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Product Hybrid Block GMRES for Nonsymmetrical Linear Systems with Multiple Right-hand Sides

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Abstract. Recently, the complementary behavior of restarted GMRES has been studied. We observed that successive cycles of restarted block BGMRES (BGMRES(*m,s*)) can also complement one another harmoniously in reducing the iterative residual. In the present paper, this characterization of BGMRES(*m,s*) is exploited to form a hybrid block iterative scheme. In particular, a product hybrid block GMRES algorithm for nonsymmetrical systems with multiple right-hand sides is proposed. The new algorithm combines the advantage of Simoncini's Hybrid Block GMRES and Zhong's Product Hybrid GMRES. Numerical experiments are conducted to show that the new algorithm can offer significant improvement over the hybrid block GMRES.

Keyword: Linear systems, block iterative method, multiple right-hand sides, Krylov subspace, matrix polynomials.

1. Introduction

We are interested in the matrix polynomial method for solving systems with multiple right-hand sides

$$AX = B \tag{1.1}$$

where $A \in R^{n\times n}$ is nonsymmetrical and nonsingular, $B = [b_1, \cdots\cdots b_s] \in R^{n\times s}$, $s << n$.

Given an initial guess X_0, the method generate a sequence of iterates $\{X_m\}$, whose block residual $\{R_m = B - AX_m\}$ satisfies $R_m = \Phi_m(A) \circ R_0$.

Here $\Phi_m(\lambda) = \sum_{i=0}^{m} \lambda^i \xi_i$ is known as a matrix polynomial in $\overline{P}_{m,s}$ ($P_{m,s}$ denotes the space of matrix polynomial $\Phi_m(\lambda) = \sum_{i=0}^{m} \lambda^i \xi_i, \xi_i \in R^{s\times s}$, of degree not greater than *m* and sides *s*, and $\overline{P}_{m,s} = \{\Phi_m(\lambda) \in P_{m,s} : \Phi_m(\lambda) = I\}$). Moreover, Φ_m solves the minimization problem

$$\min_{\Theta \in \overline{P}_{m,s}} \left\| \Theta_m \circ R_0 \right\|. \tag{1.2}$$

with which BGMRES method [8] is defined.

It is sufficient to observe that in the exact arithmetic and under certain condition on *R* (*R* is $n\times s$ residual block) and *A*, BGMRES achieves finite termination in [*n/s*] iteration. It follows that the number of iterations to termination for BGMRES is expected to decrease as the number of right-hand sides increase [3]. The property, combined with the built-in minimization of the block residual, makes BGMRES mathematically attractive. However, experiments in [5] indicated that BGMRES has great difficulty competing with the other solvers with respect to computational cost.

To limit the average work per (block) iteration, BGMRES is often restarted every steps, leading to the BGMRES(*m,s*) algorithm:

$$R_{k,m} = \Phi_{m,k}(A) \circ R_{(k-1),m}.$$

$\Phi_{m,k}(\lambda)$ selected by (1.2) based on $R_{(k-1),m}$ $(k = 2,3\cdots\cdots)$. Restarting entails, however, loss of the

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properties of finite termination and minimization over the entire Krylov subspace [1]. In particular, for small m and large n, the number of right-hand side s has to be large for an acceptable reduction of the number of iteration. But also it can increase the work per iteration.

Considerably more practical algorithms are the hybrid block iterative algorithm. This algorithm extract the matrix polynomial obtained in the course of a BGMRES step, then reapply the matrix polynomial by means of a basic one-step iterated until convergence. Unfortunately, it is known that matrices exist for which BGMRES(m,s) convergence but the hybrid block iteration may perform much disappointedly. Therefore, the question that arises is how to modify the hybrid BGMRES method in order to make it viable.

In this paper, we propose an approach for addressing the above question. Our experiments show that this approach offers substantially better performance than hybrid BGMRES [1]. The proposed method is referred to as *Product hybrid block GMRES*. It implements an the existing hybrid BGMRES algorithm, but the Richardson iteration is based on a product of several matrix polynomials rather than a single matrix polynomial.

In Section 2, some properties of hybrid BGMRES are recalled. In Section 3, the complementary behavior of BGMRES(m,s) are illustrated, which provides the main motivation of developing the product hybrid block scheme. In Section 4, the product hybrid block GMRES algorithm is developed. In Section 5, numerical examples are presented to illustrate a remarkable superiority of the new algorithm. Finally, in Section 6 the paper is concluded.

2. Hybrid BGMRES

Hybrid BGMRES [1] attempts to combine the advantage of the block approach with those of hybrid methods proposed by Joubert [15], Saylor and Smolonski [16], and especially Nachtigal et al [4].

Hybrid BGMRES algorithm

Given X_0 and $R_0 = B - AX_0$

(1) Generate V_m, H_m, L_m;

(2) $\min_{Y \in R^{ms \times n}} \left\| E_1 \chi_{0,0} - H_m Y \right\|$;

(3) $\overline{X}_m = X_0 + V_m Y$;

(4) $\theta = Eig(H_m + L_m)$;

(5) $X_m = Richardson(A, \overline{X}_m, B, \theta)$.

The matrix $\chi_{0,0}$ is chosen so that $R_0 \chi_{0,0}$ is orthonormal. The least square problem in the algorithm is solved by block QR decomposition. Hybrid BGMRES is an extension of the method used in the single right-hand side case [4]. As we show below, critical to the design of hybrid block method described in this paper is the characterization of BGMRES in terms of matrix polynomial according to the theory developed in [5].

Theorem 1. (Simoncini and Gallopoulos [5]) Let $H_m = V_m^T A V_m$. The BGMRES residual matrix polynomial Φ_m coincides with the eigenvalues of the matrix $\overline{H}_m + L_m$, where $\overline{H}_m = [I_{ms}, 0] H_m$ and $L_m = \overline{H}_m^{-T} h_{m+1}^T h_{m+1}$ with $h_{m+1} = E_{m+1}^T H_m$.

Note $E_i^T := [0_s, \cdots, I_s, \cdots, 0_s]$ is the rectangular matrix with I_s as its ith block element.

From Theorem 1, the roots of the matrix polynomial $\Phi_m(\lambda) = 0$ satisfy $(H_m + L_m)z = \lambda z$. The rank of L_m is s. Hence, the roots of the BGMRES residual are Ritz values of a rank-s modification of A.

The parameters of the Richardson process are inverse of the latent roots of Φ_m. These are the roots of the polynomial $p_{ms} := \det(\Phi_m(\lambda))$, $p_{ms} \in \overline{P}_{m,s}$ [1]. Consequently, from Theorem 1 we can get $p_{ms} = \det(\lambda I - (H_m + L_m))$. Thus, the Richardson procedure accomplishes the multiplication [1]:

$$R_m = p_{ms} \overline{R}_m .$$

3. Complementary behavior of restarted BGMRES

Suppose that at the mth BGMRES step, we have

$$\frac{\left\|R^{(m)}\right\|}{\left\|R^{(0)}\right\|}=\frac{\left\|p_{ms}(A)R^{(0)}\right\|}{\left\|R^{(0)}\right\|}=\tau$$

for some $\tau<1$.

For HBGMRES, our hope that

$$\left\|p_{ms}(A)\right\|\approx\tau \tag{3.1}$$

so that the Richardson iterative will continue to reduce the residual

$$\frac{\left\|R^{(km)}\right\|}{\left\|R^{(0)}\right\|}\approx\left(\frac{\left\|R^{(m)}\right\|}{\left\|R^{(0)}\right\|}\right)^{k},\ k\geq 0. \tag{3.2}$$

However, such a conclusion can never be guaranteed. The equation (3.1) may fail, leading us with

$$\tau=\frac{\left\|R^{(m)}\right\|}{\left\|R^{(0)}\right\|}<<\left\|p_{ms}(A)\right\|.$$

In such circumstances, (3.2) will be far from satisfied, and the Richardson iteration may convergence much more slowly than expected or may not convergence at all.

We present a theorem in support of the convergence of HBGMRES.

Theorem 2. Let $p_{ms}(A)$ be the matrix polynomial obtained in the course of a BGMRES step, Λ is the spectrum of A, HBGMRES algorithm convergence if and only if $\forall\lambda\in\Lambda,\left|p_{ms}\right|<1$.

The BGMRES residual polynomial $\left|p_{ms}(\lambda)\right|$ is likely to be considerably large for one cycle. This is fetal to the Richardson iteration. On the other hand, because of the complementary behavior of restarted GMRES, $\left|p_{ms}(\lambda)\right|$ can be correspondingly small in the next cycle.

Example 1. Take

$$A=\begin{pmatrix}0.5 & \delta & & & & \\ & 1.0 & \delta & & & \\ & & 1.5 & \delta & & \\ & & & 2.0 & \delta & \\ & & & & 2.5 & \delta \\ & & & & & 3.0\end{pmatrix};\ B=\begin{pmatrix}0.5+\delta & 0.5-\delta \\ 1.0+\delta & -1.0+\delta \\ 1.5+\delta & 1.5-\delta \\ 2.0+\delta & -2.0+\delta \\ 2.5+\delta & 2.5-\delta \\ 3.0 & -3.0\end{pmatrix},\ (\delta=0.05).$$

and run BGMRES(2,2). It is observed that the eigenvector components of residuals of every two successive cycles complement each other.

BGMRES lemniscates [5] are employed to give a clear description of the complementary behavior of BGMRES(2,2). The lemniscates of the *s*th cycles was defined as $L_\tau=\left\{z\in c:\left|p_{ms}(z)\right|=\tau_s\right\}$, in which τ_s is the convergence rate of the cycle.

In Fig.1, the complementary behavior of BGMRES(2,2) is observed clearly. The BGMRES lemniscates of the 1st to 8th restarting cycles are presented. Write the spectrum of A as $\Lambda=\{\lambda_1,\lambda_2,\lambda_3,\lambda_4,\lambda_5,\lambda_6\}=\{0.5,1.0,1.5,2.0,2.5,3.0\}$. At the 1st cycle, $\lambda_2,\lambda_3,\lambda_4,\lambda_5,\lambda_6$ are well enclosed by the BGMRES lemniscates and the corresponding eigenvector components are significantly reduced. After the 1st cycle, the residual is rich in the first eigenvector direction. For the

2nd cycle, λ_1 is well enclosed by the BGMRES lemniscates, a significant reduction in the first eigenvector is occurred. The following BGMRES cycles behave similarly to these first two, with groups of two cycles complementing each other.

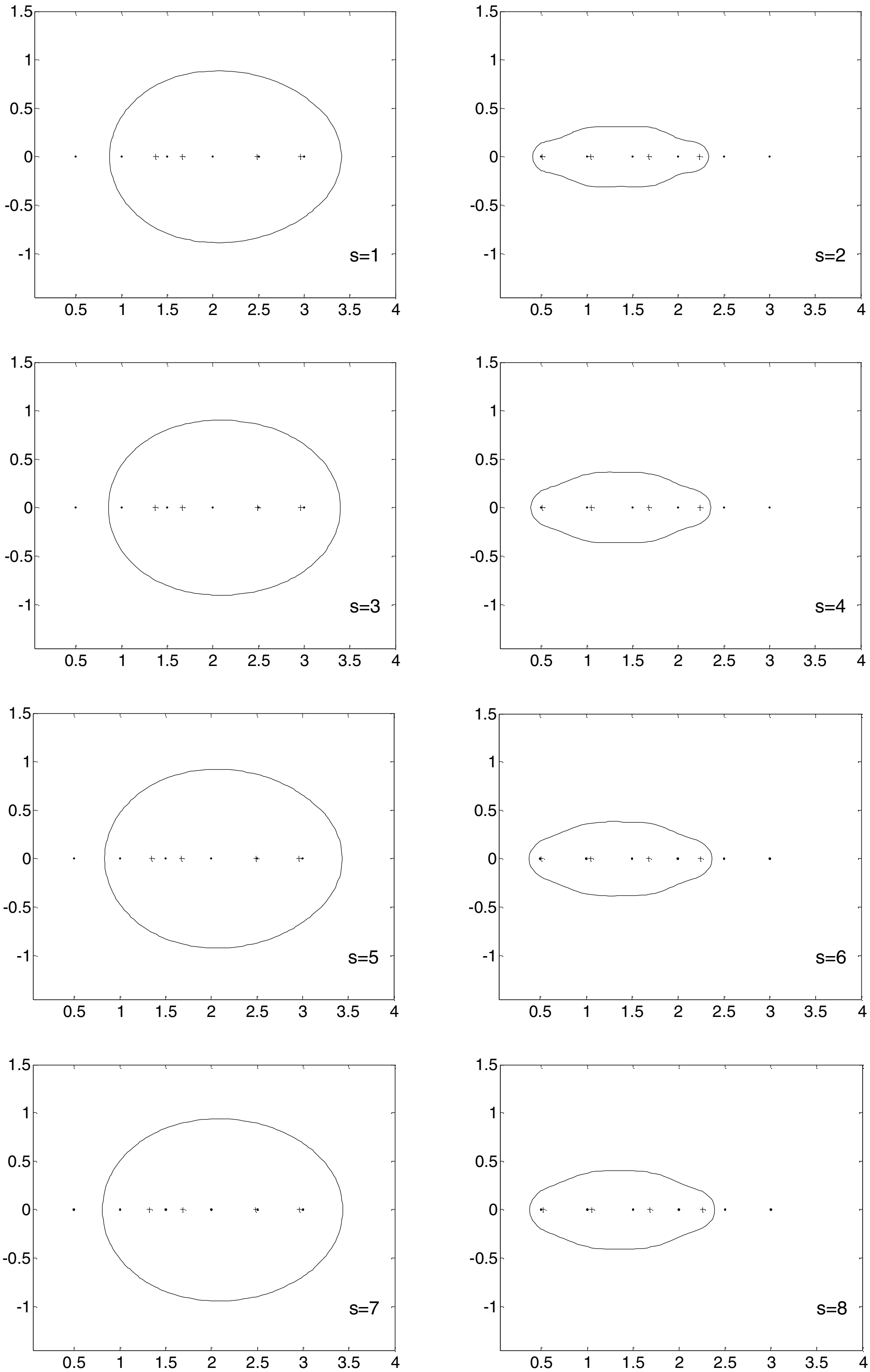

Fig. 1: BGMRES lemniscates of the 1st to 8th cycles. Eigenvalues: •; Harmonic Ritz values: +.

Let π_{ms} be a product of all the BGMRES polynomials. The lemniscates in Fig. 2 is computed by $L_\tau = \{z \in c : |\pi_{ms}(z)| = \tau_{average}\}$, in which $\tau_{average}$ is the average convergence rate of all the involved restarting cycles.

As it is seen in Fig. 2, all the eigenvalues are enclosed in the product BGMRES lemniscates, indicating that all the eigenvector components have been significant reduced by the product polynomial. In consequence, the product matrix polynomial associated with a complementary cycle can be used to form a more effective hybrid block method.

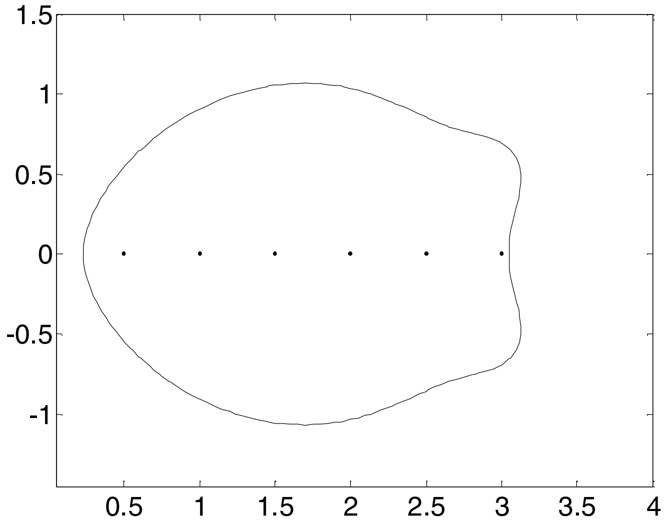

Fig. 2: BGMRES lemniscates of a product of all the cycles. Eigenvalues: •.

4. Product hybrid block GMRES

The product hybrid block GMRES algorithm is sketched in the following.

Phase (i). Run BGMRES(*m,s*) until $\|R_{km}\|$ drops by a suitable amount. Set *t*=*k* and construct the BGMRES residual polynomials $\{p_{ms,k}\}_{k=1}^{t}$

Phase (ii). Re-apply the product polynomial

$$\pi_t(z) = p_{ms,t}(z) p_{ms,(t-1)}(z) \cdots\cdots p_{ms,1}(z)$$

cyclically until convergence: $R_{mt,k} = [\pi_t(A)]^k \circ R_0$, $(k = 2,3\cdots\cdots)$.

Table1:Leading computational costs per iterative of PHBGMRES

$M \times N$	$s(m+1)+2ms^2$
n-vector DOT	$\frac{m(m+1)}{2}$
n-vector DAXPY	$s\frac{m(m+1)}{2}+s+2ms$
MGS on $n \times s$ block	$\frac{m(m+1)}{2}s^2+s$
Solve orders ms triang. system	s
Leading scalar costs	$6s^3m^2+s^2m^3+4ms^3$
Mult. of block of dim. $n \times s$ and $s \times s$	$\frac{m(m+1)}{2}$

The structure of the algorithm is practically appealing. In Phase(i) the BGMRES(*m,s*) iteration produces iterates as by-product, and its cost is only slightly greater(about $2m^2s^3$ per step) than a standard BGMRES(*m,s*) iteration, due to the calculation of $\pi_s(z)$. The computation cost of product hybrid BGMRES is summarized in Table 1.

The computational cost for the polynomial acceleration led us to re-use the same residual polynomial ($\pi_s(z)$) during the algorithm.

The new algorithm has the advantage over the original one in that its convergence behavior is well understand, as stated in the following theorem.

Theorem 3. The product hybrid BGMRES algorithm convergence if BGMRES(*m,s*) convergence.

Proof: If BGMRES(*m,s*) convergence, it holds that $\lim_{t\to\infty}\|\pi_t(z)R_0\|=0$. Then with a suitable *t*, we must have $\|\pi_t(z)\|<1$, which leads to convergence of the Richardson iteration of Phase (ii).

5. Numerical experiments

In this section experimental results of using product hybrid BGMRES to solve (1.1) is presented. Its performance is compared with other iterative methods, including hybrid BGMRES (HBGMRES) and BGMRES(*m,s*). The right-hand sides were chosen as *B*=rand(*n,s*), where function rand creates a random matrix of dimension $n\times s$ with values uniformly distributed in [0,1]. The initial guess $X_0=[0,0,\cdots\cdots,0]$, the convergence tolerance $\varepsilon=1.0e-10$, and for each example, the plot shows $\log_{10}\|R_n\|$ as a function of work measured by vector operations.

Example 2. This problem is taken from [4]. Let *A* be a large upper-triangular Toeplitz matrix of the form

$$A=\begin{pmatrix}1.0 & 1.0 & 0.5 & & & \\ & 1.0 & 1.0 & 0.5 & & \\ & & 1.0 & 1.0 & \ddots & \\ & & & \ddots & \ddots & 0.5 \\ & & & & \ddots & 1.0 \\ & & & & & 1.0\end{pmatrix}(1000\times 1000).$$

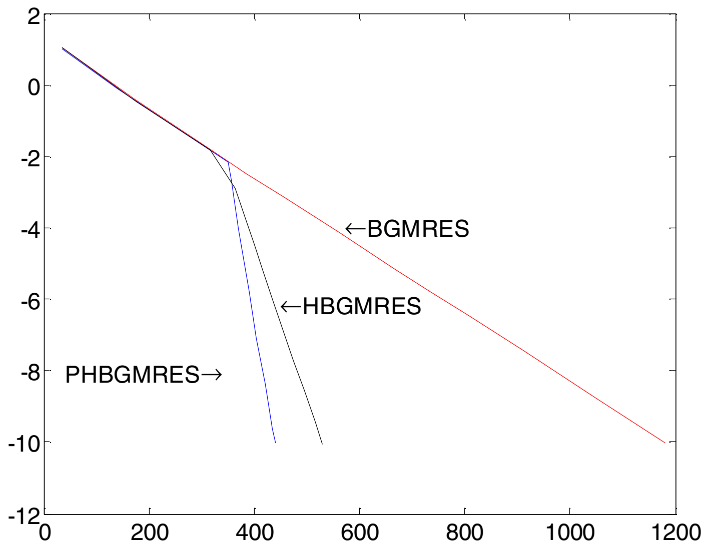

Fig. 3: Example 2. Convergence curve; Log. residual norm vs. work.

In Fig. 3, we observe that hybrid BGMRES performs well. However, PH-BGMRES is further ahead. It shows that product hybrid BGMRES consistently and significantly improved the performance of hybrid BGMRES and BGMRES(*m,s*).

Example 3. The experiment is conducted using matrix (e05r0000) that originate from the Harwell-Boeing collection.

It is seen that the hybrid BGMRES diverges, where PH-BGMRES convergence rapidly. Fig. 4 again shows that the product hybrid BGMRES approach consistently and significantly improved the performance of hybrid BGMRES and BGMRES(*m,s*). After incorporating ILU preconditioning with no additional fill-in, we see that the product hybrid BGMRES algorithm can perform even better.

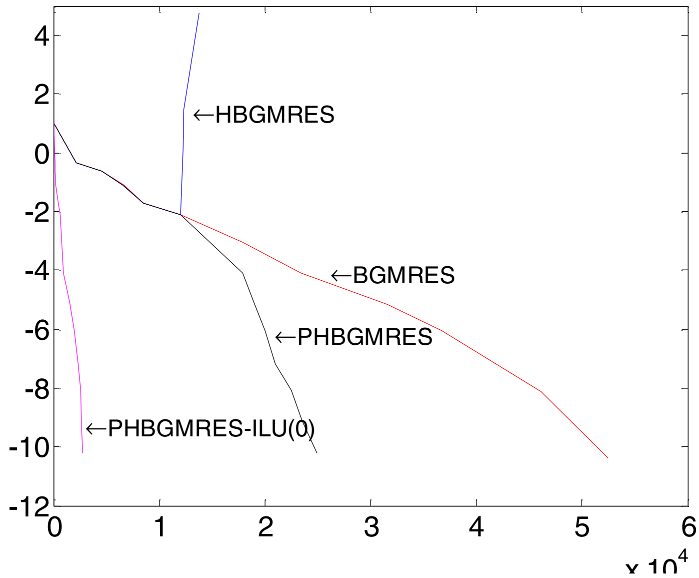

Fig. 4: Example 3. Convergence curve; Log. residual norm vs. work.

6. Conclusions

In this paper a product hybrid block GMRES algorithm for solving linear systems with multiple right-hand sides is proposed. It is achieved by computing a product of the BGMRES matrix polynomials and then applying the product polynomial via a Richardson iteration cyclically. Numerical experiments show that the new algorithm can significantly improve the performance of hybrid BGMRES and BGMRES.

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