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Block variants of the COCG and COCR methods for solving complex symmetric linear systems with multiple right-hand sides

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Abstract. In the present study, we establish two new block variants of the Conjugate Orthogonal Conjugate Gradient (COCG) and the Conjugate A-Orthogonal Conjugate Residual (COCR) Krylov subspace methods for solving complex symmetric linear systems with multiple right hand sides. The proposed Block iterative solvers can fully exploit the complex symmetry property of coefficient matrix of the linear system. We report on extensive numerical experiments to show the favourable convergence properties of our newly developed Block algorithms for solving realistic electromagnetic simulations.

1 Introduction

In this paper we are interested in the efficient solution of linear systems with multiple right-hand sides (RHSs) of the form

$$AX = B, \quad A \in \mathbb{C}^{n\times n}, \quad X, B \in \mathbb{C}^{n\times p}, \ p \ll n, \tag{1}$$

where A is a non-Hermitian but symmetric matrix, i.e, $A \neq A^H$ and $A = A^T$. Linear systems of this form arise frequently in electromagnetic scattering applications, for example in monostatic radar cross-section calculation, where each right-hand side typically corresponds to an incident wave illuminating the target at a given angle of incidence [1,2].

Roughly speaking, computational techniques for solving linear systems on modern computers can be divided into the class of direct and of iterative methods. Block iterative Krylov subspace methods are particularly designed for solving efficiently linear systems with multiple RHSs (cf. [3,4]). Block algorithms require one or more matrix product operations of the form AV, with $V \in \mathbb{C}^{n\times p}$ an arbitrary rectangular matrix, per iteration step.

Thus they can solve the typical memory bottlenecks of direct methods. However, most of them, such as the Block Bi-Conjugate Gradient (bl_bicg) [5], Block Bi-Conjugate Residual (bl_bicr) [3], Block BiCGSTAB (bl_bicgstab) [6], Block BiCRSTAB (bl_bicrstab) [3], Block QMR (bl_qmr) [7], Block IDR(s) (bl_idr(s)) [8] and Block GMRES (bl_gmres) [9] methods, do not naturally exploit any symmetry of A.

Methods that can exploit the symmetry of A are typically of (quasi) minimal residual type (i.e. bl_sqmr) [7]. Tadano and Sakurai recently proposed the Block COCG (bl_cocg) [10] method, which can be regarded as a natural extension of the COCG [11] algorithm for solving linear systems (1). Both these two methods need one operation AV per iteration step. In this paper we revisit the Block COCG method, presenting a more systematic derivation than the one presented [10], and we introduce a new Block solver (bl_cocr) that can be seen as an extension of the COCR algorithm proposed in [12]. The numerical stability of the bl_cocg and the bl_cocr methods are enhanced by the residual orthonormalization technique [13].

The paper is organized as follows. In Section 2 we present the general framework for the development of the bl_cocg and the bl_cocr solvers. In Section 3 we study their numerical stability properties and then we show how to improve their convergence by employing the residual orthonormalization technique. In Section 3, we report on extensive numerical experiments to illustrate the effectiveness of the two new iterative methods in computational electromagnetics. Finally, some conclusions arising from this work are presented in Section 4.

2 The Block COCG and Block COCR methods

Let $X^{m+1} \in \mathbb{C}^{n\times p}$ be the $(m+1)$th approximate solution of linear systems (1) satisfying the following condition

$$X_{m+1} = X_0 + Z_{m+1}, \quad Z_{m+1} \in \mathcal{K}^{\diamond}_{m+1}(A; R_0), \tag{2}$$

where $R_0 = B - AX_0$ is an initial residual and $\mathcal{K}^{\diamond}_{m+1}(A; R_0)$ is the block Krylov subspace [4] defined as

$$\mathcal{K}^{\diamond}_{m+1}(A; R_0) = \Big\{ \sum_{j=0}^{m} A^j R_0 \gamma_j \mid \gamma_j \in \mathbb{C}^{p\times p} \ (j = 0, 1, \ldots, m) \Big\}. \tag{3}$$

Compared with conventional Krylov subspace methods, where $\boldsymbol{x}^{(j)}_{m+1} - \boldsymbol{x}^{(j)}_0 \in \mathcal{K}_{m+1}(A, \boldsymbol{r}^{(j)}_0)$, note that block Krylov methods can search the approximate solutions into larger spaces, and thus they may require less iterations to converge to a given accuracy. In the next section we introduce the framework for the development of the Block COCG and the Block COCR methods.

2.1 Derivation of the Block COCG and Block COCR methods

According to Eqs. (2)–(3), the $(m+1)$th residual $R_{m+1} = B - AX_{m+1}$ of the Block COCG method [10] and the Block COCR method is computed by the following recurrence relations,

$$\begin{aligned} R_0 = P_0 = B - AX_0 &\in \mathcal{K}_1^{\diamond}(A; R_0), \\ R_{m+1} = R_m - AP_m\alpha_m &\in \mathcal{K}_{m+2}^{\diamond}(A; R_0), \\ P_{m+1} = R_{m+1} + P_m\beta_m &\in \mathcal{K}_{m+2}^{\diamond}(A; R_0). \end{aligned} \tag{4}$$

Here, $P_{m+1} \in \mathbb{C}^{n\times p}, \alpha_m, \beta_m \in \mathbb{C}^{p\times p}$. The $(m+1)$th approximate solution X_{m+1} is updated through the recurrence relation

$$X_{m+1} = X_m + P_m\alpha_m. \tag{5}$$

Similarly to the framework introduced in [14], different formulae for the $p \times p$ matrices α_m, β_m $(m = 0, 1, \ldots)$ in the recurrences (4)–(5) lead to different iterative algorithms. Denoting by $\mathcal{L}$ the *block constraints subspace*, these matrices α_m, β_m are determined by imposing the orthogonality conditions

$$R_m \perp \mathcal{L} \quad \text{and} \quad AP_m \perp \mathcal{L}. \tag{6}$$

The Block COCG and the Block COCR methods correspond to the choices $\mathcal{L} = \mathcal{K}_m^{\diamond}(\bar{A}; \bar{R}_0)$ and $\mathcal{L} = \bar{A}\mathcal{K}_m^{\diamond}(\bar{A}; \bar{R}_0)$, respectively. In Table 1, the conjugate orthogonality conditions imposed to determine α_m and β_m are summarized for the sake of clarity.

Table 1. Orthogonality conditions imposed to determine $p \times p$ matrices α_m, β_m

Matrix	Block COCG	Blcok COCR
α_m, β_m	$R_m \perp \mathcal{K}_m^{\diamond}(\bar{A}; \bar{R}_0)$	$R_m \perp \bar{A}\mathcal{K}_m^{\diamond}(\bar{A}; \bar{R}_0)$
	$AP_m \perp \mathcal{K}_m^{\diamond}(\bar{A}; \bar{R}_0)$	$AP_m \perp \bar{A}\mathcal{K}_m^{\diamond}(\bar{A}; \bar{R}_0)$

We show the complete Block COCR algorithm in Algorithm 1. We use the notation $\|\cdot\|_F$ for the Frobenius norm of a matrix, and ϵ is a sufficiently small user-defined value. We see that the Block COCR method requires two matrix products AP_{m+1}, AR_{m+1} at each iteration step. While the product AR_{m+1} is computed by explicit matrix multiplication, the product AP_{m+1} is computed by the recurrence relation at line 9, to reduce the computational complexity. Note that the Block COCG and the Block COCR methods can be derived from the Block BiCG and the Block BiCR methods, respectively, by choosing the initial auxiliary residual $\hat{R}_0 = \bar{R}_0$ and removing some redundant computations; we refer to the recent work [14] for similar discussions about the derivation of conventional non-block Krylov subspace methods for complex symmetric linear systems with single RHS.

Algorithm 1 The Block COCR method

1: $X_0 \in \mathbb{C}^{n\times p}$ is an initial guess, $R_0 = B - AX_0$,
2: Set $P_0 = R_0$, $U_0 = V_0 = AR_0$,
3: **for** $m = 0, 1, \ldots,$ until $\|R_m\|_F / \|R_0\|_F \leq \epsilon$ **do**
4: Solve $(U_m^T U_m)\alpha_m = R_m^T V_m$ for α_m,
5: $X_{m+1} = X_m + P_m\alpha_m$,
6: $R_{m+1} = R_m - U_m\alpha_m$ and $V_{m+1} = AR_{m+1}$,
7: Solve $(R_m^T V_m)\beta_m = R_{m+1}^T V_{m+1}$ for β_m,
8: $P_{m+1} = R_{m+1} + P_m\beta_m$,
9: $U_{m+1} = V_{m+1} + U_m\beta_m$,
10: **end for**

2.2 Improving the numerical stability of the Block COCG and Block COCR methods by residual orthonormalization

One known problem with Block Krylov subspace methods is that the residual norms may not converge when the number p of right-hand sides is large, mainly due to numerical instabilities, see e.g. [13]. These instabilities often arise because of the loss of linear independence among the column vectors of the $n \times p$ matrices that appear in the methods, such as R_m and P_m. Motivated by this concern, in this section we propose to use the residual orthonormalization technique to enhance the numerical stability of the Block COCG and Block COCR algorithms. This efficient technique was introduced in [13] in the context of the Block CG method [5].

Let the Block residual R_m be factored as $R_m = Q_m\xi_m$ by conventional QR factorization[1], with $Q_m^H Q_m = I_p$. Here I_p denotes the identity matrix of order p and $\xi_m \in \mathbb{C}^{p\times p}$. From (4), the following equation can be obtained

$$Q_{m+1}\tau_{m+1} = Q_m - AS_m\alpha'_k. \tag{7}$$

Here, $\tau_{m+1} \equiv \xi_{m+1}\xi_{m-1}$, $\alpha'_k \equiv \xi_m\alpha_m\xi_{m-1}$, and $S_m = P_m\xi_{m-1}$. In the new Algorithms 2-3, the matrix β'_m is defined as $\alpha'_m \equiv \xi_m\beta_m\xi_{m+1}^{-1}$. The residual norm is monitored by $\|\xi_m\|_F$ instead of $\|R_m\|_F$, since the Frobenius norm of R_m satisfies $\|R_m\|_F = \|\xi_m\|_F$. Note that the QR decomposition is calculated at each iteration. However, the numerical results shown in the next section indicate that the extra cost is amortized by the improved robustness of the two Block solvers.

3 Numerical experiments

In this section, we carry out some numerical experiments to show the potential effectiveness of the proposed iterative solution strategies in computational

[1] For our practical implementation, we use MATLAB qr-function "`qr`(W,0)" for a given matrix $W \in \mathbb{C}^{n\times p}$.

Algorithm 2 Algorithm of the Block COCG method with residual orthonormalization (bl_cocg_rq)

1: $X_0 \in \mathbb{C}^{n\times p}$ is an initial guess, and compute $Q_0\xi_0 = B - AX_0$,
2: Set $S_0 = Q_0$,
3: **for** $m = 0, 1, \ldots,$ until $\|\xi_m\|_F/\|B\|_F \leq \epsilon$ **do**
4: Solve $(S_m^T AS_m)\alpha'_m = Q_m^T Q_m$ for α'_m,
5: $X_{m+1} = X_m + S_m\alpha'_m\xi_m$,
6: $Q_{m+1}\tau_{m+1} = Q_m - AS_m\alpha'_m$ and $\xi_{m+1} = \tau_{m+1}\xi_m$,
7: Solve $(Q_m^T Q_m)\beta'_m = \tau_{m+1}^T Q_{m+1}^T Q_{m+1}$ for β'_m,
8: $S_{m+1} = Q_{m+1} + S_m\beta'_m$,
9: **end for**

Algorithm 3 Algorithm of the Block COCR method with residual orthonormalization (bl_cocr_rq)

1: $X_0 \in \mathbb{C}^{n\times p}$ is an initial guess, and compute $Q_0\xi_0 = B - AX_0$,
2: Set $S_0 = Q_0$ and $U_0 = V_0 = AQ_0$,
3: **for** $m = 0, 1, \ldots,$ until $\|\xi_m\|_F/\|B\|_F \leq \epsilon$ **do**
4: Solve $(U_m^T U_m)\alpha'_m = Q_m^T U_m$ for α'_m,
5: $X_{m+1} = X_m + P_m\alpha'_m$
6: $Q_{m+1}\tau_{m+1} = Q_m - U_m\alpha'_m$ and $\xi_{m+1} = \tau_{m+1}\xi_m$,
7: Compute $V_{m+1} = AQ_{m+1}$,
8: Solve $(Q_m^T V_m)\beta_m = \tau_{m+1}^T Q_{m+1}^T V_{m+1}$ for β'_m,
9: $S_{m+1} = Q_{m+1} + S_m\beta'_m$,
10: $U_{m+1} = V_{m+1} + U_m\beta'_m$,
11: **end for**

electromagnetics. We compare the bl_cocg, bl_cocg_rq, bl_cocr, bl_cocr_rq methods against other popular block Krylov subspace methods such as bl_qmr, bl_bicgstab, bl_bicrstab, bl_idr(s) (selecting matrix $P = rand(n, sp)$, see [8]) and restarted bl_gmres(m). We use the value $m = 80$ for the restart in bl_gmres(m). The experiments have been carried out in double precision floating point arithmetic with MATLAB 2014a (64 bit) on PC-Intel(R) Core(TM) i5-3470 CPU 3.20 GHz, 8 GB of RAM.

The different Block algorithms are compared in terms of number of iterations, denoted as *Iters* in the tables, and $\log_{10}$ of the final true relative residual norm defined as $\log_{10}(\|B - AX_{\text{final}}\|_F/\|B\|_F)$, denoted as *TRR*. The iterative solution is started choosing $X_0 = O \in \mathbb{C}^{n\times p}$ as initial guess. The stopping criterion in our runs is the reduction of the norm of the initial Block residual by eight orders of magnitude, i.e., $\|R_m\|_F/\|B\|_F \leq Tol = 10^{-10}$. The right-hand side B is computed by the MATLAB function `rand`. In the tables, the symbol "†" indicates no convergence within n iterations, or n/m cycles for the bl_gmres(m) method.

Table 2. The numerical results of different iterative solvers for the first example.

Method	`young2c` ($p = 10$)			`young3c` ($p = 8$)			`young1c` ($p = 8$)		
	Iters	*TRR*	CPU	*Iters*	*TRR*	CPU	*Iters*	*TRR*	CPU
bl_cocg	238	-10.03	0.17	†	†	†	329	-10.16	0.16
bl_cocg_rq	142	-10.14	0.13	151	-10.00	0.09	177	-10.29	0.12
bl_cocr	201	-10.07	0.15	145	-9.95	0.04	221	-10.07	0.12
bl_cocr_rq	138	-10.18	0.13	146	-10.03	0.05	180	-10.18	0.13
bl_sqmr	154	-9.87	0.29	131	-10.39	0.09	188	-9.88	0.25
bl_bicgstab	395*	-10.09	0.41	†	†	†	433*	-10.04	0.35
bl_bicrstab	356*	-9.96	0.46	†	†	†	417*	-9.71	0.44
bl_idr(4)	269*	-8.57	0.28	†	†	†	334*	-10.10	0.27
bl_gmres(m)	3**	-10.08	24.5	†	†	†	†	†	†

The first test problems are three matrices extracted from the Matrix Market collection[2], arising from modeling acoustic scattering problems. They are denoted as `young1c, young2c`, and `young3c`. The results of our experiments are presented in Table 2. The symbol * used for the bl_bicgstab, bl_idr(4), and bl_bicrstav methods indicate that these three methods require no less than two matrix products AV per iteration step. The symbol ** refers to the number of outer iterations in the Block GMRES(m) method, when it can achieve convergence; refer to [15] for details. This notation is used throughout this section.

Table 2 shows the results with nine different Block Krylov solvers. Although the bl_cocg and bl_cocr methods required more *Iters*, they are more competitive than the bl_sqmr method in terms of CPU time and *TRR* (except the case of `young3c`). Bl_cocr method is more robust than bl_cocg in terms of *Iters*, CPU time and *TRR*. The bl_cocg_rq and bl_cocr_rq variant are very efficient in terms of *TRR* and CPU time. The bl_bicgstab, bl_bicrstab, bl_idr(4), and bl_gmres(m) methods cannot solve the test problem (`young3c`), while bl_cocg and bl_cocr converge rapidly. Due to the long iterative recurrence, the bl_gmres(m) method is typically expensive.

In the second experiment we consider three dense matrices arising from monostatic radar cross-section calculation; they are denoted as `sphere2430`, `parallelepipede`, `cube1800`. These problems are available from our GitHub repository[3], and we choose $p = 8$. Although rather small, the selected dense problems are representative of realistic radar-cross-section calculation [2]. Larger problems would require a Fortran or C implementation of the solvers and will be considered in a separate study. Numerical results for each test problem are summarized in Table 3.

[2] `http://math.nist.gov/MatrixMarket/matrices.html`
[3] `https://github.com/Hsien-Ming-Ku/Test_matrices/tree/master/Example2`

Table 3. The numerical results of different iterative solvers for Example 1.

Method	sphere2430			parallelepipede			cube1800		
	Iters	*TRR*	CPU	*Iters*	*TRR*	CPU	*Iters*	*TRR*	CPU
bl_cocg	189	-10.07	4.16	176	-10.02	2.40	174	-10.21	1.94
bl_cocg_rq	169	-10.00	3.77	156	-10.13	2.13	156	-10.08	1.74
bl_cocr	186	-10.03	4.12	174	-10.02	2.35	169	-10.00	1.84
bl_cocr_rq	166	-10.05	3.77	152	-10.15	2.11	151	-10.09	1.73
bl_sqmr	172	-9.84	4.15	161	-9.91	2.42	159	-9.97	2.11
bl_bicgstab	379^{*}	-10.04	16.5	370^{*}	-10.04	9.94	396^{*}	-10.29	8.42
bl_bicrstab	392^{*}	-9.57	17.3	355^{*}	-9.85	9.98	303^{*}	-8.38	6.70
bl_idr(4)	409^{*}	-9.64	22.1	474^{*}	-10.11	16.5	334^{*}	-9.43	10.2
bl_gmres(m)	2^{**}	-10.07	38.2	2^{**}	-10.04	33.3	2^{**}	-10.09	22.1

Table 3 displays the results with again nine different Block Krylov solvers. We can see that the bl_sqmr method requires less *Iters* to converge compared to the bl_cocg and bl_cocr methods. However, it is more expensive in terms of CPU time except on the `sphere2430` problem. Besides, the true residual norms produced by the bl_sqmr method are larger than those of both bl_cocg and bl_cocr. Furthermore, bl_cocg_rq and bl_cocr_rq are the most effective and promising solvers in terms of *Iters* and CPU time. Specifically, the bl_cocr_rq method is slightly more efficient than the bl_cocg_rq method in terms of *TRR*.

4 Conclusions

In this paper, a framework for constructing new Block iterative Krylov subspace methods is presented. Two new matrix solvers that can exploit the symmetry of A for solving complex symmetric non-Hermitian linear systems (1) are introduced. Stabilization techniques based on residual orthonormalization strategy are discussed for both methods. The numerical experiments show that the solvers can be viable alternative to standard Krylov subspace methods for solving complex symmetric linear systems with multiple RHSs efficiently. Obviously, for solving realistic electromagnetic problems they both need to be combinated with suitable preconditioners that reflect the symmetry of A; we refer the reader to, e.g., [16,17,18] for some related studies.

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