big(\widehat{\mathbf{z}}_{m+1}\beta_m + \widetilde{\mathbf{G}}_m^{(\sigma)}\widehat{\mathbf{y}}_m^{(\sigma)}\big) + \sigma\begin{bmatrix}\mathbf{E}\mathbf{F} & \mathbf{0}\end{bmatrix}\widehat{\mathbf{y}}_m^{(\sigma)}.\end{aligned} \tag{20}$$

Observe that in the general case, $\mathbf{r}_0 \in \mathcal{C} \oplus \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$ while the right-hand side of (20) has a non-zero component in $\mathcal{R}(\mathbf{E}) = (\mathcal{C} \oplus \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0))^{\perp}$. Thus, we state the conditions for existence (and nonexistence) of the collinear residual in the following theorem.

Theorem 1. *Suppose we have approximations* $\mathbf{x}_0$ *and* $\mathbf{x}_0^{(\sigma)}$ *to the solutions of* (3) *and* (4)*, respectively, such that the residuals* $\mathbf{r}_0$ *and* $\mathbf{r}_0^{(\sigma)}$ *are collinear, and* $\mathbf{r}_0 \in \mathcal{C}^{\perp}$*. Let* $\mathbf{r}_m$ *be the minimum residual solution produced by Recycled GMRES over the augmented Krylov subspace* $\mathcal{U} + \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$*. Then one of the following mutually exclusive statements is true:*

- $\mathcal{U} + \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0) \subset \mathcal{C} \oplus \mathcal{K}_{m+1}(\mathbf{PA}, \mathbf{r}_0)$
- *There exists* ***no*** *approximation* $\mathbf{x}_m^{(\sigma)} \in \mathcal{U} + \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$ *to* (4) *such that* $\mathbf{r}_m^{(\sigma)}$ *is collinear to* $\mathbf{r}_m$*, i.e.,* $\mathbf{r}_m^{(\sigma)} \neq \beta_m \mathbf{r}_m$*, for* ***all*** $\beta_m \in \mathbb{C}$.

4. A method with the collinearity approach

We have shown in Theorem 1 that the ideal algorithm, i.e., one where all shifted systems are solved with the same approximation subspace and with fixed storage, generally does not exist. However, by removing one of the two requirements, we can derive viable methods. First, in this section, we consider a method which imposes the collinearity of the residuals, thus allowing the use of the same subspace for all shifts, at the cost of building different deflation subspaces for each of the shifts with their dimensions small enough to not incur excessive memory costs. In other words, additional storage is required for each new shift. We do so by extending the work of Frommer and Glässner [11] to this situation.

Let $\mathbf{x}_{-1}$ and $\mathbf{x}_{-1}^{(\sigma)}$ be initial approximations so that the initial residuals are collinear, i.e., $\mathbf{r}_{-1} = \beta_0 \mathbf{r}_{-1}^{(\sigma)}$. The update,

$$\mathbf{x}_0 = \mathbf{x}_{-1} + \mathbf{U}\mathbf{C}^*\mathbf{r}_{-1} \quad \text{and} \quad \mathbf{r}_0 = \mathbf{r}_{-1} - \mathbf{C}\mathbf{C}^*\mathbf{r}_{-1} \tag{21}$$

cheaply yields a residual $\mathbf{r}_0 \in \mathcal{C}^{\perp}$. In order to effect a similar update of $\mathbf{x}_{-1}^{(\sigma)}$, we need $\mathbf{U}^{(\sigma)}$ such that

$$\mathbf{C} = \mathbf{A}\mathbf{U} = (\mathbf{A} + \sigma \mathbf{I})\mathbf{U}^{(\sigma)}. \tag{22}$$

This requires an additional k vectors of storage for each shift. Given an initial subspace $\mathcal{U}$, we can derive $\mathbf{U}^{(\sigma)}$ for each value of σ. For details, see [33], where in addition to a description of how to efficiently build the family of deflation spaces, an analysis is presented on the relation between the value of the shift and the degradation of the orthogonality of the columns of the matrix in (22).

As described in Section 3, (3) can be solved using Recycled GMRES while for (4), we can compute

$$\mathbf{x}_m^{(\sigma)} = \mathbf{x}_0^{(\sigma)} + \mathbf{U}^{(\sigma)}\mathbf{y}_m^{(1,\sigma)} + \mathbf{V}_m \mathbf{y}_m^{(2,\sigma)}$$

such that the collinearity condition $\mathbf{r}_m^{(\sigma)} = \beta_m^{(\sigma)} \mathbf{r}_m$ holds; cf. (18). The vector

$$\mathbf{y}_m^{(\sigma)} = \begin{bmatrix} \mathbf{y}_m^{(1,\sigma)} \\ \mathbf{y}_m^{(2,\sigma)} \end{bmatrix}$$

together with the scalar $\beta_m^{(\sigma)}$ are solved simultaneously from an augmented system, as was done in [11]. Just as Recycled GMRES can be viewed as applying GMRES to a projected linear system, this method can be shown to reduce to applying the shifted GMRES method to a projected, shifted linear system.

Such an augmented system is also used in our second approach presented in the next section; cf. (24). The procedure for the method presented in this section with multiple deflation spaces is fully developed in [33], but omitted here for sake of brevity. We observe though, that the approximation with collinear residual is drawn from $\mathbf{U}^{(\sigma)} + \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$ rather than from $\mathbf{U} + \mathcal{K}_m(\mathbf{PA}, \mathbf{r}_0)$, from which the minimal residual correction of the base system is extracted.

5. A method with fixed storage

Inspired by the results of Theorem 1, we consider a different alternative than that briefly discussed in Section 4. If we enforce the fixed-storage requirement (i.e., only one recycled subspace $\mathcal{U}$ is stored and all approximations are drawn from the same augmented Krylov subspace) then a prospective algorithm must overcome two obstacles.

First, we cannot conveniently update the residual of the shifted system. For the shifted system, we construct approximations of the form (11). As already discussed, without a $\mathbf{U}^{(\sigma)}$ defined as in (22), we cannot project $\mathbf{r}_{-1}^{(\sigma)}$ and update $\mathbf{x}_{-1}^{(\sigma)}$, as in (21). As a remedy, we can perform an update of the shifted system approximation which implicitly updates the residual by the perturbation of an orthogonal projection. We set

$$\mathbf{x}_0^{(\sigma)} = \mathbf{x}_{-1}^{(\sigma)} + \mathbf{U}\mathbf{C}^*\mathbf{r}_{-1}^{(\sigma)}.$$

The updated residual can be written as

$$\begin{aligned} \mathbf{r}_0^{(\sigma)} &= \mathbf{b} - (\mathbf{A} + \sigma \mathbf{I})\mathbf{x}_0^{(\sigma)} \\ &= \mathbf{b} - (\mathbf{A} + \sigma \mathbf{I})\left(\mathbf{x}_{-1}^{(\sigma)} + \mathbf{U}\mathbf{C}^*\mathbf{r}_{-1}^{(\sigma)}\right) \\ &= \mathbf{r}_{-1}^{(\sigma)} - (\mathbf{A} + \sigma \mathbf{I})\mathbf{U}\mathbf{C}^*\mathbf{r}_{-1}^{(\sigma)} \\ &= \underbrace{\mathbf{r}_{-1}^{(\sigma)} - \mathbf{C}\mathbf{C}^*\mathbf{r}_{-1}^{(\sigma)}}_{\text{true orthogonal projection}} \underbrace{- \sigma \mathbf{U}\mathbf{C}^*\mathbf{r}_{-1}^{(\sigma)}}_{\text{perturbation}}. \end{aligned} \tag{23}$$

Second, the collinear residual does not exist. Deriving this result yields clues to another way forward. Neglecting a term from (20) allows us to solve a nearby approximate collinearity condition (which we will explain shortly, after Algorithm 5.1) and update the approximation for the shifted system. This update is of the form (11) with $\mathbf{s}_m^{(\sigma)} \in \mathcal{U}$. These corrections tend to improve the residual but do not lead to convergence for the shifted system, which will start with an expected improved approximation. We present analysis showing how much improvement is possible with this method. After convergence of the base system, the algorithm can be applied recursively on the remaining unconverged systems. This recursive method of solving one seed system at a time while choosing corrections for the approximations for the other systems has been previously suggested in the context of linear systems with multiple right-hand sides; see e.g., [6,31].

We begin by providing an overview of the strategy we are proposing and encode this into a schematic algorithm. This algorithm solves the base system with Recycled GMRES while cheaply computing better initial approximations for the shifted systems. We present this outline in Algorithm 5.1.

Algorithm 5.1: Schematic of shifted Recycled GMRES with an approximate collinearity condition

Input : $\mathbf{A} \in \mathbb{C}^{n\times n}$; $\{\sigma^{(\ell)}\}_{\ell=1}^{L} \subset \mathbb{C}$; $\mathbf{U}, \mathbf{C} \in \mathbb{C}^{n\times k}$ such that $\mathbf{AU} = \mathbf{C}$ and $\mathbf{C}^*\mathbf{C} = \mathbf{I}_k$; Initial Approximations $\mathbf{x}_0$ and $\mathbf{x}_0^{(\sigma^{(\ell)})}$ such that residuals are collinear; $\varepsilon > 0$

$\mathbf{x} \leftarrow \mathbf{x}_0$, $\mathbf{r} = \mathbf{b} - \mathbf{Ax}$

$\mathbf{x} \leftarrow \mathbf{x} + \mathbf{UC}^*\mathbf{r}$, $\mathbf{r} \leftarrow \mathbf{r} - \mathbf{CC}^*\mathbf{r}$; `Project base residual`

$\mathbf{x}^{(\sigma^{(\ell)})} \leftarrow \mathbf{x}_0^{(\sigma^{(\ell)})}$, $\mathbf{r}^{(\sigma^{(\ell)})} = \mathbf{b} - \mathbf{Ax}^{(\sigma^{(\ell)})}$ for all ℓ

for $\ell = 1$ *to* L **do**

  $\mathbf{x}^{(\sigma^{(\ell)})} \leftarrow \mathbf{x}^{(\sigma^{(\ell)})} + \mathbf{UC}^*\mathbf{r}^{(\sigma^{(\ell)})}$; `Update shifted approximation, but not an implicit residual projection`

while $\|\mathbf{r}\| > \varepsilon$ **do**

  Construct a basis of the subspace $\mathcal{K}_m((\mathbf{I} - \mathbf{CC}^*)\mathbf{A}, \mathbf{r})$

  Compute update $\mathbf{t} \in \mathcal{R}(\mathbf{U}) + \mathcal{K}_m((\mathbf{I} - \mathbf{CC}^*)\mathbf{A}, \mathbf{r})$ by minimizing residual using Recycled GMRES

  $\mathbf{x} \leftarrow \mathbf{x} + \mathbf{t}$; $\mathbf{r} \leftarrow \mathbf{b} - \mathbf{Ax}$

  for $\ell = 1$ *to* L **do**

    Compute update $\mathbf{t}^{(\sigma^{(\ell)})} \in \mathcal{R}(\mathbf{U}) + \mathcal{K}_m((\mathbf{I} - \mathbf{CC}^*)\mathbf{A}, \mathbf{r})$ according to the approximate collinearity condition (24)

    $\mathbf{x}^{(\sigma^{(\ell)})} \leftarrow \mathbf{x}^{(\sigma^{(\ell)})} + \mathbf{t}^{(\sigma^{(\ell)})}$

  Compute updated recycled subspace information $\mathbf{U}$ and $\mathbf{C}$

Clear any variables no longer needed

if $L > 2$ **then**

  Make a recursive call to Algorithm 5.1 with $\mathbf{A} \leftarrow \mathbf{A} + \sigma^{(1)}\mathbf{I}$, shifts $\{\sigma^{(\ell)} - \sigma^{(1)}\}_{\ell=2}^{L}$, approximations $\{\mathbf{x}^{(\sigma^{(\ell)})}\}_{\ell=2}^{L}$ and updated recycled subspace matrix $\mathbf{U}$

else

  Apply Recycled GMRES to the last unconverged system

This algorithm relies on dropping the term $\mathbf{EF}(\tilde{\mathbf{y}}_m)_{1:k}$ from (20), which yields an augmented linear system on the new variables $\tilde{\mathbf{y}}_m^{(\sigma)}$ and $\tilde{\beta}_m$ that can be solved directly,

$$\mathbf{z}_{m+1}\tilde{\beta}_m + \widetilde{\mathbf{G}}_m^{(\sigma)}\tilde{\mathbf{y}}_m^{(\sigma)} = \beta_0\|\mathbf{r}_0\|\mathbf{e}_{k+1}^{(m+1)}, \quad \text{or}$$
$$\left[\widetilde{\mathbf{G}}_m^{(\sigma)} \quad \mathbf{z}_{m+1}\right]\begin{bmatrix}\tilde{\mathbf{y}}_m^{(\sigma)} \\ \tilde{\beta}_m\end{bmatrix} = \beta_0\|\mathbf{r}_0\|\mathbf{e}_{k+1}^{(m+1)}. \tag{24}$$

Thus, we proceed by solving this nearby problem and updating the shifted solution,

$$\mathbf{x}_m^{(\sigma)} = \mathbf{x}_0^{(\sigma)} + \widehat{\mathbf{V}}_m\tilde{\mathbf{y}}_m^{(\sigma)}. \tag{25}$$

For each restart cycle, we repeat this process for the shifted system. We stop when the base residual norm is below tolerance. When the residual norm for the base system reaches the desired tolerance, the residual norm of the shifted system will have been reduced at little additional cost; but, generally, the reduction is insufficient. Thus, we apply the GMRES with recycling algorithm with this approximate collinearity scheme to the remaining unsolved systems, taking one of the shifted systems as our new base system. This method is amenable to recursion on the number of shifts. When only one system remains, Recycled GMRES is applied.

Observe that for any number of shifts, we can easily form $\widetilde{\mathbf{G}}_m^{(\sigma)}$ for each σ at little additional cost. The matrices $\mathbf{Y}$ and $\mathbf{Z}$ in (16) must be computed only once per cycle, regardless of the number of shifted systems we are solving. However, additional shifts will require more recursive calls to the algorithm and, thus, more iterations.

Why does the approximate collinearity condition produce an improved approximation to the solution of the shifted system? How well we can expect the algorithm to perform? The following analysis answers these questions and also yields a cheap way in which we can monitor the progress of the residuals of the shifted systems. Theorem 2 shows how the algorithm behaves when we start with already non-collinear residuals. This allows for the treatment of the case when the perturbed initial projection of the residual (25) renders collinearity invalid at the start.

Theorem 2. *Suppose we begin the cycle as in (20), with approximate collinearity between the base and shifted residuals, satisfying the relation*

$$\mathbf{r}_0^{(\sigma)} = \tilde{\beta}_0 \mathbf{r}_0 + \mathbf{w}^{(\sigma)}. \tag{26}$$

If we perform a cycle of Recycled GMRES to reduce the residual of the base system and apply the approximate collinearity condition (24) to the shifted residual, then we have the relation

$$\tilde{\mathbf{r}}_m^{(\sigma)} = \tilde{\beta}_m \mathbf{r}_m - \sigma \mathbf{E}\mathbf{F}\big(\tilde{\mathbf{y}}_m^{(\sigma)}\big)_{1:k} + \mathbf{w}^{(\sigma)}. \tag{27}$$

Proof. We can write the residual produced by the approximate collinearity procedure for the shifted system as follows, using (19),

$$\begin{aligned}
\tilde{\mathbf{r}}_m^{(\sigma)} &= \mathbf{b} - (\mathbf{A} + \sigma \mathbf{I})\mathbf{x}_m^{(\sigma)} \\
&= \mathbf{r}_0^{(\sigma)} - (\mathbf{A} + \sigma \mathbf{I})\widehat{\mathbf{V}}_m \tilde{\mathbf{y}}_m^{(\sigma)} \\
&= \tilde{\beta}_0 \mathbf{r}_0 + \mathbf{w}^{(\sigma)} - (\mathbf{A} + \sigma \mathbf{I})\widehat{\mathbf{V}}_m \tilde{\mathbf{y}}_m^{(\sigma)} \\
&= \tilde{\beta}_0 \mathbf{r}_0 - \big(\widehat{\mathbf{W}}_{m+1}\widetilde{\mathbf{G}}_m^{(\sigma)} + \sigma\,[\,\mathbf{E}\mathbf{F} \quad \mathbf{0}\,]\big)\tilde{\mathbf{y}}_m^{(\sigma)} + \mathbf{w}^{(\sigma)} \\
&= \tilde{\beta}_0 \|\mathbf{r}_0\| \widehat{\mathbf{W}}_{m+1}\mathbf{e}_{k+1}^{(m+1)} - \widehat{\mathbf{W}}_{m+1}\widetilde{\mathbf{G}}_m^{(\sigma)}\tilde{\mathbf{y}}_m^{(\sigma)} - \sigma\,[\,\mathbf{E}\mathbf{F} \quad \mathbf{0}\,]\,\tilde{\mathbf{y}}_m^{(\sigma)} + \mathbf{w}^{(\sigma)} \\
&= \tilde{\beta}_0 \|\mathbf{r}_0\| \widehat{\mathbf{W}}_{m+1}\mathbf{e}_{k+1}^{(m+1)} - \widehat{\mathbf{W}}_{m+1}\widetilde{\mathbf{G}}_m^{(\sigma)}\tilde{\mathbf{y}}_m^{(\sigma)} - \tilde{\beta}_m \widehat{\mathbf{W}}_{m+1}\mathbf{z}_{m+1} + \tilde{\beta}_m \widehat{\mathbf{W}}_{m+1}\mathbf{z}_{m+1} - \sigma\,[\,\mathbf{E}\mathbf{F} \quad \mathbf{0}\,]\,\tilde{\mathbf{y}}_m^{(\sigma)} + \mathbf{w}^{(\sigma)} \\
&= \widehat{\mathbf{W}}_{m+1}\big(\tilde{\beta}_0 \|\mathbf{r}_0\| \mathbf{e}_{k+1}^{(m+1)} - \widetilde{\mathbf{G}}_m^{(\sigma)}\tilde{\mathbf{y}}_m^{(\sigma)} - \tilde{\beta}_m \mathbf{z}_{m+1}\big) + \tilde{\beta}_m \widehat{\mathbf{W}}_{m+1}\mathbf{z}_{m+1} - \sigma\,[\,\mathbf{E}\mathbf{F} \quad \mathbf{0}\,]\,\tilde{\mathbf{y}}_m^{(\sigma)} + \mathbf{w}^{(\sigma)}.
\end{aligned}$$

Now using the approximate collinearity condition (24) and the fact that by definition $\mathbf{r}_m = \widehat{\mathbf{W}}_{m+1}\mathbf{z}_{m+1}$, we have that

$$\tilde{\mathbf{r}}_m^{(\sigma)} = \tilde{\beta}_m \mathbf{r}_m - \sigma\,[\,\mathbf{E}\mathbf{F} \quad \mathbf{0}\,]\,\tilde{\mathbf{y}}_m^{(\sigma)} + \mathbf{w}^{(\sigma)},$$

which can be rewritten in the form (27). □

It should be noted that the term $-\sigma \mathbf{E}\mathbf{F}(\tilde{\mathbf{y}}_m^{(\sigma)})_{1:k} + \mathbf{w}^{(\sigma)}$ is a function of the quality of the recycled subspaces as well as of σ. With the use of simple inequalities, we obtain an important corollary estimating the amount of residual norm reduction we can expect for the shifted systems.

Corollary 1. *The shifted system residual norm satisfies the following inequality,*

$$\big\|\tilde{\mathbf{r}}_m^{(\sigma)}\big\| \leqslant |\tilde{\beta}_m| \|\mathbf{r}_m\| + |\sigma| \|\mathbf{E}\mathbf{F}\| \big\|\big(\tilde{\mathbf{y}}_m^{(\sigma)}\big)_{1:k}\big\| + \big\|\mathbf{w}^{(\sigma)}\big\|. \tag{28}$$

As long as $|\tilde{\beta}_m|\|\mathbf{r}_m\|$ dominates the right-hand side, we will observe a reduction of the shifted residual norm. This reduction is controlled by $|\sigma|$, $\|\mathbf{E}\mathbf{F}\|$, and $\|(\tilde{\mathbf{y}}_m^{(\sigma)})_{1:k}\|$. We cannot control $\|(\tilde{\mathbf{y}}_m^{(\sigma)})_{1:k}\|$, and σ is dictated by the problem. The size of $\|\mathbf{E}\mathbf{F}\|$ is connected to the quality of $\mathbf{U}$ as an approximation to an invariant subspace of $\mathbf{A}$. This can seen by writing

$$\mathbf{E}\mathbf{F} = \mathbf{U} - (\mathbf{C}\mathbf{Y} + \mathbf{V}_{m+1}\mathbf{Z}) \tag{29}$$

and observing that the norm of this difference decreases as $\mathbf{U}$ becomes a better approximation of an invariant subspace of $\mathbf{A}$. Thus, choosing $\mathbf{U}$ as an approximate invariant subspace may improve performance of the method.

Ideally, we would like to detect when $|\tilde{\beta}_m|\|\mathbf{r}_m\|$ ceases to dominate (28) in order to cease updating the approximations to the shifted system once such an update no longer leads to a decrease in residual norm. Our analysis gives us a way to monitor both quantities. Observe that given σ, $\mathbf{U}$, and $\mathbf{C}$, if we compute $\tilde{\mathbf{y}}_m^{(\sigma)}$ according to (24), then from (29), we can compute the product $\mathbf{E}\mathbf{F}(\tilde{\mathbf{y}}_m^{(\sigma)})_{1:k}$. Thus, we can keep track of the vector $\mathbf{w}^{(\sigma)}$, and use it to construct $\mathbf{r}_m^{(\sigma)}$ using (27). Rather than detecting that $|\tilde{\beta}_m|\|\mathbf{r}_m\|$ ceases to dominate (28), it is simpler to calculate $\|\mathbf{r}_m^{(\sigma)}\|$ after each cycle and detect when it has ceased to be reduced by the correction from that cycle. At this point, we cease updating $\mathbf{x}_m^{(\sigma)}$ for the remaining cycles.

It should be noted that $\mathbf{w}^{(\sigma)}$ can be easily accumulated. At the beginning of Algorithm 5.1, we compute an initial value of $\mathbf{w}^{(\sigma)}$ according to (26). At Line 5 of Algorithm 5.1, we update $\mathbf{w}^{(\sigma)} \leftarrow \mathbf{w}^{(\sigma)} - \sigma \mathbf{U}\mathbf{C}^*\tilde{\mathbf{r}}^{(\sigma)}$ according to (23). At Line 11, we update $\mathbf{w}^{(\sigma)} \leftarrow \mathbf{w}^{(\sigma)} - \sigma \mathbf{E}\mathbf{F}(\tilde{\mathbf{y}}_m)_{1:k}$ according to (27).

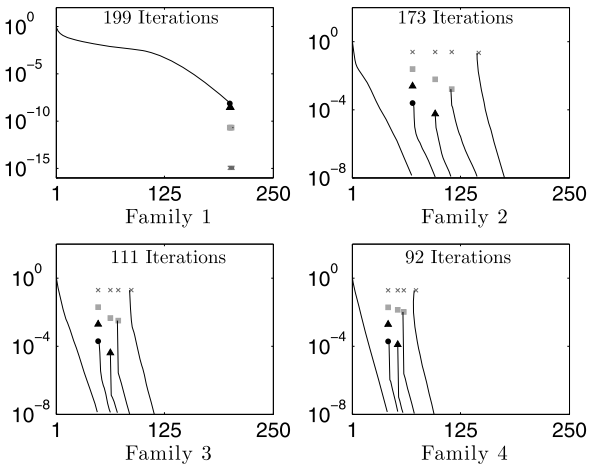

Fig. 1. Recycled GMRES (RGMRES) for shifted systems with recursion on the number of unconverged shifted systems, on a sequence of four families (of five systems each) of 1000×1000 bidiagonal matrices, $m = 100$ and $k = 50$, and shifts 10^{-2}, 10^{-1}, 1, and 10. For the shifted systems, the residuals are only computed at the end of each cycle, with residual norms represented by the **circle**, **triangle**, **square**, and **cross**, respectively. Curves originating from these symbols are convergence curves for RGMRES for each shifted system when that system becomes the base system during a recursive call.

6. Numerical experiments

We performed a series of numerical experiments illustrating the applicability of the method described in Section 5, i.e., using an implementation of Algorithm 5.1. Following [23], we constructed recycled subspaces from harmonic Ritz vectors of the coefficient matrix associated with the base system (3) with respect to the augmented subspace. In the figures reported here, for each recursive call to the algorithm, the solid black line represents the convergence curve for the base system, while the different markers indicate residual norms for the shifted systems at the end of each restart cycle.

In all experiments, when solving the first family of shifted systems in the sequence, there is no initial recycled subspace. Thus, (15) holds at the end of each cycle, and $\mathbf{E} = \mathbf{0}$. Therefore, the approximate collinearity condition (24) becomes an exact collinearity condition. This is equivalent to applying shifted GMRES-DR for shifted systems [7]. Observe in the convergence plots, that all residuals are reduced in norm below tolerance when solving the base system.

Our first experiment, presented in Fig. 1, illustrates the performance of the Recycled GMRES method for shifted linear systems on a sequence of four bidiagonal matrices. The first matrix, $\mathbf{B}_1$, used in [7], is a bidiagonal matrix with $\{0.1, 1, 2, \ldots, 998, 999\}$ on the diagonal and ones on the first superdiagonal, and the other matrices are random bidiagonal perturbations of $\mathbf{B}_1$; we use the Matlab function `sprand()`. We use four shifts: 10^{-2}, 10^{-1}, 1, and 10, and values of $m = 100$ and $k = 50$. We see that, as predicted by Corollary 2, the amount of residual reduction achieved for the shifted systems is affected by the size of the shift. For the shift $\sigma_1 = 10^{-2}$, the relative residual is reduced to $\mathcal{O}(10^{-4})$ during the solution of the base system while for $\sigma_4 = 10$, the relative residual is only reduced to $\mathcal{O}(10^{-1})$. This experiment is more for illustrative purposes than to demonstrate superior performance. Nevertheless, after convergence for the base system, we take one of the shifted systems as our new base system and reapply the algorithm for the smaller family of systems.

For comparison, we present in Fig. 2 the convergence curves if we simply apply Recycled GMRES to each shifted system sequentially. It can be appreciated that while applying Recycled GMRES sequentially requires a total of 1107 matrix–vector products for all systems with all shifts, the proposed approach requires only 575 matrix–vector products, an improvement of about 50%.

Our choice of $m = 100$, $k = 50$ represent simply typical values. Our aim with these experiments is to illustrate the effectiveness of the method, and not to advocate for specific values of m or k. We have performed experiments with various values of m and k, and there are many other pairs for which the overall performance is superior to that shown here. At the same time, small values of m and k tend to exhibit convergence in more iterations, though the overall pattern is similar to that observed in Figs. 1 and 2.

For our second and third experiments, we test two sequences of six QCD matrices from the University of Florida sparse matrix collection [8]. In the second experiment, we work with six 3072×3072 sample matrices (called $\mathbf{D}_1$ through $\mathbf{D}_6$) with filename prefix `conf5.0-0014x4`. We can construct the coefficient matrix $\mathbf{A}_i = \mathbf{I} - \kappa^{(i)}\mathbf{D}_i$ where $\kappa^{(i)}$ is a parameter associated to the QCD problem. For each matrix, there exists some critical value $\kappa_c^{(i)}$ representing the shift for which the real part of one of the eigenvalues of the shifted matrix becomes zero. For values of $0 \leqslant \kappa^{(i)}$ smaller than $\kappa_c^{(i)}$ the shifted matrix is expected to be a real-positive matrix. For each $\mathbf{D}_i$, $\kappa_c^{(i)}$ is included with the matrix, and in these experiments, all are in the interval $[0.20, 0.22]$. Frequently in QCD computations, we wish to solve with multiple parameters.

We chose $\{0.001, 0.002, 0.003, -0.6, -0.5\}$ as our family of shifts. Observe that by the definition of $\mathbf{A}_i$ and $\kappa_c^{(i)}$, the two shifted coefficient matrices associated with the two negative shifts are not real-positive. These are not physically relevant for QCD computations. We chose negative shifts merely to demonstrate the robustness of the algorithm. In this experiment,

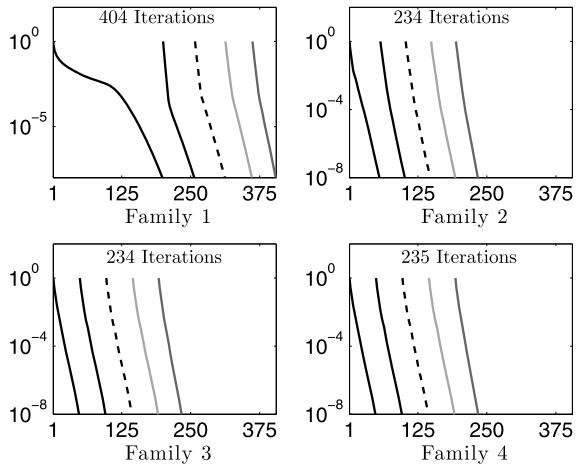

Fig. 2. Convergence curves when we apply Recycled GMRES to each shifted bidiagonal system sequentially. As in the previous experiment, $m = 100$ and $k = 50$.

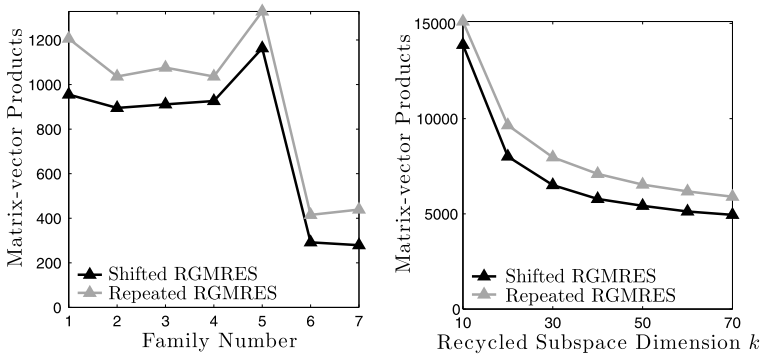

Fig. 3. RGMRES for shifted systems on a sequence of seven small Wilson fermion matrices. For each matrix, we solve the base system and those associated with the shifts 0.001 , 0.002, 0.003, −0.6, and −0.5. Left: RMGRES(100, 50) for shifted systems as compared to repeated applications of RGMRES(100, 50). Right: comparison of recycled subspaces of different size with $m = 100$ fixed.

GMRES for shifted systems was unable to produce approximations for long sequences of iterations (due to numerical singularity of the augmented collinearity matrix). Since the shifted GMRES method did not converge for some systems, its performance was not included in the figure. However, as we have noted, it is not difficult to modify this algorithm to gracefully handle this situation by applying restarted GMRES to any unconverged shifted systems at the end of the process. We compared with another strategy, repeated applications of Recycled GMRES [23] for the base and shifted system. In Fig. 3 we present the matrix–vector product counts for each system for a particular recycled subspace dimension as well as the totals over seven systems for various recycled subspace dimensions. We see that our method is able to produce a 20% reduction in the number of matrix–vector products needed to solve these systems, when compared to repeated applications of Recycled GMRES. In Fig. 4, we present the convergence curves for the first six QCD matrices. Observe that two of the shifted systems (corresponding to the negative shifts) require more work than the others for each base system *including* the first system, in which we started with no recycled subspace. These are the two shifts for which shifted GMRES (or shifted GMRES-DR) would not converge. Notice that in this case, we are still able to converge by applying Recycled GMRES at the end.

In the third experiment, we worked with another sequence of six QCD matrices from the University of Florida Sparse Matrix Collection [8] with filename prefixes `conf5.4` and `conf6.0`. These matrices of size $49\,152 \times 49\,152$. We used the critical $\kappa_c^{(i)}$ to construct our system matrices, and we choose the shifts $\{0.001, 0.002, 0.003, 0.01, 0.02\}$, the first three of which are as in the second experiment. In Fig. 5, we see the convergence of our algorithm for these systems.

In the fourth experiment, we work with a sequence of eleven QCD matrices obtained from [18]. These matrices were delivered already shifted to be positive-real. As in the previous experiment, they are also of size $49\,152 \times 49\,152$.

In Table 1, we illustrate the performance of the proposed algorithm when the total dimension of the augmented space increases. We also ran a comparable instance of the shifted GMRES algorithm. More specifically, we compared the performance of shifted GMRES with cycle length m versus our algorithm with a $k = \lfloor m/2 \rfloor$ dimension deflation space and $m - k$ cycle length. In this experiment, there are two shifts, $\{0.8, 0.81\}$. Here we see the potential benefits that our algorithm can yield as the deflation dimension increases. In particular, in the last example, the gain as compared with RGMRES is of 16%. We mention though that for a larger number of shifts (or different values for the shifts) RGMRES may not be more

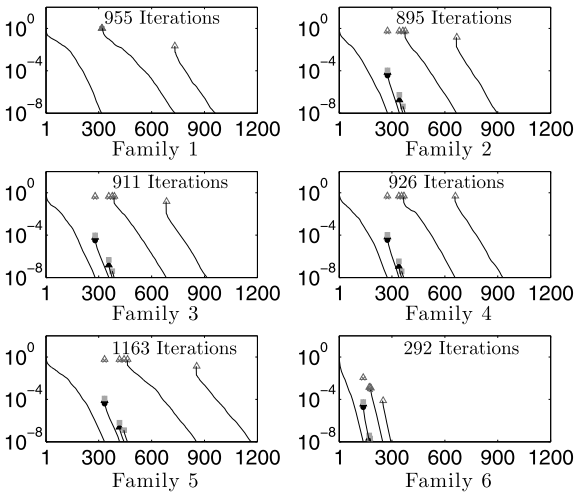

Fig. 4. Same experiment as in Fig. 3 but only for the first six systems, $m = 100$ and $k = 50$.

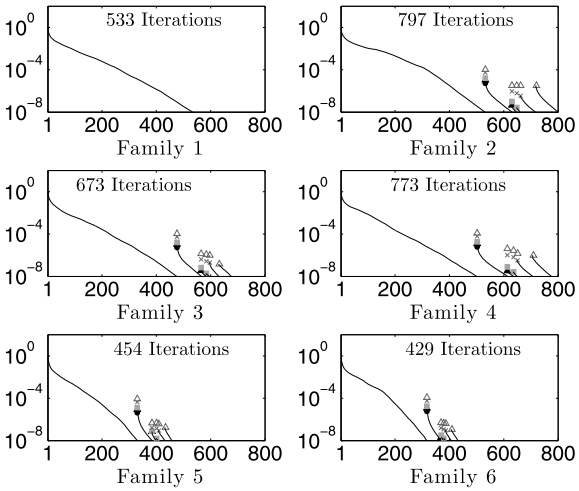

Fig. 5. Convergence curves for another sequence of six Wilson fermion matrices, of size $49\,152 \times 49\,152$ with $m = 100$ and $k = 50$.

Table 1
A comparison, in terms of iteration counts of the shifted GMRES algorithm (SGMRES) with the Recycled GMRES algorithm for shifted systems (RGMRES) in terms of iteration count for different cycle lengths m. The results presented are the total iterations for solving a sequence of eleven QCD systems from [18].

m	k	SGMRES(m)	RGMRES($m-k,k$)	Ratio
25	12	4297	3880	0.90
50	25	3284	2980	0.91
75	37	3108	2816	0.91
100	50	3028	2697	0.89
125	67	3058	2612	0.85
150	75	2958	2546	0.86
175	87	2962	2499	0.84
200	100	2947	2458	0.83
225	112	2860	2410	0.84

advantageous. This follows from the fact that each shift incurs an additional recursive call to the algorithm and additional iterations. There is no such increase for shifted GMRES. Therefore, for sufficiently large number of shifts, shifted GMRES will have an advantage. Which method will perform better depends on several factors including the number of shifts (as we just mentioned), the magnitude of the shifts, the size of deflation space, and the deflation space selection technique. What we have shown is that for certain problems, the recycling strategy is definitely worth considering.

7. Conclusions

We have shown that the ideal method that solves a family of shifted systems simultaneously using one augmented subspace with subspace recycling generally does not exist under a fixed storage requirement independent of the number of shifts. As an alternative, we present two methods, each of which relax one of the two requirements, yielding two possible algorithms. One solves the family of shifted systems using the same subspace but requires the construction of multiple deflation spaces. The other constructs approximations over a single augmented Krylov subspace, but not all shifted systems are solved to tolerance at the same time. Instead, we showed some theoretical results indicating that the latter approach produces improved initial approximate solutions for the shifted systems. This was confirmed in our numerical experiments, which also showed that the fixed-memory method can be quite effective, especially when the shifts are all located in a small interval.

Acknowledgements

We would like to thank David Day and Michael Parks for engaging in fruitful discussions with the first author. We also thank Andreas Frommer for his extensive comments, including the suggestion that Algorithm 5.1 is amenable to recursion. We also publicly thank the two anonymous referees for their comments and questions, which helped improve our presentation.

References

[1] A. Adbel-Rehim, R.B. Morgan, W. Wilcox, Seed methods for linear equations in lattice QCD problems with multiple right-hand sides, in: Proceedings of Science, Lattice 2008, 2008, paper 038.
[2] M.I. Ahmad, D.B. Szyld, M.B. van Gijzen, Preconditioned multishift BiCG for $\mathcal{H}_2$-optimal model reduction, Research Report 12-06-15, Department of Mathematics, Temple University, Jun. 2012.
[3] A.H. Baker, E.R. Jessup, T. Manteuffel, A technique for accelerating the convergence of restarted GMRES, SIAM J. Matrix Anal. Appl. 26 (2005) 962–984.
[4] S.L. Campbell, I.C.F. Ipsen, C.T. Kelley, C.D. Meyer, GMRES and the minimal polynomial, BIT Numer. Math. 36 (1996) 664–675.
[5] M.R. Celis, J.E. Dennis, R.A. Tapia, A trust region strategy for nonlinear equality constrained optimization, in: P.T. Boggs, R.H. Byrd, R.B. Schnabel (Eds.), Numerical Optimization, Boulder, Colo., 1984, SIAM, Philadelphia, 1985, pp. 71–82.
[6] T.F. Chan, W.L. Wan, Analysis of projection methods for solving linear systems with multiple right-hand sides, SIAM J. Sci. Comput. 18 (1997) 1698–1721.
[7] D. Darnell, R.B. Morgan, W. Wilcox, Deflated GMRES for systems with multiple shifts and multiple right-hand sides, Linear Algebra Appl. 429 (2008) 2415–2434.
[8] T.A. Davis, Y. Hu, The University of Florida sparse matrix collection, ACM Trans. Math. Softw. 38 (2011) 1:1–1:25.
[9] M. Eiermann, O.G. Ernst, O. Schneider, Analysis of acceleration strategies for restarted minimal residual methods, J. Comput. Appl. Math. 123 (2000) 261–292.
[10] A. Frommer, BiCGStab(l) for families of shifted linear systems, Computing 70 (2003) 87–109.
[11] A. Frommer, U. Glässner, Restarted GMRES for shifted linear systems, SIAM J. Sci. Comput. 19 (1998) 15–26.
[12] A. Frommer, P. Maass, Fast CG-based methods for Tikhonov–Phillips regularization, SIAM J. Sci. Comput. 20 (1999) 1831–1850.
[13] A. Frommer, S. Güsken, T. Lippert, B. Nöckel, K. Schilling, Many masses on one stroke: economic computation of quark propagators, Int. J. Mod. Phys. C 6 (1995) 627–638.
[14] P.C. Hansen, Discrete Inverse Problems: Insight and Algorithms, SIAM, Philadelphia, 2010.
[15] B. Jegerlehner, Krylov space solvers for sparse linear systems, Tech. Rep. IUHET-353, Indiana University, 1996.
[16] M.E. Kilmer, E. de Sturler, Recycling subspace information for diffuse optical tomography, SIAM J. Sci. Comput. 27 (2006) 2140–2166.
[17] S. Kirchner, IDR-Verfahren zur Lösung von Familien geshifteter linearer Gleichungssysteme, Master's thesis, Bergische Universität Wuppertal, Department of Mathematics, Wuppertal, Germany, 2011.
[18] B. Leder, N. Bozovic, 2012, Personal communication.
[19] R.B. Lehoucq, D.C. Sorensen, Deflation techniques for an implicitly restarted Arnoldi iteration, SIAM J. Matrix Anal. Appl. 17 (1996) 789–821.
[20] K. Meerbergen, The solution of parametrized symmetric linear systems, SIAM J. Matrix Anal. Appl. 24 (2003) 1038–1059.
[21] R.B. Morgan, Implicitly restarted GMRES and Arnoldi methods for nonsymmetric systems of equations, SIAM J. Matrix Anal. Appl. 21 (2000) 1112–1135.
[22] R.B. Morgan, GMRES with deflated restarting, SIAM J. Sci. Comput. 24 (2002) 20–37.
[23] M.L. Parks, E. de Sturler, G. Mackey, D.D. Johnson, S. Maiti, Recycling Krylov subspaces for sequences of linear systems, SIAM J. Sci. Comput. 28 (2006) 1651–1674.
[24] Y. Saad, Analysis of augmented Krylov subspace methods, SIAM J. Matrix Anal. Appl. 18 (1997) 435–449.
[25] Y. Saad, Iterative Methods for Sparse Linear Systems, second ed., SIAM, Philadelphia, 2003.
[26] Y. Saad, M.H. Schultz, GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM J. Sci. Stat. Comput. 7 (1986) 856–869.
[27] V. Simoncini, Restarted full orthogonalization method for shifted linear systems, BIT Numer. Math. 43 (2003) 459–466.
[28] V. Simoncini, D.B. Szyld, On the occurrence of superlinear convergence of exact and inexact Krylov subspace methods, SIAM Rev. 47 (2005) 247–272.
[29] V. Simoncini, D.B. Szyld, Recent computational developments in Krylov subspace methods for linear systems, Numer. Linear Algebra Appl. 14 (2007) 1–59.
[30] V. Simoncini, D.B. Szyld, Interpreting IDR as a Petrov–Galerkin method, SIAM J. Sci. Comput. 32 (2010) 1898–1912.
[31] C.F. Smith, A.F. Peterson, R. Mittra, A conjugate gradient algorithm for treatment of multiple incident electromagnetic fields, IEEE Trans. Antennas Propag. 37 (1989) 1490–1493.
[32] P. Sonneveld, M.B. van Gijzen, IDR(s): a family of simple and fast algorithms for solving large nonsymmetric systems of linear equations, SIAM J. Sci. Comput. 31 (2008) 1035–1062.
[33] K.M. Soodhalter, D.B. Szyld, F. Xue, Krylov subspace recycling for sequences of shifted linear systems, Arxiv Preprint, arXiv:1301.2650, 2013.
[34] A. Stathopoulos, K. Orginos, Computing and deflating eigenvalues while solving multiple right-hand side linear systems with an application to quantum chromodynamics, SIAM J. Sci. Comput. 32 (2010) 439–462.
[35] E. de Sturler, Nested Krylov methods based on GCR, J. Comput. Appl. Math. 67 (1996) 15–41.

[36] E. de Sturler, Truncation strategies for optimal Krylov subspace methods, SIAM J. Numer. Anal. 36 (1999) 864–889.
[37] E. de Sturler, Convergence bounds for approximate invariant subspace recycling for sequences of linear systems, in: Program of the Householder Symposium XVIII on Numerical Linear Algebra, 2011, pp. 51–52.
[38] H.A. van der Vorst, K. Vuik, The superlinear convergence behaviour of GMRES, J. Comput. Appl. Math. 48 (1993) 327–341.
[39] G. Wu, Y.-C. Wang, X.-Q. Jin, A preconditioned and shifted GMRES algorithm for the PageRank problem with multiple damping factors, SIAM J. Sci. Comput. 34 (2012) A2558–A2575.