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Improving GMRES(m) using an adaptive switching controller

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Summary

The restarted generalized minimal residual (denoted as GMRES(m)) normally used for solving a linear system of equations of the form $Ax = b$ has the drawback of eventually presenting a stagnation or a slowdown in its rate of convergence at certain restarting cycles. In this article, a switching controller is introduced to modify the structure of the GMRES(m) when a stagnation is detected, enlarging and enriching the subspace. In addition, an adaptive control law is introduced to update the restarting parameter to modify the dimension of the Krylov subspace. This combination of strategies is competitive from the point of view of helping to avoid the stagnation and accelerating the convergence with respect to the number of iterations and the computational time. Computational experiments corroborate the theoretical results.

KEYWORDS

acceleration, adaptive restarting parameter, control Lyapunov law, GMRES(m)

1 | INTRODUCTION

The generalized minimal residual method (GMRES)[1] is a popular iterative method for solving the large nonsymmetric system of linear equations

$$Ax = b; \quad A \in \mathbb{C}^{n\times n}; \quad x, b \in \mathbb{C}^n. \tag{1}$$

To limit the computational cost and storage requirements, the method is usually restarted after a fixed number of steps. The resulting method is called restarted GMRES, denoted by GMRES(m). When restarted, the resulting approximate solution is used as the initial guess for the next step. This process repeats until the residual norm is small enough. The group of m iterations between successive restarts is referred to as a cycle, and m is referred to as the restart parameter. In this article, the jth restart cycle number is denoted by a superscript, while the iteration number is denoted by a subscript, that is, $x_k^{(j)}$ ($r_k^{(j)} := b - Ax_k^{(j)}$) is the approximate solution (residual) after j cycles at the kth internal iteration with $1 \le k \le m$.

The approximate solution at the end of the jth cycle is $x_m^{(j)} = x_m^{(j-1)} + q_{m-1}^{(j)}(A)r_m^{(j-1)}$, where $q_{m-1}^{(j)}(A)$ is a polynomial of degree at most $m-1$ and $q_{m-1}^{(j)}(A)r_m^{(j-1)}$ is an element of the Krylov subspace, span$\{r_m^{(j-1)}, Ar_m^{(j-1)}, \dots A^{m-1}r_m^{(j-1)}\}$. The residual vector at the end of the cycle is $r_m^{(j)} = b - Ax_m^{(j)} = r_m^{(j-1)} - Aq_{m-1}^{(j)}(A)r_m^{(j-1)} = p_m(A)r_m^{(j-1)}$, where p is a polynomial of degree m or less with $p(0) = 1$.

A drawback with the GMRES(m) is that its rate of convergence can deteriorate and even stagnate.[2,3] The latter means that the new subspace generated is close to the previous one so that the approximation does not make

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any progress.[4] The problem of improving the rate of convergence and avoiding stagnation has been addressed using several strategies; see, for instance, References 5-12 and the references therein. In this article, two strategies are used to ensure that the residual has monotonically decreasing behavior. The first strategy consists of the augmentation of the search subspace by a subspace that contains information about the previous cycles.[6,13] This strategy accelerates the GMRES(m) but it is not helpful when the method stagnates. The second strategy consists of enriching the search subspace by the inclusion of spectral information about the matrix A.[9] This enrichment of the subspace is commonly associated with the smallest eigenvalues and it can improve the convergence by helping to avoid stagnation. However, enrichment of the subspace can be expensive when many eigenvalues have to be computed at each step.

In order to combine the advantages of each of the aforementioned strategies at each cycle of the restarted GMRES, we explore an appropriate articulation of the strategies by considering the adaptive variation of the strategies in the process of resolution of the restarted GMRES. This is done by introducing a switching logic into the structure of the GMRES(m). The logic is defined so as to combine the desirable properties of variation of the restart parameter and subspace enrichment in accordance with the evolution of the GMRES(m)algorithm (ie, by monitoring the residues). This kind of switching strategy, based on the state of the system, is referred to in the feedback control literature as variable structure control.[14,15] With the implementation of the several strategies using the variable structure approach, in principle, it is possible to enrich the search subspace whenever it is necessary to accelerate the convergence and avoid stagnation.[16-19]

This article proposes a strategy about when and how to augment and choose the enrichment information to include in the search subspace. At each restart cycle, the strategy decides which part of the available subspace should be kept to augment the Krylov subspace at the next restart. The new search subspace is composed of some of the previously kept vectors, as well as the vectors generated in the current cycle. Unfortunately, in some cases even with the augmentation and the enrichment, it is possible to obtain a poor performance. Moreover, the selection of the appropriate augmentation or enrichment at each cycle does not ensure the right rate of convergence and the restarted GMRES can still present stagnation if the m value is not selected correctly. For this reason, we also consider the modification of the restart parameter for adjusting the dimension of the Krylov subspace. Several approaches have been encountered in the literature with regard to the appropriate adjustment of the restart parameter appropriately,[3,5,8,12,20] but the best way to select m has still not been established.[5,12] We will use an adaptive rule inspired by the ones presented in Reference 5,20 but with different criteria allowing the increase of the restart parameter whenever stagnation is detected.

This work is organized as follows. In Section 2, the control theoretical formulation for stagnation of GMRES(m) is characterized and ways to measure its rate of convergence are defined. In Section 3, techniques are presented to overcome the stagnation and improve the rate of convergence. The techniques are parts of the proposed switching control strategy and the control law for the adjustment of the restart parameter. The convergence is guaranteed by using a control Lyapunov function, designed to evaluate the convergence, and forcing negativity of its decrement by choice of the switching control as well as the variation of the restart parameter m. The switching rule allows the combination of the augmentation and the enrichment of the subspace and allows one to identify if the dimension of the search subspace needs to be modified. The latter is done using a rule inspired by a proportional derivative control which is used to update the value of m. Numerical examples are presented in Section 4 and concluding remarks in Section 5. It is observed that the combination of the methods results in a better rate of convergence and a more adequate trade-off between the rate of convergence and the computational time, with only a moderate increase in memory requirements.

Matlab notation has been used for matrices and vectors. Given a vector u, u^T denotes its transpose and u^* its conjugate transpose or Hermitian transpose, $u_{k:m}$ denotes its kth through mth components; its kth single component is denoted by u_k. An analogous notation is used for matrices. Throughout the article, $\|\cdot\|$ denotes the 2-norm for vectors and the induced 2-norm for matrices. The inner product is denoted as $\langle\cdot,\cdot\rangle$.

2 | CONTROL FORMULATION FOR STAGNATION

The GMRES(m) approximates the solution to the system (1) at jth cycle from a residual $r_m^{(j-1)}$ which is used to construct a Krylov subspace of dimension m. At the jth cycle one obtains the vector $x_m^{(j)}$ that solves the least squares problem

$$\min_{x_m^{(j)} \in \mathcal{K}_m(A,v)} \|b - Ax_m^{(j)}\| \tag{2}$$

over the Krylov subspace $\mathcal{K}_m(A, v) = \text{span}\{v, Av, \dots A^{m-1}v\}$. To solve this problem, an orthonormal basis for the Krylov subspace is developed using the Arnoldi relationship given by

$$AV_m^{(j)} = V_{m+1}^{(j)}\tilde{H}_m^{(j)} = V_m^{(j)}H_m^{(j)} + h_{m+1,m}v_{m+1}^{(j)}e_m^T, \tag{3}$$

where $V_m^{(j)} \in \mathbb{C}^{n\times m}$ and $V_{m+1}^{(j)} := [V_m^{(j)}\ v_{m+1}^{(j)}] \in \mathbb{C}^{n\times(m+1)}$ has orthonormal columns. The matrix $\tilde{H}_m^{(j)} \in \mathbb{C}^{(m+1)\times m}$ is upper Hessenberg by construction, with upper $m \times m$ block $H_m^{(j)}$, and the $(m+1, m)$ entry is $h_{m+1,m}$. If the Arnoldi process is initiated with $v = r_m^{(j-1)}/\|r_m^{(j-1)}\|$, then at the jth cycle, one obtains the Krylov subspace of dimension m denoted by $\mathcal{K}_m(A, v) = \text{span}(V_m^{(j)})$.

At the jth cycle of GMRES(m), the functional to be minimized in expression (2) is

$$J(y^{(j)}) = \|b - Ax_m^{(j)}\| = \|b - A(x_m^{(j-1)} + V_m^{(j)}y^{(j)})\|. \tag{4}$$

Using the Arnoldi relation $AV_m^{(j)} = V_{m+1}^{(j)}\tilde{H}_m^{(j)}$ the expression above takes the form:

$$\begin{aligned} J(y^{(j)}) &= \|b - Ax_m^{(j-1)} - AV_m^{(j)}y^{(j)}\| \\ &= \|V_{m+1}^{(j)}(\beta e_1^{(m+1)} - \tilde{H}_m^{(j)}y^{(j)})\|, \end{aligned}$$

where $\beta = \|r_m^{(j-1)}\|$ and $e_i^{(n)}$ is the ith column of the $n \times n$ identity matrix. Since matrix $V_{m+1}^{(j)}$ is orthogonal, then one obtains

$$J(y^{(j)}) = \|\beta e_1^{(m+1)} - \tilde{H}_m^{(j)}y^{(j)}\|. \tag{5}$$

Hence, GMRES(m) gives a vector $y^{(j)}$ which minimizes (5), and the minimization of functional (5) is equivalent to the minimization of the expression (2). For solving expression (5) by least squares, in practice a QR decomposition of matrix $\tilde{H}_m^{(j)}$ is computed, obtaining:

$$Q_m^{(j)}\tilde{H}_m^{(j)} = \begin{bmatrix} R_m^{(j)} \\ 0 \end{bmatrix}, \tag{6}$$

where $Q_m^{(j)}$ is a unitary matrix of dimension $(m+1)\times(m+1)$ and $R_m^{(j)}$ an upper triangular matrix of dimension $m \times m$ which is nonsingular, since $\tilde{H}_m^{(j)}$ has full rank. Hence using the QR factorization the problem of minimizing (5) has the form

$$\min_{y^{(j)}\in\mathbb{C}^m} \|\beta e_1^{(m+1)} - \tilde{H}_m^{(j)}y^{(j)}\| = \min_{y^{(j)}\in\mathbb{C}^m} \left\| Q_m^{(j)*}\left(\beta Q_m^{(j)}e_1^{(m+1)} - \begin{bmatrix} R_m^{(j)} \\ 0 \end{bmatrix} y^{(j)}\right)\right\| \tag{7}$$

$$= \min_{y_j^{(j)}\in\mathbb{C}^m} \left\| \beta Q_m^{(j)}e_1^{(m+1)} - \begin{bmatrix} R_m^{(j)} \\ 0 \end{bmatrix} y^{(j)} \right\| \tag{8}$$

$$= \min_{y^{(j)}\in\mathbb{C}^m} \left\| \begin{bmatrix} \beta q_{1:m,1} - R_m^{(j)}y^{(j)} \\ \beta q_{m+1,1} \end{bmatrix} \right\| \tag{9}$$

where $Q_m^{(j)}e_1^{(m+1)} = \left[q_{1:m,1}; q_{m+1,1}\right]$ denotes the first column of $Q_m^{(j)}$. Recalling that $\beta = \|r_m^{(j-1)}\|$, the unique solution of the above least squares problem is $y^{(j)} = \beta R_m^{(j)-1}q_{1:m,1}$ and $\|r_m^{(j)}\| = \beta|q_{m+1,1}|$.

In terms of the control theory, an iterative method for solving linear systems can be represented as Reference 14:

$$\begin{cases} x_m^{(j)} = x_m^{(j-1)} + u^{(j)}, \\ r_m^{(j-1)} = b - Ax_m^{(j-1)}, \\ u^{(j)} = \phi(r_m^{(j-1)}, A, m). \end{cases} \tag{10}$$

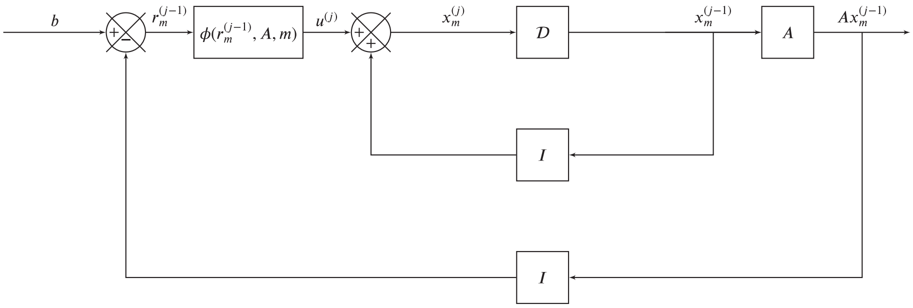


FIGURE 1 Control theoretical block diagram of GMRES(m) (10). The block labeled $\mathcal{D}$ delays its input by one cycle, that is, $x^j = \mathcal{D}(x^{j+1})$. GMRES, generalized minimal residual

where $u^{(j)}$ is the control signal and $\phi(\cdot)$ is the control law. It is desired to choose the the control law $\phi(\cdot)$ to provide a sequence of control signals $u^{(j)}$ to guide the residual $\|r^{(j)}\|$ to zero as $j \to \infty$. The GMRES(m) control law $\phi(\cdot)$ is $\phi(r_m^{(j-1)}, A, m) = V_m^{(j)} y^{(j)}$ where $y^{(j)}$ is obtained by minimizing expression (5). Figure 1 is the block diagram representing the GMRES(m) from the control theory perspective.

It is important to observe that the control law $\phi(r_m^{(j-1)}, A, m)$ determines the behavior of system (10) and consequently, in order to improve its convergence, the control law $\phi(\cdot)$ must be modified. At this point it is important: (a) to characterize the stagnation and slowdown of convergence for GMRES(m) modeled by system (10), and (b) to specify how to measure the behavior in terms of the residuals allowing the measurement of the quality of the convergence and the modification of the control law $\phi(\cdot)$ in order to ensure the convergence of system (10).

In this article, two types of GMRES(m) stagnation are considered. The first one is known as partial stagnation meaning that the residual norm of consecutive cycles remains approximately constant, that is, $\|r_m^{(j)}\| \approx \|r_m^{(j-1)}\|$, $j = k, \ldots, p$, where $k > 0$ and p is a finite value. Subsequently, at the $(p+1)$th cycle, a decrease in the residual norm ($\|r_m^{(p+1)}\| < \|r_m^{(p)}\|$) is obtained (for instances of this kind of stagnation, see the experimental results in Figure 3 for GMRES(30)). The difference between p and k is known as the complementary frequency.[21]

Partial stagnation can be detected by comparing the size of the residual norm form two consecutive cycles. This, in turn, can be achieved by observing the entry $q_{m+1,1}$, since $\|r_m^{(j)}\| = \beta |q_{m+1,1}|$ with $\beta = \|r_m^{(j-1)}\|$ (see expression 9). If $|q_{m+1,1}| = 1$, then the GMRES(m) will not converge (ie, stagnates completely at the jth cycle with respect to the previous one) and it will be necessary to take some action to overcome the stagnation. A more general situation can occurs when it happens that Reference 3: $\|r_m^{(j)}\| < \|r_m^{(j-1)}\|$, $j = 1, 2, \ldots, k$; followed by $\|r_m^{(j)}\| = \|r_m^{(j-1)}\|$, $j = k+1, \ldots, p$; with $p \to \infty$.

Although complete stagnation can happen, in practice, it is more common to observe a deterioration in the rate of convergence. We are interested in the characterization of this slowdown in the convergence when the reduction in the residual norms at consecutive cycles is very small, that is, $\|r_m^{(j)}\| \approx \|r_m^{(j-1)}\|$.

Definition 1. When the residual norms at consecutive jth and $(j-1)$th cycles satisfy $\|r_m^{(j)}\| = (1-\epsilon)\|r_m^{(j-1)}\|$, for any positive $\epsilon \ll 1$, it is said that GMRES(m) presents a *slowdown convergence* in its rate of convergence.

To relate the concepts above with the quality of the convergence and the convergence itself, we introduce an energy Lyapunov function based on the residuals as follows Reference 20.

Definition 2. The function $V(r) : \mathbb{R}^n \to \mathbb{R}$ is said to be a *candidate Lyapunov function* on a subset $\mathcal{H}$ of $\mathbb{R}^n$, if (i) V is continuous on $\mathcal{H}$ and (ii) locally positive definite $V(0) = 0$ and $V(r) > 0$, $\forall r \in \mathcal{H} \setminus \{0\}$ with $\mathcal{H}$ being a neighborhood of $r = 0$; in addition $V(r)$ is a Lyapunov function if its increment $\Delta V(r)$ is negative definite (denoted < 0), whenever $r \in \mathcal{H}$.

The importance of Lyapunov functions arises from the fact that the GMRES(m) is asymptotically stable (this implies that $\lim \|r_m^{(j)}\| \to 0$ as $j \to \infty$) whenever $\Delta V(r_m^{(j)}) < 0$ for the sequence $x_m^{(j)}$. We use the 2-norm squared of the residual at the current cycle as a candidate Lyapunov function, that is, $V(r_m^{(j)}) = \langle r_m^{(j)}, r_m^{(j)} \rangle$ at the jth cycle.

Definition 3. Let the residuals at cycles j, $(j-1)$ and $(j-2)$ be $R_m^{(j)}$, $r_m^{(j-1)}$ and $r_m^{(j-2)}$, respectively. Let the control Lyapunov function be chosen as $V(r_m^{(j)}) = \langle r_m^{(j)}, r_m^{(j)} \rangle$. The local increment $\Delta V(r_m^{(j)})$ and the skip local increment $\Delta \tilde{V}(r_m^{(j)})$ at the jth cycle are defined as

$$\Delta V(r_m^{(j)}) := \|r_m^{(j)}\|^2 - \|r_m^{(j-1)}\|^2 \tag{11}$$

and

$$\Delta\tilde{V}(r_m^{(j)}) := \left(\Delta V(r_m^{(j)}) + \Delta V(r_m^{(j-1)})\right) = \left(\|r_m^{(j)}\|^2 - \|r_m^{(j-2)}\|^2\right); \tag{12}$$

the relative skip increment rate $D(r_m^{(j)})$ with respect to the $(j-1)$th cycle is defined as:

$$D(r_m^{(j)}) := \left(\|r_m^{(j)}\| - \|r_m^{(j-2)}\|\right) / \left(\|r_m^{(j-1)}\|\right). \tag{13}$$

Let consider now the behavior of the angles between consecutive residual cycles in terms of stagnation and the skip local increment $\Delta\tilde{V}(r_m^{(j)})$ and the relative skip increment rate $D(r_m^{(j)})$. Let the residuals at the mth iteration at the cycles j, $(j-1)$, and $(j-2)$ be given by $R_m^{(j)}$, $r_m^{(j-1)}$ and $r_m^{(j-2)}$, respectively. The angles $\alpha_m^{(j)} := \angle(r_m^{(j)}, r_m^{(j-1)})$ and $\gamma_m^{(j)} := \angle(r_m^{(j)}, r_m^{(j-2)})$ are called sequential and skip angles, respectively. Following Reference 6, consider that the angles are always between 0 and $\pi/2$. To obtain an expression for the sequential angle note that

$$\langle r_m^{(j)}, r_m^{(j-1)}\rangle = \langle r_m^{(j)}, r_m^{(j)} + AV_m^{(j)}y^{(j)}\rangle, \tag{14}$$

$$= \|r_m^{(j)}\|^2 + \langle r_m^{(j)}, AV_m^{(j)}y^{(j)}\rangle, \tag{15}$$

where $V_m^{(j)}$ is a basis for the Krylov subspace $\mathcal{K}_m(A, r_m^{(j-1)})$. In addition, since $r_m^{(j)} \perp AV_m^{(j)}y^{(j)}$ by construction, one obtains $\langle r_m^{(j)}, r_m^{(j-1)}\rangle = \|r_m^{(j)}\|^2$. This motivates the following definition for the sequential angle $\angle(r_m^{(j)}, r_m^{(j-1)})$ (details are in References 6,22).

Definition 4. The sequential angle $\alpha_m^{(j)} = \angle(r_m^{(j)}, r_m^{(j-1)})$ between the residual vectors at the end of the jth and $(j-1)$th restart cycles, denoted by $R_m^{(j)}$ and $r_m^{(j-1)}$, respectively; is given by the following implicit relationship:

$$\cos(\alpha_m^{(j)}) = \frac{\langle r_m^{(j)}, r_m^{(j-1)}\rangle}{\|r_m^{(j)}\|\ \|r_m^{(j-1)}\|} = \frac{\|r_m^{(j)}\|}{\|r_m^{(j-1)}\|}. \tag{16}$$

Next, a formulation for the stagnation and slowdown convergence in terms of the Lyapunov function (Definition 2) and the local increment (11)) is obtained. Since $\|r_m^{(j)}\| \leq \|r_m^{(j-1)}\|$, dividing the Equation (11) by $\|r_m^{(j-1)}\|^2 > 0$, one gets

$$\frac{\Delta V(r_m^{(j)})}{\|r_m^{(j-1)}\|^2} = \frac{\|r_m^{(j)}\|^2}{\|r_m^{(j-1)}\|^2} - 1, \tag{17}$$

so that $\Delta V(r_m^{(j)})$ is negative definite (ie, $\Delta V(r_m^{(j)}) < 0$) if $0 \leq \|r_m^{(j)}\|/\|r_m^{(j-1)}\| < 1$.

Remark 1. Notice that if $\Delta V(r_m^{(j)}) < 0$ then the algorithm is locally convergent at jth cycle. Moreover, the more negative $\Delta V(r_m^{(j)})$, the faster the reduction of the residual with respect to the previous one, which means that convergence is accelerated. If $\Delta V(r_m^{(j)})/\|r_m^{(j-1)}\|^2 \approx -1$, then $\|r_m^{(j)}\|/\|r_m^{(j-1)}\| \approx 0$. On other hand, if $\Delta V(r_m^{(j)})/\|r_m^{(j-1)}\|^2 \approx 0$ then $\|r_m^{(j)}\| \approx \|r_m^{(j-1)}\|$ (which implies local stagnation with respect to $\|r_m^{(j-1)}\|$). Conversely, if $\|r_m^{(j)}\| \approx \|r_m^{(j-1)}\|$, that is, $\|r_m^{(j)}\| = (1-\epsilon)\|r_m^{(j-1)}\|$ for some $\epsilon \ll 1$, then $\Delta V(r_m^{(j)})/\|r_m^{(j-1)}\|^2 = \mathcal{O}(\epsilon)$.

Based on the determination of the quality of the rate of convergence measured with the concepts introduced in this section, the adaptive switching controller (introduced in the following section) decides either to modify the restart parameter or the structure in the GMRES(m). This is discussed in the following section.

3 | ADAPTIVE SWITCHING CONTROLLER

The adaptive switching controller is composed of three parts: the adaptive part that modifies the restart parameter,[11,12,20] and another two parts that form the switching controller itself. The strategy behind the techniques for avoiding stagnation rely on modifying the search subspace. Some alternatives are to modify the initial vector that is usually the last residual vector,[7,11,23,24] to include other information or a combination of strategies.[5,9,25,26] In the following section, the three parts that form the controller are introduced.

3.1 | Controllers to modify the restart parameter

The next results show that a possible action to avoid stagnation consists of the increase of the restart parameter in the next cycle, after a complete stagnation is observed. Of course, this is always possible, however, the important point here is that not always is necessary to modify the parameter m and, in case it is, then to decide exactly how to change it.

First, observe that a complete stagnation (and convergence slowdown) has repercussions in structural terms of the matrices in the Arnoldi relation (3) as follows.

Proposition 1. *GMRES(m) presents complete stagnation if and only if at any jth cycle the vector $y^{(j)}$ is a null vector.*

Proof. According to Lemma 2.5 of Reference 27 and Theorem 3.1 of Reference 28, if complete stagnation happens, then at the jth cycle we have:

$$[h_{1,1} \quad h_{1,2} \quad \dots \quad h_{1,m}] = [0 \quad 0 \quad \dots \quad 0]$$

Denoting $y^{(j)}(k)$ the kth entry of vector $y^{(j)}$ at the jth cycle, and recalling that $y^{(j)}$ minimizes $J(y^{(j)})$, from the above expression

$$\begin{bmatrix} h_{2,1} & h_{2,2} & \dots & h_{2,m} \\ 0 & h_{3,2} & \dots & h_{3,m} \\ \vdots & \ddots & \vdots & \\ 0 & \dots & h_{m,m-1} & h_{m,m} \\ 0 & \dots & 0 & h_{m+1,m} \end{bmatrix} \begin{bmatrix} y^{(j)}(1) \\ y^{(j)}(2) \\ \vdots \\ y^{(j)}(m) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{18}$$

The matrix in (18) is upper triangular and has linearly independent rows because $h_{i,i-1} \neq 0, i = 2, \dots m+1$, thus $y^{(j)}(k) = 0$ for all $k = 1, \dots, m$ in the expression above.

Conversely, denoting by $K^{(j)}$ the $n \times m$ matrix of Krylov vectors $K^{(j)} = [r_m^{(j-1)} \quad Ar_m^{(j-1)} \quad \dots \quad A^{m-1}r_m^{(j-1)}]$, from Section 4 of Reference 29, $V_m^{(j)}y^{(j)} = K^{(j)}C_m^{(j)}y^{(j)}$; it follows that the vector $C_m^{(j)}y^{(j)}$ contains the coefficients of the polynomial $q_{m-1}(z)$ so that

$$C_m^{(j)}y^{(j)} = [\alpha_0 \cdots \alpha_{m-1}]^T, \quad q_{m-1}(z) = \alpha_0 + \alpha_1 z + \cdots + \alpha_{m-1}z^{m-1}. \tag{19}$$

Since vector $y^{(j)}$ is the null vector, one obtains $q_{m-1}(z) = 0 + 0z + \cdots + 0z^{m-1}$ and since $p_m(z) = 1 - zq_{m-1}(z)$, this gives the coefficients of $p_m(z)$ as well. Finally $p_m(z) = 1$ and $r_m^{(j-1)} = r_m^{(j)} = \cdots = r_m^{(p)}$. ■

The next result characterizes convergence slowdown.

Proposition 2. *If GMRES(m) presents a convergence slowdown at jth cycle, then the first row of the corresponding Hessenberg matrix has all first row entries much smaller than one, that is*

$$\tilde{H}_m^{(j)}(1,:) = [h_{1,1} \quad h_{1,2} \quad \dots \quad h_{1,m}] = [\epsilon_1 \quad \epsilon_2 \quad \dots \quad \epsilon_m],$$

where $|\epsilon_k| \ll 1, \forall k = 1 : m$.

Proof. If GMRES(m) presents convergence slowdown then this implies that $\|r_k^{(j)}\| \approx \|r_{k-1}^{(j)}\|,\ \forall k = 1 : m$. By construction, $r_0^{(j)} = r_m^{(j-1)}$ and $v_1^{(j)} = r_0^{(j)}/\|r_0^{(j)}\|$. Since $\|r_1^{(j)}\| \approx \|r_0^{(j)}\|$ (due to the deterioration in the convergence), the angle $\theta_1^{(j)} = \angle(r_0^{(j)}, Av_1^{(j)}) = \angle(v_1^{(j)}, Av_1^{(j)}) \approx \frac{\pi}{2}$. Computing the components of the Hessenberg matrix

$$h_{1,1} = \langle v_1^{(j)}, Av_1^{(j)} \rangle = \|v_1^{(j)}\| \|Av_1^{(j)}\| \cos(\theta_1^{(j)}) = \epsilon_1$$

where $\epsilon_1 \ll 1$ and is positive. Analogously, if $r_2^{(j)} \approx r_1^{(j)} \approx r_0^{(j)}$, and computing $h_{1,2} = \langle v_1^{(j)}, Av_2^{(j)} \rangle$ then $\langle r_1^{(j)}, AV_2^{(j)}y \rangle \approx 0$, where $y \in \mathbb{C}^2$ and $AV_2^{(j)}y$ is a linear combination of the columns of $AV_2^{(j)}$, we obtain

$$y(1)\langle r_1^{(j)}, Av_1^{(j)} \rangle + y(2)\langle r_1^{(j)}, Av_2^{(j)} \rangle \approx 0.$$

Since $\langle r_1^{(j)}, Av_1^{(j)} \rangle = \|r_0^{(j)}\| \langle v_1^{(j)}, Av_1^{(j)} \rangle = \|r_0^{(j)}\| |\epsilon_1|$, thus in order to keep the left side of the above expression as small as possible, it is necessary that $\langle r_1^{(j)}, Av_2^{(j)} \rangle = \|r_0^{(j)}\| \langle v_1^{(j)}, Av_2^{(j)} \rangle = \|r_0^{(j)}\| |\epsilon_2|$ with $|\epsilon_2| \ll 1$, implying $h_{1,2} = |\epsilon_2|$. Analogously, for the other components, $h_{1,k} = \epsilon_k \; \forall k = 3, \dots, m$. ∎

When the entries of the first row of the Hessenberg matrix $\tilde{H}_m^{(j)}(1,:)$ show the property mentioned in Proposition 2, its QR-decomposition has the form shown in (20) bellow.

Proposition 3. *If GMRES(m) presents convergence slowdown, then the matrix $Q_m^{(j)}$ associated with the QR - decomposition of the matrix $\tilde{H}_m^{(j)}$ has the form*

$$Q_m^{(j)} = \begin{bmatrix} \epsilon & 1 & 0 & \dots & 0 \\ -\epsilon & \epsilon^2 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (-1)^m \epsilon & (-1)^m \epsilon^2 & (-1)^m \epsilon^2 & \dots & 1 \\ (-1)^{m+1} & (-1)^{m+1}\epsilon & (-1)^{m+1}\epsilon & \dots & (-1)^{m+1}\epsilon \end{bmatrix}. \tag{20}$$

where ϵ is a small positive number.

Proof. The matrix $Q_m^{(j)}$ is constructed as a product of Givens rotations.[22,30]

$$Q_m^{(j)} = G_m^{(j)} \begin{bmatrix} G_{m-1}^{(j)} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} G_{m-2}^{(j)} & 0 \\ 0 & I_{m-2} \end{bmatrix} \dots \begin{bmatrix} G_1^{(j)} & 0 \\ 0 & I_{m-1} \end{bmatrix}, \tag{21}$$

where,

$$G_k^{(j)} := \begin{bmatrix} I_{k-1} & 0 & 0 \\ 0 & \cos(\theta_k^{(j)}) & \sin(\theta_k^{(j)}) \\ 0 & -\sin(\theta_k^{(j)}) & \cos(\theta_k^{(j)}) \end{bmatrix}. \tag{22}$$

for $k = 1, 2, \dots, m$. Considering a convergence slowdown, that is, $\theta_k^{(j)} \approx \pi/2$, that is, $\cos(\theta_k^{(j)}) \approx \epsilon$ and $\sin(\theta_k^{(j)}) \approx 1$, for $k = 1, 2, \dots, m$. Performing the matrix multiplication operations, the proposition is proved. ∎

A generalization of the above proposition is stated as follows:

Theorem 1. *GMRES(m) presents convergence slowdown if and only if at any jth cycle the vector $y^{(j)}$ has $\|y^{(j)}\| = \epsilon$ for any $\epsilon \ll 1$.*

Proof. Minimizing the expression (5) and using the QR factorization

$$\|r_m^{(j)}\| = \min_{y^{(j)} \in \mathbb{C}^m} \|\beta e_1^{(m+1)} - \tilde{H}_m^{(j)} y^{(j)}\| = \min_{y^{(j)} \in \mathbb{C}^m} \left\| \begin{bmatrix} \beta q_{1:m,1} - R_m^{(j)} y^{(j)} \\ \beta q_{m+1,1} \end{bmatrix} \right\|. \tag{23}$$

According to Proposition 3, one obtains $|q_{k,1}| = \epsilon, \forall k = 1, \dots, m$ and the component $q_{m+1,1} = 1$, consequently it is necessary to solve the linear system $R_m^{(j)} y^{(j)} = \beta q_{1:m,1}$ where $R_m^{(j)}$ is an upper triangular matrix. Using back substitution one obtains the components of the vector $y^{(j)}(k) \ll 1, \forall k = 1, \dots, m$ therefore $\|y^{(j)}\| = \epsilon$. Conversely, if $\|y^{(j)}\| = \epsilon$, the components of $y^{(j)}(k) = \epsilon, \forall k = 1, \dots, m$ where $|\epsilon| \ll 1$, therefore $\tilde{H}_m^{(j)} y^{(j)} = z^{(j)}$ with $|z^{(j)}(k)| = |\epsilon| \ll 1, \forall k = 1, \dots, m$. Hence in equation (23) it follows that $\|r_m^{(j)}\| \approx \|\beta\|$, thus $\|r_m^{(j)}\| \approx \|r_m^{(j-1)}\|$. ∎

Proposition 4. *If GMRES(m) presents complete stagnation, then a decrease in the residual norm at the next restart cycle is obtained by increasing the restart parameter m, if the entry $h_{1,m+1}$ of the Hessenberg matrix associated to the Arnoldi decomposition in the GMRES process is nonzero.*

Proof. According to lemma 2.5 of Tebbens and Meurant[27] and theorem 3.1 of Strikwerda and Stodder,[28] the GMRES(m) presents complete stagnation when the first row of the Hessenberg matrix has zero components.

Because the vector $y^{(j)}$ minimizes $J(y^{(j)})$ and the Hessenberg matrix without the first row is upper triangular with linearly independent rows, the residual norm at jth cycle is $\|r_m^{(j)}\| = \|r_m^{(j-1)}\|$ because the vector $y^{(j)} = 0$ (see Proposition 1).

Considering any decrease in m at the jth cycle, there is no improvement in the rate of convergence because the vector $y^{(j)}$ remains a zero vector. Thus, the only alternative to achieve a decrease in the residual norm is by increasing the parameter m. Assuming an increase of one unit in m and $h_{1,m+1} \neq 0$, the expression for $J(\hat{y}^{(j)})$ becomes

$$J(\hat{y}^{j}) = \left\| \begin{bmatrix} \beta \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & \dots & h_{1,m+1} \\ h_{2,1} & h_{2,2} & \dots & h_{2,m+1} \\ 0 & h_{3,2} & \dots & h_{3,m+1} \\ \vdots & \ddots & \vdots & \\ 0 & \dots & h_{m+1,m} & h_{m+1,m+1} \\ 0 & \dots & 0 & h_{m+2,m+1} \end{bmatrix} \begin{bmatrix} \hat{y}^{(j)}(1) \\ \hat{y}^{(j)}(2) \\ \vdots \\ \hat{y}^{(j)}(m+1) \end{bmatrix} \right\|,$$

consequently, $\|r_m^{(j)}\| < \|r_m^{(j-1)}\|$. Further increments of the restart parameter m produce similar results. ■

Reasoning similar to that used in Proposition 4 applies to the case of convergence slowdown. Hence, since convergence slowdown can be characterized using the Hessenberg matrix of the corresponding GMRES Arnoldi process by having the entries $h_{1,k} \approx \epsilon$ with $k = 1, \dots, m$, it follows that a decrease in the residual norm at the next restart cycle is obtained if at least $h_{1,m+1} > \epsilon$.

3.2 | Including error approximations in the search subspace

The inclusion of the relative error between the approximate solution at subsequent cycles of restarted GMRES is used in several algorithms for improving convergence. For instance, the algorithm denominated LGMRES introduced in Reference 6 and GMRES-E method introduced in Reference 9, based on appending vectors to the standard Krylov space, are used as acceleration techniques and to avoid alternating behavior.[6,25] The error of consecutive cycles solution approximation of GMRES(m) is defined as:

$$\psi^{(j-1)} := x_m^{(j-1)} - x_m^{(j-2)}. \tag{24}$$

This error approximation vector is used to augment the next approximation space $\mathcal{K}_m(A, r_m^{(j-1)})$. Note that $\psi^{(j-1)} \in \mathcal{K}_m(A, r_m^{(j-2)})$. Therefore, this error approximation $\psi^{(j-1)}$ in some sense represents the space $\mathcal{K}_m(A, r_m^{(j-2)})$ generated in the previous cycle and subsequently discarded when the restart is performed.[6] The LGMRES(m, l) augments the standard Krylov approximation space with l previous approximations to the error. Therefore, at the end of jth restart cycle, the LGMRES(m, l) obtains an approximate solution to (1) as follows:

$$x_m^{(j)} = x_m^{(j-1)} + q_{m-1}(A)\tilde{r}_s^{(j-1)} + \sum_{k=(j-l)}^{j-1} \alpha_{jk}(A)\psi^{(k)} \tag{25}$$

where the polynomial $q_{m-1}(A)$ and coefficients $\alpha_{jk}(A)$ are chosen such that the residual norm is minimized. Note that $l = 0$ corresponds to standard GMRES(m).[6] The residual vector using the LGMRES(m, l) approaches is denoted as $\tilde{r}_s^{(j)}$, where the residual norm is

$$\|\tilde{r}_s^{(j)}\| = \min_{\tilde{p}_m \in \tilde{\pi}_j} \|\tilde{p}_m(A)\tilde{r}_s^{(j-1)}\| \tag{26}$$

where $\tilde{\pi}_j$ is the set of polynomials $p_m(A) + \sum_{k=(j-l)}^{j-1} \alpha_{jk}(A)A\psi^{(k)}$, $\tilde{p}_m(A)$ is a polynomial of degree m with the value one at the origin. The augmented approximation space $S = \mathcal{K}_m(A, \tilde{r}_s^{(j-1)}) \cup span\{\psi^{(k)}\}, k = j - l : j - 1$, has dimension $s = m + l$. The sequence of residual norms generated by LGMRES(m, l) is nonincreasing similar to other methods that satisfy the minimum residual condition (there are exceptions[10]), that is, $\|\tilde{r}_s^{(j)}\| \leq \|\tilde{r}_s^{(j-1)}\|$.

Observing that if GMRES(m) presents a stagnation, this implies $\psi^{(k)} = x_m^{(k)} - x_m^{(k-1)} = 0$ for all $k = j - l : j - 1$. Thus, one obtains $h_{1,i} = (v_1^{(j)}, A\psi^{(k)}) = 0, \forall i = m + 1 : m + l$; therefore, $\|\tilde{r}_s^{(j)}\| = \|\tilde{r}_s^{(j-1)}\|$. This observation implies that the LGMRES is not adequate for helping to overcome stagnation but rather for accelerating convergence. This feature motivates its inclusion in the switching proposal.

3.3 | Deflation by the inclusion of the approximate eigenvectors

In a deflation strategy, the general goal consists of the elimination of components that supposedly slow down convergence.[9,31] A natural strategy in GMRES(m) consists of enlarging the Krylov subspace to produce an automatic deflation. Although this strategy is normally used, this strategy is not convenient with regard to memory and computational requirements, especially when the subspace is enlarged without any control, since a priori the increase in subspace size is not known since it is not known. Methods for adaptively enlarging the space in a controlled manner are discussed in References 5,20 and references therein. Another strategy consists of enriching the subspace by introducing eigenvectors associated to the problematic eigenvalues. In practice, this requires is working with approximate eigenvalues (harmonic Ritz values) and the corresponding approximate eigenvectors per cycle.[9,12,25,26]

Definition 5. If $\mathcal{V}_m$ is a linear subspace of $\mathbb{C}^n$ then ϑ is a Ritz value of A with respect to $\mathcal{V}_m$ with Ritz vector μ if

$$\mu \in \mathcal{V}_m, \quad \mu \neq 0, \quad A\mu - \vartheta\mu \perp \mathcal{V}_m. \tag{27}$$

The Ritz pair (ϑ, μ) approximates an eigenpair (λ, v) of the matrix A depending on the angle between v and $\mathcal{V}_m$.[32]

For GMRES, it is more convenient to use harmonic Ritz values that correspond to the inverse of the Ritz approximations for A^{-1}[33,34] and they are defined as follows:

Definition 6 (32,34). A value $\tilde{\vartheta} \in \mathbb{C}$ is a harmonic Ritz value of A with respect to some linear subspace $\mathcal{W}_m := A\mathcal{V}_m$ if $\tilde{\vartheta}^{-1}$ is a Ritz value of A^{-1} with respect to $\mathcal{W}_m$.

Following Reference 34, expression $(\tilde{\vartheta}^{-1}, A\varphi)$ is a Ritz pair of A^{-1} with respect to $\mathcal{W}_m$. In the context of Krylov subspace methods with restarts, $\mathcal{V}_m$ is the Krylov subspace $\mathcal{K}_m(A, r_m^{(j-1)})$, hence an approximate eigenvector $\varphi = V_m^{(j)} g_m$ is sought in $\mathcal{K}_m(A, r_m^{(j-1)})$. Since the minimal residual criterion requires that the residual of eigenvalue equation be orthogonal to $A\mathcal{K}_m(A, r_m^{(j-1)})$ hence one obtains

$$\varphi \in \mathcal{V}_m, \quad \varphi \neq 0, \quad A\varphi - \tilde{\vartheta}\varphi \perp A\mathcal{V}_m. \tag{28}$$

Using the Arnoldi relation (3) one obtains a generalized eigenvalue problem

$$\tilde{H}_m^{(j)*} \tilde{H}_m^{(j)} g_m = \tilde{\vartheta} H_m^{(j)*} g_m. \tag{29}$$

The vector φ is denoted as the harmonic Ritz vector associated with the harmonic Ritz value $\tilde{\vartheta}$ and $(\tilde{\vartheta}, \varphi)$ is a harmonic Ritz pair. If $H_m^{(j)}$ is singular, the harmonic Ritz value becomes ∞ and the GMRES(m) residual curve stagnates, thus $r_m^{(j)} = r_m^{(j-1)}$.[33,35]

In this article, we use the GMRES-E(m, d) to denote the restarted GMRES method augmented with approximate eigenvectors corresponding to the d smallest harmonic Ritz values in magnitude. Following the strategy of enrichment of the Krylov subspace, the GMRES-E(m, d) which appends approximate eigenvectors to the Krylov subspace corresponding to a few of the smallest eigenvalues in magnitude is proposed in Reference 9. The correction vector is found in a $(m + d)$ dimensional subspace constituted by the m dimensional standard Krylov subspace and d approximate eigenvectors. At each jth restart cycle, the GMRES-E(m, d) seeks approximate solution $x_m^{(j)}$ of the form

$$x_m^{(j)} = x_m^{(j-1)} + q_{m-1}(A)\hat{r}_s^{(j-1)} + \sum_{k=1}^{d} \beta_{jk}(A)\varphi_k^{(j-1)}, \tag{30}$$

where $\varphi_k^{(j-1)}$, $k = 1 : d$, is a group of vectors constituted by d harmonic Ritz vectors associated with d smallest (in magnitude) harmonic Ritz values calculated in the $(j-1)$th cycle. In a manner analogous to that of LGMRES(m, l), the residual vector using the GMRES-E(m, d) approach is denoted as $\hat{r}_s^{(j)}$ and the residual norm is

$$\|\hat{r}_s^{(j)}\| = \min_{\hat{p}_m \in \hat{\pi}_j} \|\hat{p}_m(A)\hat{r}_s^{(j-1)}\|, \tag{31}$$

where $\hat{\pi}_j$ is the set of polynomial $p_m(A) + \sum_{k=1}^{d} \beta_{jk}(A)A\varphi_k^{(j-1)}$, $\hat{p}_m(A)$ is a polynomial of degree m with the value one at the origin. The augmented approximation space $S = \mathcal{K}_m(A, \hat{r}_s^{(j-1)}) \cup span\{\varphi_k^{(j-1)}\}$, $k = 1 : d$, has dimension $s = m + d$. The harmonic Ritz vectors help only for that cycle and may need to be recalculated in the next cycle.[9,10] The sequence of the residual norm of the GMRES-E(m, d) has the property of being nonincreasing, that is, $\|\hat{r}_s^{(j)}\| \leq \|\hat{r}_s^{(j-1)}\|$. The GMRES-E is not really needed for easy problems where few restarts are used[9] and the LGMRES proposal is less computationally expensive and can accelerate the convergence.

3.4 | The convergence of switching control

The proposed strategy has two parts: the first part is the detection of stagnation and the appropriate enrichment (or augmentation) of the subspace using a switching controller that changes the structure when the stagnation is detected. An acceleration technique is used in order to speed up the convergence. This latter is important in order to keep the overall cost of the algorithm competitive, since the enrichment of the subspace has an additional cost. In the second part, a strategy for adjusting the restart parameter is implemented when stagnation is detected and enrichment does not guarantee the recovery of the convergence. In this case, the size of the search subspace is increased via the increment of the value of m and preserving the selected enrichment. In case that the rate of convergence is recovered, then the value of m can be decreased subsequently.

Switching control of LGMRES-E(m, l, d). This method is denoted by SLGMRES-E (m, l, d) (or in short SLGMRES-E), where the parameters m, l, and d remain constant at every cycle. The switch controller at the end of jth cycle seeks the approximate solution $x_m^{(j)}$ of the form

$$x_m^{(j)} = x_m^{(j-1)} + u^{(j)}, \tag{32}$$

where $u^{(j)} \in \mathcal{K}_m^{(j)}(A, r_s^{(j-1)}) \cup \mathcal{U}$. The Krylov subspace $\mathcal{K}_m^{(j)}(A, r_s^{(j-1)})$ is augmented by using a subspace $\mathcal{U}$ built in such way as maintain the residual norm minimized. In this section, we analyze the switching of the subspace $\mathcal{U}$ between two possibilities: first, considering $\mathcal{U} = \mathcal{U}_l$ being an appropriate linear combination of l error approximations. Then the approximate solution takes the form of expression (25). In practice, the LGMRES method can be used (see Section 3.2). Second, supposing that $\mathcal{U} = \mathcal{U}_d$ is the appropriate linear combination of the d harmonic Ritz vectors associated with the corresponding d smallest harmonic Ritz values in magnitude. In practice the GMRES-E can be used (see Section 3.3).

Observing the behavior of LGMRES(m) clearly when a convergence slowdown happens, it is necessary to switch in order to enrich the subspace. Unfortunately, there is no clear identification of when to switch. To overcome this problem, observe that from the expression (7), the residual is concentrated at $|q_{m+1,1}|$ by $\|r_m^{(j)}\| = \beta |q_{m+1,1}|$ where $\beta = \|r_m^{(j-1)}\|$, thus by Definition 1 one obtains the following relation for the residual norm between two cycles,

$$\frac{\|r_m^{(j)}\|}{\|r_m^{(j-1)}\|} = |q_{m+1,1}| = (1 - \epsilon), \tag{33}$$

which characterizes the relation between the residuals at consecutive cycles in terms of ϵ and $|q_{1,m+1}|$. Hence, as a practical rule, augmentation of the Krylov subspace can be carried out by using the (switching) rule:

$$\mathcal{U} = \begin{cases} \mathcal{U}_l = \displaystyle\sum_{k=j-l}^{j-1} \alpha_{jk} \psi^{(k)} & \forall \epsilon > \epsilon_0, \\ \mathcal{U}_d = \displaystyle\sum_{k=1}^{d} \beta_{jk} \varphi_k^{(j-1)} & \forall \epsilon \leq \epsilon_0, \end{cases}$$

where ϵ_0 is defined as the stagnation threshold parameter, slow convergence being considered to occur when $\epsilon \leq \epsilon_0$. If the strategy of augmenting the subspace with approximations of the errors does not achieve a good rate of convergence, then an enrichment of the subspace using harmonic Ritz vectors is carried out by applying the GMRES-E method.

To analyze the convergence using the switching rule, the switching residual at jth cycle is defined as

$$r_s^{(j)} := \sigma \tilde{r}_s^{(j)} + (1 - \sigma) \hat{r}_s^{(j)}, \tag{34}$$

where $\tilde{r}_s^{(j)}$ is the residual of LGMRES and $\hat{r}_s^{(j)}$ is the residual of GMRES-E. In addition, the parameter σ has two values in accordance with the following rule:

$$\sigma = \begin{cases} 1 & \forall \epsilon > \epsilon_0 \\ 0 & \forall \epsilon \leq \epsilon_0. \end{cases} \tag{35}$$

Hence given a candidate Lyapunov function defined by $V(r_s^{(j)}) := \langle r_s^{(j)}, r_s^{(j)} \rangle$, the increment $\Delta V(r_m^{(j)})$ is negative definite for all positive $0 < \epsilon_0, \epsilon < 1$. The next result ensures the local convergence of the SLGMRES-E.

Theorem 2. *Given a candidate Lyapunov function $V(r_s^{(j)}) := \langle r_s^{(j)}, r_s^{(j)} \rangle$ where $r_s^{(j)}$ is defined by the expression (34). Let the parameter σ be defined as in rule (35). Then for all positive $0 < \epsilon_0, \epsilon < 1$, the increment $\Delta V(r_m^{(j)})$ is negative definite.*

Proof. Considering the definition of $V(r_s^{(j)})$ and $r_s^{(j)}$ given by the expression (34):

$$V(r_s^{(j)}) = \langle r_s^{(j)}, r_s^{(j)} \rangle = \sigma^2 \langle \tilde{r}_s^{(j)}, \tilde{r}_s^{(j)} \rangle + 2\sigma(1-\sigma)\langle \tilde{r}_s^{(j)}, \hat{r}_s^{(j)} \rangle + (1-\sigma)^2 \langle \hat{r}_s^{(j)}, \hat{r}_s^{(j)} \rangle.$$

Considering the local increment given by (similar to Definition 3):

$$\Delta V(r_s^{(j)}) = \Delta V(r_s^{(j)}) - \Delta V(r_s^{(j-1)})$$

and dividing by $\beta^2 := \langle r_s^{(j-1)}, r_s^{(j-1)} \rangle$,:

$$\frac{\Delta V(r_s^{(j)})}{\beta^2} = \sigma^2 \frac{\langle \tilde{r}_s^{(j)}, \tilde{r}_s^{(j)} \rangle}{\beta^2} + 2\sigma(1-\sigma)\frac{\langle \tilde{r}_s^{(j)}, \hat{r}_s^{(j)} \rangle}{\beta^2} + (1-\sigma)^2 \frac{\langle \hat{r}_s^{(j)}, \hat{r}_s^{(j)} \rangle}{\beta^2} - 1. \tag{36}$$

From Sections 3.2 and 3.3, then there exists ϵ_1 and ϵ_2 such that $\|\tilde{r}_s^{(j)}\| = (1-\epsilon_1)\beta$ and $\|\hat{r}_s^{(j)}\| = (1-\epsilon_2)\beta$ for all positive $\epsilon_1, \epsilon_2 < 1$. By simplicity it is considered that $\epsilon_1 = \epsilon_2 = \epsilon$. Thus, (36) can be written as:

$$\frac{\Delta V(r_s^{(j)})}{\beta^2} = (2\sigma^2 - 2\sigma + 1)(1-\epsilon)^2 + 2\sigma(1-\sigma)\frac{\langle \tilde{r}_s^{(j)}, \hat{r}_s^{(j)} \rangle}{\beta^2} - 1. \tag{37}$$

Considering the rule (35), the expression (37) takes the form:

$$\frac{\Delta V(r_s^{(j)})}{\beta^2} = -\epsilon(2-\epsilon), \tag{38}$$

which is negative for all $0 < \epsilon < 1$ with respect to $0 < \epsilon_0 < 1$. ■

Theorem 2 shows that $\|r_s^{(j)}\| < \|r_s^{(j-1)}\|$ for both cases $\epsilon > \epsilon_0$ and $\epsilon < \epsilon_0$ for $0 < \epsilon_0, \epsilon < 1$. Hence, for $\epsilon \neq 0$, it is possible to decrease the residual at consecutive cycles. Theorem 2 is only a sufficient condition for ensuring the convergence. If $\epsilon = 1$ the convergence of the SLGMRES-E is achieved. However, if $\epsilon = 0$ the method stagnates completely. A necessary condition for $\epsilon = 0$ is presented in the next theorem.

Theorem 3. *Giving the switching residual $r_s^{(j)}$ and $\epsilon = 0$. If $h_{1,k} = v_1^* A \varphi_{k-m}^{(j-1)} \neq 0, \forall k > m$, then $\|r_s^{(j)}\| < \|r_s^{(j-1)}\|$.*

Proof. Consider now $\epsilon = 0$. In this case, the proposed method SLGMRES-E presents complete stagnation. Assuming stagnation in the first m iterations of the jth cycle, then in the next iteration using the harmonic Ritz vector one obtains

$$\tilde{H}_{s+1}^{(j)}(1,:) = [0 \quad 0 \ldots 0 \quad v_1^* A \varphi_1^{(j-1)}].$$

Observe that if $v_1^* A \varphi_1^{(j-1)} = 0$ then $H_m^{(j)*}$ is singular; and consequently, following Reference 36 one obtains that the generalized eigenvalue problem $\tilde{H}_m^{(j)*}\tilde{H}_m^{(j)} g_m = \tilde{\vartheta} H_m^{(j)*} g_m$ has an eigenvalue $\tilde{\vartheta} = \infty$. Following Reference 33, this implies that

$\|r_s^{(j)}\| = \|r_s^{(j-1)}\|$. A similar analysis can be performed for other harmonic Ritz vectors in the same jth cycle, therefore if $h_{1,k} = v_1^* A\varphi_{k-m}^{(j-1)} = 0$ with $k = m+1 : m+d$, the residual has completely stagnated. ■

Theorem 3 means that if a vector $\varphi_1^{(j-1)}$ is added to $\mathcal{K}_m(A, r_s^{(j-1)})$ with $(r_s^{(j-1)}, A\varphi_1^{(j-1)}) = 0$, then SLGMRES-E does not have any progress. A possible strategy to overcome this problem consists in modifying the restart parameter based on Proposition 4.

Switching control LGMRES-E(m, l, d) using adjustment of the restart parameter. An update law is used when slow convergence is observed, that is, $\epsilon < \epsilon_0$. In this case, the control update law for the restart parameter is used. We denote this method by Adaptive-Switched LGMRES-E(m_j, l, d) or in short A-SLGMRES-E. The dimension of the search space is $s = m_j + l + d$ with fixed l and d values. Several authors have proposed varying the restart parameter of the GMRES(m) (see References 3,5,8,12,20). Following Reference 20, in this article we use the discrete proportional-derivative controller (denoted PD) with different parameters but the same form:

$$m_j = m_{j-1} + \left\lfloor \alpha_P \frac{\|r_s^{(j)}\|}{\|r_s^{(j-1)}\|} + \alpha_D \frac{\|r_s^{(j)}\| - \|r_s^{(j-2)}\|}{2\|r_s^{(j-1)}\|} \right\rfloor. \tag{39}$$

where $\alpha_P, \alpha_D \in \mathbb{R}$ and $\lfloor(.)\rfloor$ denotes the integer part. The effect of the proportional $\alpha_P(\cdot)$ and derivative $\alpha_D(\cdot)$ parts can be summarized qualitatively as follows:

- If A-SLGMRES-E presents poor convergence with respect to the previous cycle, that is, $\angle(r_s^{(j)}, r_s^{(j-1)}) \approx 0$; then $\|r_s^{(j)}\|/\|r_s^{(j-1)}\| \approx 1$ and with $\alpha_P > 0$, the value of m_j is increased because $(\|r_s^{(j)}\| - \|r_s^{(j-2)}\|)/2\|r_s^{(j-1)}\| \approx 0$.
- If A-SLGMRES-E presents an appropriate good convergence with respect to the previous cycle, that is, $\angle(r_s^{(j-1)}, r_s^{(j-2)}) > 0$; then $(\|r_s^{(j)}\| - \|r_s^{(j-2)}\|)/2\|r_s^{(j-1)}\| < 0$. The derivative part is always less or equal to zero, since the residual norm cannot increase in the next cycle, so the derivative part only can remain constant or decrease the value of m_j.

The proposed strategy to adjust the restart parameter is inspired by the rules introduced in References 5,20 but we seek to increase the restart parameter using an appropriate selection of the PD rule parameters in order to avoid slowdown of convergence. This is based on the observation of Proposition 4 that maintaining the restart parameter as a constant does not help in improving the convergence when stagnation occurs. Thus, we choose the parameters α_P and α_D in order to increase the value of m_j.

To maintain the values of m between certain maximum and minimum values, an upper and lower bound μ are defined as the maximal increment and decrement of the restart parameter in the next cycle, which is achieved by imposing:

$$-\mu \leq \left\lfloor \alpha_P \frac{\|r_s^{(j)}\|}{\|r_s^{(j-1)}\|} + \alpha_D \frac{\|r_s^{(j)}\| - \|r_s^{(j-2)}\|}{2\|r_s^{(j-1)}\|} \right\rfloor \leq \mu. \tag{40}$$

The proposed PD rule is used when $\|r_s^{(j)}\|/\|r_s^{(j-1)}\| \geq 1 - \epsilon_0$ and $\|r_s^{(j-1)}\|/\|r_s^{(j-2)}\| \geq 0.1$. If the previous condition is not met, it is not necessary to modify the restart parameter. Considering the stagnation threshold parameter chosen in Section4.1, $\epsilon_0 = 0.01$, two extreme cases are considered for the selection of α_P and α_D. The first one, when the GMRES(m) presents slowdown of convergence in the jth, $(j-1)$th, and $(j-2)$th cycles. In this case, using $\|r_s^{(j)}\|/\|r_s^{(j-1)}\| \geq 0.99$ and $\|r_s^{(j-1)}\|/\|r_s^{(j-2)}\| \geq 0.99$, the relation (40) for the case of the upper limit becomes:

$$0.99\alpha_P - 0.01\alpha_D \leq \mu.$$

The second case considers a poor rate of convergence in the jth cycle (condition to use the PD rule) and good convergence in the $(j-1)$th cycle. In this case, using $\|r_s^{(j)}\|/\|r_s^{(j-1)}\| \geq 0.99$ and $\|r_s^{(j-1)}\|/\|r_s^{(j-2)}\| \geq 0.1$, the relation (40) for the case of the lower limit becomes:

$$0.99\alpha_P - 4.505\alpha_D \geq -\mu.$$

Next, considering the extreme cases of convergence above, in order to obtain the appropriate values of α_P and α_D, it is necessary to satisfy the following linear system of inequalities,

$$\begin{bmatrix} 0.99 & -0.01 \\ -0.99 & 4.51 \end{bmatrix} \begin{bmatrix} \alpha_P \\ \alpha_D \end{bmatrix} \leq \begin{bmatrix} \mu \\ \mu \end{bmatrix}. \tag{41}$$

It is observed through numerical experiments in Section 4.3 (see Table 4), that the choice $\mu = 2$ present a better performance for A-SLGMRES-E and PD-GMRES methods in the problems where the GMRES(m) does not converge. The proportional and derivative constants that satisfy the expression (40) with $\mu = 2$ are $\alpha_P = 2$ and $\alpha_D = 0.8$. These values are used for the numerical experiments in the following section. The pseudo-code of the Adaptive SLGMRES-E(m_j, d, l) is presented in Algorithm 1.

Algorithm 1. The jth cycle of Adaptive SLGMRES-E(m, d, l)

Require: Given $r_s^{(j-1)}$, $\beta = \| r_s^{(j-1)} \|$, $v_1 = r_s^{(j-1)}/\beta$, m_j, *flag-stagnation*.
Ensure: $r_s^{(j)}$, m_{j+1}, *flag-stagnation*.
  if flag-stagnation = 0 **then**
    $s = m_j + l$
    Generate Arnoldi basis and matrix $\tilde{H}_s$, using error approximation vectors $\psi^{(k)}$, $k = j - l, \dots, j - 1$.
  else
    $s = m_j + d$
    Generate Arnoldi basis and matrix $\tilde{H}_s$, using harmonic Ritz vectors $\varphi_k^{(j)}$, $k = 1, \dots, d$.
  end if
  Find $y^{(j)} = argmin_{y \in \mathbb{C}^s} \| \beta e_1 - \tilde{H}_s^{(j)} y \|$, compute $x_s^{(j)}$ and $r_s^{(j)}$;
  if $\| r_s^{(j)} \| < tolerance$ **then**
    stop;
  end if
  if have stagnation **then**
    flag-stagnation = 1;
    Compute the harmonic Ritz vectors, $\varphi_k^{(j)}$, $k = 1, \dots, d$;
    Compute m_{j+1} from PD rule;
  else
    flag-stagnation = 0;
    Compute the error approximation vectors, $\psi^{(j)}$;
  end if
  $j = j + 1$

4 | NUMERICAL EXPERIMENTS

This section reports on numerical results based on matrices from the Matrix Market Collection.[37] The problems involve matrices that are nonsymmetric with a high condition number. The matrices considered are listed in Table 1, where n is the size of A, nnz is the number of nonzero elements and *Cond* is the condition number. For problems in which the right-hand side are not specified, the vector b is generated randomly using a uniform distribution with values between the minimum and maximum values $A(i, j)$.

Two kinds of problems are considered with respect to the convergence of the GMRES(m): *problem group 1* corresponding to problems where the GMRES(m) converge before the preestablished maximum number of cycles, and *problem group 2* corresponding to problems with a slowdown of convergence, that do not converge before the preestablished maximum number of cycles. In the context of this set of experiments, the latter group is denoted as hard problems, corresponding to the last six problems in Table 1.

In Section 4.1, the threshold parameter that allows the best performance is experimentally obtained. In Section 4.2, the proposed method SLGMRES-E(m, l, d) is compared with other methods using enriched subspace. These methods are: LGMRES(m, l),[6] GMRES-E(m, d),[9] and LGMRES-E($m, l, d,$).[25] All these methods employ fixed restart and enrichment

TABLE 1 Matrices information used in this section extracted from the Matrix Market Collection[37]

Id	Problem	n	nnz	Cond	Application area
1	Add20	2395	13 151	1.20e+04	Circuit simulation problem
2	Circuit_2	4510	21 199	1.32e+05	Circuit simulation problem
3	Raefsky1	3242	293 409	1.29e+04	Computational fluid dynamics problem sequence
4	Raefsky2	3242	293 551	4.25e+03	Subsequent computational fluid dynamics problem
5	Fpga_trans_01	1220	7382	1.22e+04	Circuit simulation problem sequence
6	Sherman1	1000	3750	1.60e+04	Computational fluid dynamics problem
7	Sherman4	1104	3786	2.18e+03	Computational fluid dynamics problem
8	Orsreg_1	2205	14 133	6.75e+03	Computational fluid dynamics problem
9	Cdde1	961	4681	2.41e+03	Computational fluid dynamics problem sequence
10	Orsirr_1	1030	6858	7.71e+04	Computational fluid dynamics problem
11	Pde2961	2961	14 585	6.42e+02	2D/3D Problem
12	Rdb2048	2048	12 032	7.31e+02	Computational fluid dynamics problem
13	Steam2	600	5660	3.78e+06	Computational fluid dynamics problem
14	Wang2	2903	19 093	2.31e+04	Subsequent semiconductor device problem
15	Watt_1	1856	11 360	4.36e+09	Computational fluid dynamics problem
16	Memplus	17 758	99 147	1.29e+05	Circuit simulation problem
17	Cavity05	1182	32 632	5.77e+05	Computational fluid dynamics problem sequence
18	Sherman5	3312	20 793	1.88e+05	Computational fluid dynamics
19	Sherman3	5005	920 033	5.01e+17	Computational fluid dynamics
20	Cavity10	2597	76 171	2.96e+06	Computational fluid dynamics
21	Young3c	841	3988	9.30e+03	Acoustics problem
22	Ex40	7740	456 188	2.75e+06	Computational fluid dynamics
23	Wang4	26 068	177 196	4.03e+04	Semiconductor device problem

parameters. In Section 4.3, an approach of automatically adjusting the subspace value m is examined. The proposed method is called Adaptive SLGMRES-E(m, l, d). The adaptive strategy allows achieving convergence for problems where the methods used in Section 4.2 did not. The methods used for all the tests were carried out without preconditioning and the initial configurations for the algorithms are: the initial solution is $x^{(0)} = 0$, the stopping criterion is $\|r_m^{(j)}\|/\|r^{(0)}\| \leq 10^{-9}$ and the maximum number of cycles is 1000. The harmonic Ritz vectors are computed using an initial vector of ones instead of using a random vector (as it is the default of the *eigs* Matlab function). This is done in order to maintain at a constant the number of restarts for converging when a problem is run several times in order to obtain its statistics. All the experiments were run on a computer Intel Celeron 1.60 GHz×2, using the software MatLab 9.1.0 (R2016b) for Ubuntu 18.04.1 LTS.

In this section, the stagnation threshold parameter ϵ_0 is tested between 0 and 0.1. The results are shown in Table 2, where the Cycles row number indicates the total restart cycles required to achieve the solution with a prespecified tolerance, while the Time row indicates the rounded average time (in seconds) of five runs corresponding to each stagnation threshold. The value of ϵ is computed using the expression (33) and cycles of Problems that have some cycle with $\epsilon \leq \epsilon_0$ are indicated with an underline. The time corresponding to the best performance is indicated by boldface. If the method does not converge after 1000 cycles, this is denoted by NC. The problems Ex40 and Wang4 do not achieve convergence for any of the stagnation thresholds tested when the method maintains constant the restart parameter, so they were omitted in Table 2.

It can be observed that for the *problem group 1* the choice of the threshold stagnation parameter, in general, does not affect the performance of the proposed switching method. This is due to the fact that in general, the computed ϵ is larger than the prescribed ϵ_0. Observe that for a larger ϵ_0 the condition for commutation in the switching rule allows

TABLE 2 Impact of the stagnation threshold parameter

		Stagnation threshold parameter ϵ_0						
Problem		**0**	**1e-06**	**1e-03**	**1e-02**	**5e-02**	**3e-02**	**0.1**
1	Cycles	18	18	18	18	18	18	18
	Time	0.71	0.70	0.66	***0.65***	0.66	0.66	0.66
2	Cycles	21	21	21	21	21	21	21
	Time	1.48	1.38	1.26	1.39	1.34	1.36	***1.24***
3	Cycles	30	30	30	30	30	30	30
	Time	***2.93***	2.95	2.94	2.98	3.13	2.94	2.95
4	Cycles	97	97	97	97	97	97	<u>81</u>
	Time	9.40	9.38	9.60	9.38	9.45	9.56	***9.34***
5	Cycles	33	33	33	33	33	33	33
	Time	0.56	0.55	0.55	0.55	0.54	***0.53***	0.57
6	Cycles	27	27	27	27	27	27	27
	Time	0.44	0.41	0.41	***0.40***	0.45	0.43	0.41
7	Cycles	16	16	16	16	16	16	16
	Time	0.30	0.25	***0.23***	0.24	0.24	0.24	0.24
8	Cycles	18	18	18	18	18	18	18
	Time	0.43	0.42	0.43	0.44	0.44	***0.41***	0.43
9	Cycles	22	22	22	22	22	22	22
	Time	0.35	0.32	***0.31***	0.32	0.32	0.32	0.32
10	Cycles	70	70	70	70	70	70	70
	Time	1.10	1.09	***1.08***	1.11	1.11	1.14	1.35
11	Cycles	18	18	18	18	18	18	18
	Time	0.70	0.65	0.65	0.65	***0.63***	***0.63***	0.65
12	Cycles	17	17	17	17	17	17	17
	Time	0.40	***0.35***	0.36	0.36	0.36	0.36	0.37
13	Cycles	23	23	23	23	23	23	23
	Time	0.30	***0.29***	***0.29***	0.30	***0.29***	0.31	0.31
14	Cycles	27	27	27	27	27	27	27
	Time	1.06	0.99	1.00	0.99	1.00	***0.98***	1.00
15	Cycles	29	29	29	29	29	29	29
	Time	0.63	0.63	***0.61***	0.62	***0.61***	***0.61***	***0.61***
16	Cycles	51	51	51	51	51	51	51
	Time	10.89	10.94	***10.88***	10.90	10.93	10.61	10.64
17	Cycles	76	76	76	76	<u>79</u>	<u>82</u>	<u>70</u>
	Time	***2.35***	2.63	2.70	2.49	3.61	2.62	2.92
18	Cycles	<u>NC</u>	<u>NC</u>	<u>NC</u>	<u>343</u>	<u>272</u>	<u>369</u>	<u>478</u>
	Time	NC	NC	NC	20.99	***16.50***	24.61	35.22
19	Cycles	271	271	271	271	<u>NC</u>	<u>NC</u>	<u>NC</u>
	Time	19.65	***19.25***	19.45	20.39	NC	NC	NC

(Continues)

TABLE 2 (Continued)

Problem		Stagnation threshold parameter ϵ_0						
		0	1e-06	1e-03	1e-02	5e-02	3e-02	0.1
20	Cycles	103	103	103	131	122	131	131
	Time	***5.83***	6.04	6.35	9.88	8.79	9.38	9.16
21	Cycles	387	387	387	319	371	277	328
	Time	5.63	5.63	5.59	***5.29***	9.03	6.83	8.95

Note: The Cycles row indicate the total restart cycles required to achieve the solution for a given specified tolerance. The Time row indicates an average time in seconds of five runs corresponding to each stagnation threshold. Best performance is indicated by boldface and cycles of Problems that have some cycle with $\epsilon \leq \epsilon_0$ are indicated with an underline. The SLGMRES-E switches between the LGMRES and GMRES-E.
Abbreviation: GMRES, generalized minimal residual.

more commutations between LGMRES and GMRES-E. This implies more computations since larger values imply more computation of the harmonic Ritz vectors and consequently, larger computational time. Hence, this fact establishes a trade-off in the choice of ϵ_0. In the following sections, we use the value $\epsilon_0 = 0.01$ for the threshold stagnation parameter since it allows convergence for all problems in Table 2. This means that the harmonic Ritz vectors are only computed when the norm of the residual is smaller than 1% with respect to the residual norm of the preceding cycle.

4.1 | Comparison of methods with fixed restart parameter

In this section, we use the proposed method SLGMRES-E(m, l, d) but maintain the restart parameter m as a constant. The following values are considered for each method: GMRES(m), $m = 30$, LGMRES(m, l), $m = 28$, $l = 2$; GMRES-E(m, d), $m = 28$, $d = 2$; LGMRES-E(m, l, d), $m = 27$, $d = 2$, $l = 1$; SLGMRES-E(m, l, d), $m = 28$, $d = 2$, $l = 2$. The results of running time in seconds and cycles necessary for convergence are shown in Table 3. The best values of running time obtained for every problem are indicated in boldface. The nonconverging problems are denoted by *NC*. It can be observed that problems Ex40 and Wang4 does not converge for any of the methods employed using a fixed restart parameter m.

Problem 18 (Sherman5) corresponds to an oil reservoir simulation problem where the matrix is real nonsymmetric with relatively small eigenvalues in magnitude with positive and negative real parts. In accordance to Reference 38, Problem 18 is difficult without preconditioning. The eight eigenvalues nearest to the origin are 0.047, 0.13, 0.40, 0.58, 0.62, 0.85, 0.91, and 1.0. The largest positive and negative eigenvalues are 595 and −189. An interesting observation is that GMRES-E(18,2) stagnates and makes little progress after 1000 restart cycles, while GMRES-E(28,2) performs better. Here it can be observed that with a slightly larger Krylov subspace, the method performs better. However, this is not known a priori.

Figure 2A shows the residual convergence behavior of the tested methods. The parameters employed correspond to the ones used in Table 3. In Figure 2A it can be observed that all tested methods do not converge to the prespecified tolerance in 450 cycles, with the exceptions of the GMRES-E and SLGMRES-E. The latter achieves the lowest computational time.

Problem 19 (Sherman3) is a difficult real problem involving a nonsymmetric matrix with a high condition number (see Table 1). It is observed that GMRES-E stagnates with the selected parameters (see Table 3). Figure 2B shows residual convergence behavior curves using the methods and parameters of Table 3. The converging methods maintain a rate of convergence almost linearly up to the prespecified tolerance. It can be observed that the method SLGMRES-E(28,2,2) is a standard LGMRES(28,2) because the threshold stagnation defined is not overcome (see Table 2).

Problems 17 and 20 are known as Cavity05 and Cavity10, respectively. They involve a real nonsymmetric matrix with a small eigenvalue in magnitude, arising from finite element modeling. Figure 3A,B shows the residual convergence behavior of the tested methods. It is observed that all methods maintain its corresponding rate of convergence up to a certain tolerance; below this tolerance, the rate of convergence deteriorates. All methods that use the strategy of enrichment subspace have the rate of convergence improved except GMRES(30) that does not converge within the prespecified maximum number of cycles for Problem 20 and presents a slowdown of convergence for Problem 17. LGMRES-E(m, l, d) has better performance with respect to the number of cycles, but requires a larger time than the other methods in these two

TABLE 3 Mean time required for convergence and cycles required for $\|r_s^{(j)}\|/\|r^{(0)}\| \leq 10^{-9}$) (in parentheses) are listed for each problem

Problem	GMRES (m)	LGMRES (m, l)	GMRES-E (m, d)	LGMRES-E (m, l, d)	SLGMRES-E (m, l, d)
1	0.86 (35)	**0.62** (21)	0.96 (23)	3.52 (2)	0.70 (20)
2	2.05 (29)	**1.45** (21)	2.39 (27)	1.84 (21)	1.49 (21)
3	11.04 (110)	2.95 (30)	2.76 (21)	**2.37** (18)	2.98 (30)
4	15.63 (156)	9.85 (97)	12.95 (95)	**7.12** (51)	9.97 (97)
5	1.17 (101)	**0.54** (33)	2.45 (75)	1.02 (32)	0.57 (33)
6	1.96 (124)	0.43 (27)	1.33 (44)	0.74 (25)	**0.41** (27)
7	0.39 (25)	0.26 (16)	0.30 (9)	**0.22** (8)	0.26 (16)
8	0.59 (26)	0.43 (18)	1.00 (24)	0.75 (19)	**0.43** (18)
9	0.56 (35)	0.35 (22)	**0.30** (9)	0.32 (9)	0.34 (22)
10	1.95 (120)	**1.09** (70)	5.03 (71)	2.21 (71)	1.13 (70)
11	**0.57** (13)	0.70 (18)	1.07 (15)	1.06 (18)	0.78 (18)
12	0.45 (19)	**0.42** (17)	0.81 (20)	0.68 (17)	**0.36** (17)
13	**0.16** (12)	0.34 (23)	0.42 (13)	0.43 (15)	0.34 (23)
14	2.65 (68)	**1.05** (27)	1.53 (27)	1.26 (21)	**1.05** (27)
15	2.50 (115)	**0.64** (29)	1.00 (17)	0.65 (17)	0.65 (29)
16	24.78 (137)	**11.42** (51)	30.36 (131)	23.28 (49)	11.62 (51)
17	8.95 (416)	2.57 (76)	**2.14** (55)	10.03 (45)	3.41 (76)
18	NC (NC)	NC (NC)	31.44 (410)	NC (NC)	**22.87** (343)
19	NC (NC)	**19.98** (271)	NC (NC)	20.96 (221)	20.70 (271)
20	NC (NC)	**8.05** (103)	9.82 (143)	13.05 (73)	10.30 (131)
21	NC (NC)	5.94 (387)	7.27 (236)	**3.56** (118)	5.23 (319)
22	NC (NC)	NC (NC)	NC (NC)	NC (NC)	NC (NC)
23	NC (NC)	NC (NC)	NC (NC)	NC (NC)	NC (NC)

Note: Best performance (lowest mean time) is indicated by boldface. Parameters for each methods are: GMRES(m), $m = 30$, LGMRES(m, l), $m = 28$, $l = 2$; GMRES-E(m, d), $m = 28$, $d = 2$; LGMRES-E(m, l, d), $m = 27$, $d = 2$, $l = 1$; SLGMRES-E(m, l, d), $m = 28$, $d = 2$, $l = 2$, $\epsilon_0 = 0.01$.
Abbreviation: GMRES, generalized minimal residual.

problems. Observe that an improvement in the number of restart cycles required for convergence does not necessarily imply in a decrease in the computational running time.

4.2 | Influence of adjusting the restart parameter m

This section analyzes the modification of the restart parameter m in the methods SLGMRES-E(m, l, d) and GMRES(m) using a controller PD as an adjustment rule.[20] To denote the adaptive nature of the restart parameter m in this section we introduce the m_j nomenclature, that is, A-SLGMRES-E(m_j, l, d) and PD-GMRES(m_j).

The values selected for the proportional and derivative parameters in general increases the restart parameter m if there is slowdown of convergence. The PD rule used in this section was introduced in Section 3. The values (α_P, α_D) that satisfies the expression (40) are (1.0; 0.4), (2.0; 0.8), and (3.0; 1.3) for $\mu = 1$, $\mu = 2$, and $\mu = 3$, respectively. The performances of the A-SLGMRES-E and PD-GMRES are presented in Table 4 for problems of group 2. Observe that $\mu = 1$ and $\mu = 2$ have the better performance but $\mu = 2$ has the lower time for the problems Ex40 and Wang4. The A-SLGMRES-E does not use the PD rule for problems of group 1 because $\epsilon > \epsilon_0$, therefore it is equivalent to the LGMRES method.

This section uses the same values for the subspace enrichment parameter as the previous subsection. The results considering time in seconds and cycles necessary for convergence are shown in Table 5. The best values obtained each

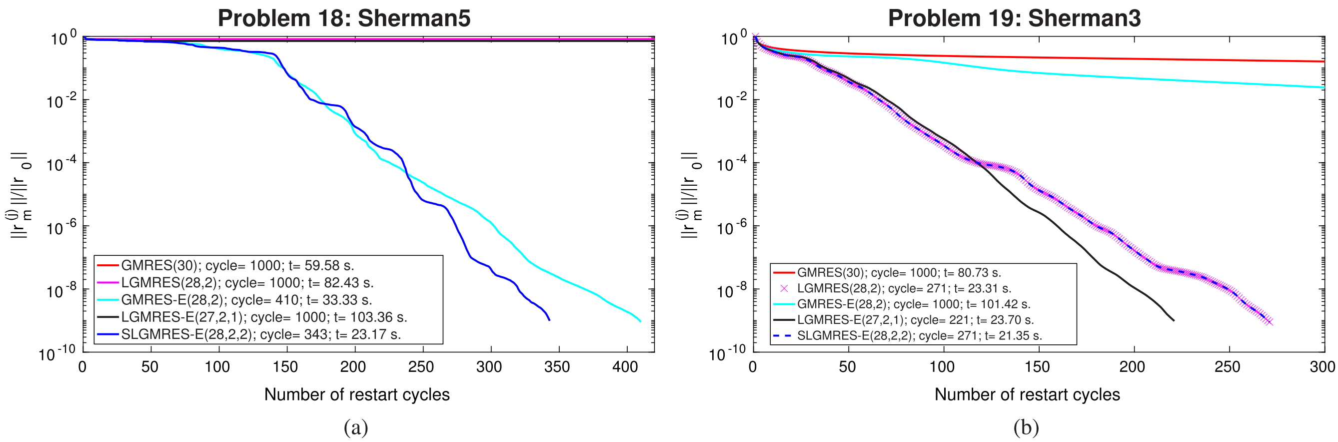


FIGURE 2 Logarithm of the relative residual norm vs the number of restart cycles necessary for converging to the prespecified tolerance. A, Problem 18 (Sherman5) and B, Problem 19 (Sherman3). See Table 3 for details about the running parameters of each method

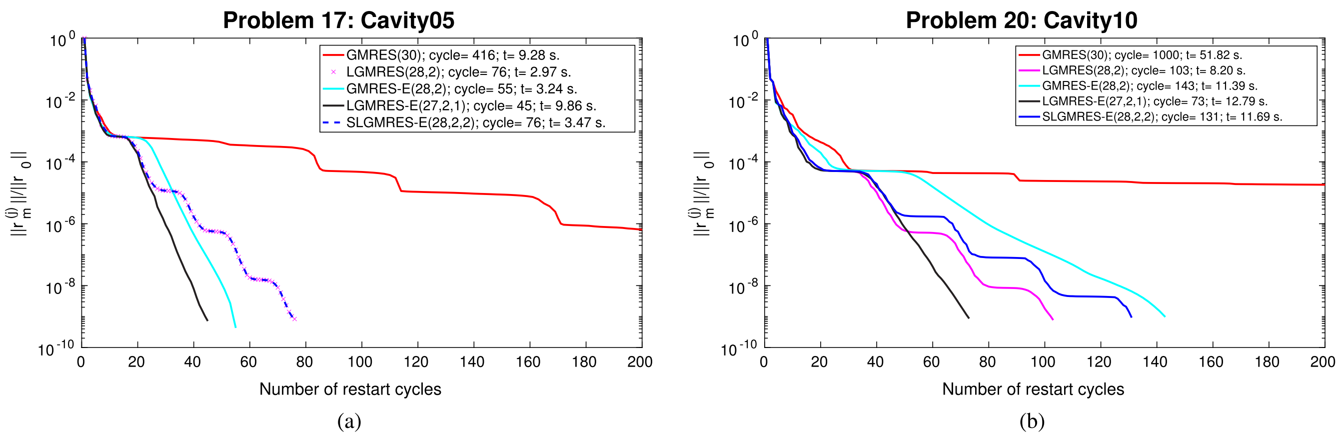


FIGURE 3 Logarithm of the relative residual norm vs the number of restart cycles necessary for converging to the prespecified tolerance. A, Problem 17 (Cavity05) and B, Problem 20 (Cavity10). The SLGMRES-E(28,2,2) method behaves as the standard LGMRES(28,2) since during the running does not overcome the threshold stagnation parameter, $\epsilon_0 = 0.01$ (see Table 3)

problem are indicated in boldface. Observe that the A-SLGMRES-E has the best performance for obtaining convergence (considering computational time) for all problems of group 2 (hard problems) for all tested methods.

Problem 22 (Ex40) is generated from a computational fluid dynamics problem. Figure 4A shows the residual convergence behavior for GMRES(m) with $m = 30$; LGMRES(m, l) with $m = 28$ and $l = 2$; GMRES-E(m, d), with $m = 28$ and $d = 2$; LGMRES-E(m, l, d) with $m = 27$, $d = 2$ and $l = 1$, and the A-SLGMRES-E(m, l, d) with $m = 28$, $d = 2$ and $l = 2$. It is observed that standard methods using enriched subspace present a slowdown of the rate of convergence, and in fact they do not converge within the prespecified maximum number of cycles. On the contrary, the method with an adaptive restart parameter converges in less than the prespecified maximum number of cycle.

In Figure 5A, the A-SLGMRES-E(m_j, l, d) is compared with the PD-GMRES(m_j). Both methods use the same rule to adjust the restart parameter. In this case, both methods converge, but A-SLGMRES-E has the best time (see Table 5), this is due to fact that A-SLGMRES-E requires lowers values for the restart parameter with respect to the ones required by the PD-GMRES. This assertion can be visualized in Figure 5B.

Problem 23 (Wang4) involves a relatively large, sparse and nonsymmetric matrix generated from a semiconductor device problem. As observed in Figure 4B, using only subspace enrichment strategy is not enough to achieve convergence when a fixed restart parameter is employed. Figure 6 shows the residual of A-SLGMRES-E(28,2,2) and the PD-GMRES(30). It is observed that A-SLGMRES-E(28,2,2) requires less computational time than PD-GMRES(30), but it

TABLE 4 Mean time and cycles required for convergence for μ = 1, 2, 3

Problem	Method	$\mu = 1$ Time (cycles)	$\mu = 2$ Time (cycles)	$\mu = 3$ Time (cycles)
18	A-SLGMRES-E	***25.52*** (151)	37.32 (108)	52.52 (89)
	PD-GMRES	118.26 (145)	204.70 (106)	***112.85*** (78)
19	A-SLGMRES-E	21.06 (274)	***20.04*** (271)	21.17 (271)
	PD-GMRES	***113.05*** (131)	122.45 (91)	128.25 (75)
20	A-SLGMRES-E	8.85 (82)	***7.04*** (67)	19.93 (78)
	PD-GMRES	103.01 (160)	***100.61*** (103)	123.41 (88)
21	A-SLGMRES-E	***5.60*** (202)	6.23 (234)	7.09 (227)
	PD-GMRES	***112.34*** (198)	147.08 (125)	175.66 (104)
22	A-SLGMRES-E	860.83 (941)	***749.50*** (920)	874.19 (936)
	PD-GMRES	7019.60 (443)	***6910.44*** (289)	7411.83 (219)
23	A-SLGMRES-E	133.58 (133)	***116.28*** (85)	191.18 (87)
	PD-GMRES	231.46 (111)	257.91 (66)	***156.18*** (54)

Note: Parameters for each method are: PD-GMRES(m_j), m_0=30; A-SLGMRES-E(m_j, d, l), m_0=28, l=2, d=2, $\epsilon_0 = 0.01$. Best performance of every method is indicated by boldface.
Abbreviations: GMRES, generalized minimal residual; PD, proportional-derivative.

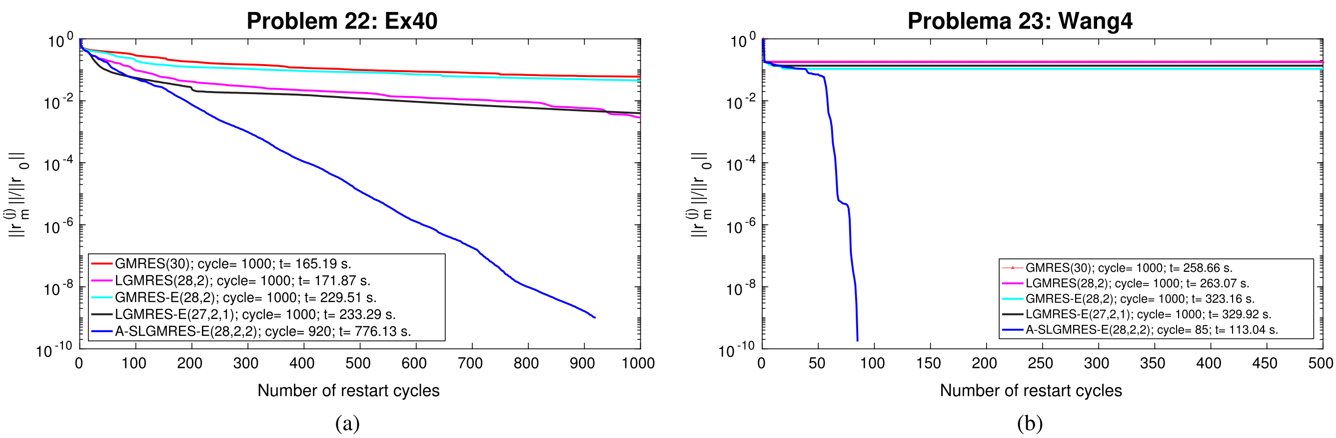


FIGURE 4 A, Problem 22: Ex40 and B, Problem 23: Wang4. For the method A-SLGMRES-E(m_j, l, d), the PD rule is used to adjust the restart parameter. In both problems, the A-SLGMRES-E(m_j, l, d) is the only that converges before the maximum number of restart cycles. PD, proportional-derivative

requires a slightly larger number of restart cycles with respect to PD-GMRES(30) (see Figure 6A). An important observation is that at each cycle the A-SLGMRES-E(28,2,2) employs lower values of the restart parameter m in comparison with its counterpart PD-GMRES (see Figure 6B). It can be observed that there is a trade-off between the computational time required for converging in terms of cycles and the computational time required for the orthogonalization of the search subspace (associated to the restart parameter m). Hence, for both Problems 22 and 23, (Figures 5 and 6, respectively), the A-SLGMRES-E(28,2,2) requires more cycles, but requires less computational time to converge in comparison with the PD-GMRES(30).

In problems where the SGMRES-E stagnates, the A-SLGMRES-E may have a decreasing in the number of cycles required for convergence. This is due to the fact that the adaptive part of the control law allows to vary the value of m, modifying the dimension of the Krylov subspace. Eventually, the control law increases the dimension of the Krylov subspace contributing to improve the approximation of the eigenvalues of matrix A, and improving the information for the new search subspace of the restarted cycle. For problems, where the GMRES(m) does not present any stagnation

TABLE 5 Mean time required for convergence (cycles required for $\|r_s^{(j)}\|/\|r^{(0)}\| \leq 10^{-9}$) are listed for each problem

Problem	A-SLGMRES-E(m, l, d)	PD-GMRES(m)
1	**0.70** (20)	0.75 (2)
2	**1.64** (21)	1.72 (18)
3	**3.14** (30)	13.27 (40)
4	**10.09** (97)	15.26 (44)
5	**0.60** (33)	0.84 (24)
6	**0.43** (27)	1.66 (34)
7	**0.29** (16)	0.37 (21)
8	**0.44** (18)	0.63 (21)
9	**0.36** (22)	0.49 (21)
10	**1.18** (70)	2.23 (38)
11	0.74 (18)	**0.53** (16)
12	**0.40** (17)	0.41 (17)
13	0.34 (23)	**0.24** (19)
14	**1.20** (27)	3.75 (34)
15	**0.66** (29)	2.44 (36)
16	**13.25** (51)	19.02 (33)
17	**2.82** (76)	16.51 (70)
18	**37.32** (108)	204.70 (106)
19	**27.48** (271)	171.66 (91)
20	**6.64** (70)	100.61 (103)
21	**6.23** (234)	147.08 (125)
22	**749.50** (920)	6910.44 (289)
23	**116.28** (85)	161.83 (67)

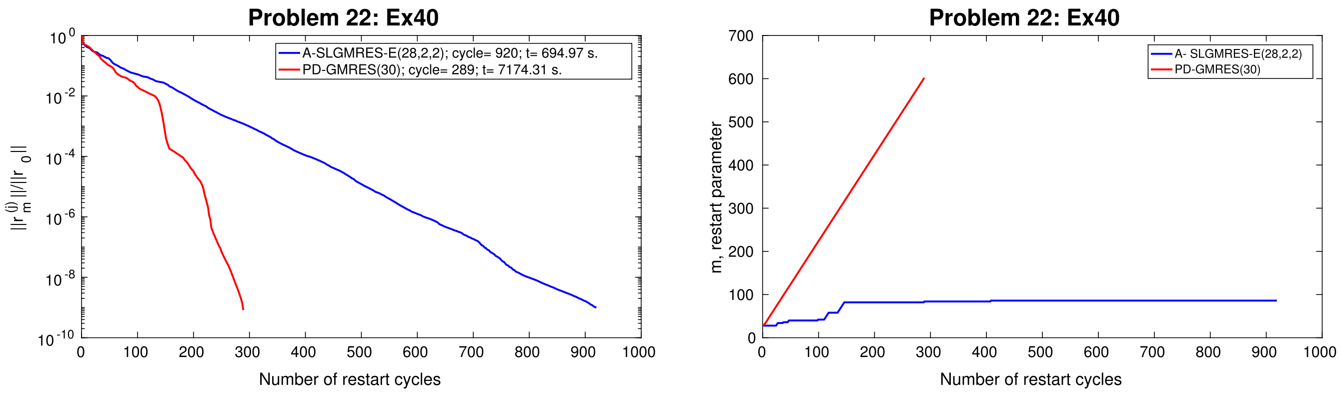
Note: Best performance (lowest mean time) is indicated by boldface. Parameters for each methods are: PD-GMRES(m_j), $m_0 = 30$; A-SLGMRES-E(m_j, l, d), $m_0 = 28$, $d = 2, l = 2, \epsilon_0 = 0.01$.
Abbreviations: GMRES, generalized minimal residual; PD, proportional-derivative.

problems, the proposed methods SLGMRES-E and A-SLGMRES-E, present similar behavior, that is, they require a similar number of cycles to achieve convergence. This is because according to the rule of variation of m it is not necessary to vary this parameter (see expression (40)).

4.3 | Effectiveness preconditioned problems

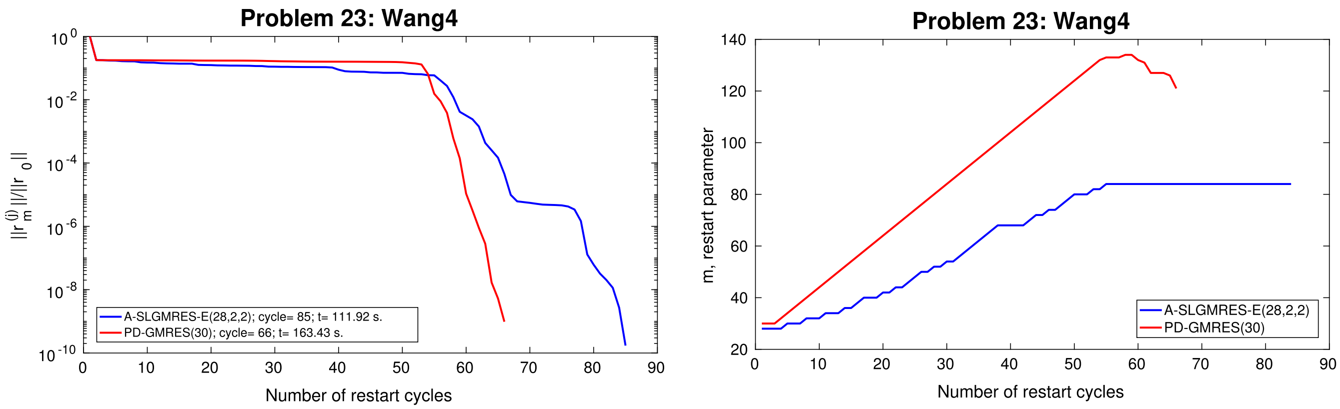
A common strategy in the iterative solution of linear systems is the use of preconditioners. There exist generic preconditioners that can be used for a wide range of problems; but in general, the design of preconditioners requires information about the problem. In this subsection, left preconditioners denoted by P^{-1} are applied to system (1). It is shown experimentally that the proposed methods with preconditioners have similar convergence properties to its nonpreconditioned counterparts. In addition, when an effective preconditioner is used, it generally improves the methods (including the proposed ones) for all problems tested. This is in accordance to results encountered at the literature.[30,39]

Three preconditioners are used: Jacobi, SOR with $\omega = 1$ denoted as Gauss-Seidel and the incomplete LU factorization denoted as ILU. The Jacobi and SOR preconditioners are very simple to implement but both can fail if any of the diagonal elements of the matrix A is zero.[30,40] For the ILU preconditioner, we used the ILUTP version of MatLab 9.1.0 (R2016b) with the value *droptol* $= 10^{-6}$. For fairness in comparing the performance of the preconditioners for improving the rate of convergence of the methods, the tables do not include the running time for computing the preconditioner matrix $P^{-1}A$.



(a) (b)

FIGURE 5 Problem 22: Ex40. A, Plot of the logarithm relative residual norm vs the number of restart cycles necessary to get the tolerance. B, The restart value m_j vs number of restart cycles. The PD rule is used to adjust the restart parameter in the GMRES(m) and the proposed switch method. GMRES, generalized minimal residual; PD, proportional-derivative



(a) (b)

FIGURE 6 Problem 23: Wang4. A, Plot of the logarithm relative residual norm vs the number of restart cycles necessary to achieve the specified tolerance. B, The restart value m_j vs number of restart cycles. The PD rule is used to adjust the restart parameter in the GMRES(m) and the proposed switching method. GMRES, generalized minimal residual; PD, proportional-derivative

The left preconditioning minimizes the preconditioned residual norm ($||P^{-1}r||$), the stopping criterion is based on this preconditioned residual norm as usual.

The above mentioned preconditioners cannot be used for some of the test problems of this article. For instance, Problems 2, 5, 17, 20, and 22 of Table 1 have zeros in the diagonal, therefore the Jacobi and SOR preconditioners cannot be implemented. For Problems 16 and 23, the ILU version of MatLab requires large memory requirements which exceed the computer capacity. For these reasons, it is selected the efficient preconditioner for the numerical comparisons.

In Table 6, is listed the necessary cycles to converge of the SLGMRES-E and A-SLGMRES-E methods when it is chosen the best effective preconditioner for every problem of Table 1. Comparing Tables 3 and 6, it is observed that the preconditioned SLGMRES-E method decreases the number of cycles necessary for converging for all problems. Observe that for certain problems (problems 22 and 23) the preconditioner improves the convergence in such a way that the preconditioned SLGMRES-E converges before 1000 cycles while its nonpreconditioned counterpart does not.

For the first 16 problems of Table 6, it is observed that the SLGMRES-E and the A-SLGMRES-E methods require similar number of cycles to converge. Since both methods without preconditioner requires similar cycles to converge and the preconditioner similarly accelerates both methods, then the ratio between the preconditioned and nonpreconditioned cycles are similar (compare the respective cycles in Tables 3,5, and 6).

For Problems 17 up to 23 of Table 6, the preconditioner speeds up the SLGMRES-E and the A-SLGMRES-E methods differently. Figure 7 shows the cycle number ratio between the SLGMRES-E and A-LGMRES-E using the best preconditioner respect to SLGMRES-E and A-LGMRES-E without a preconditioner. Values less than 1 represents that the proposed

Problem	Preconditioner	SLGMRES-E(m, l, d)	A-SLGMRES-E(m_j, l, d)
1	Jacobi	8	8
2	ILU(0)	3	3
3	SOR	15	15
4	SOR	18	18
5	ILU(0)	3	3
6	SOR	11	11
7	SOR	7	7
8	SOR	11	11
9	SOR	19	19
10	ILU(0)	4	4
11	Jacobi	16	16
12	SOR	14	14
13	Jacobi	3	3
14	Jacobi	15	15
15	Jacobi	15	15
16	Jacobi	9	9
17	ILU(0)	3	3
18	ILU(0)	3	3
19	ILU(0)	7	7
20	ILU(0)	3	3
21	ILU(0)	217	162
22	ILU(0)	3	3
23	Jacobi	408	199

Abbreviation: GMRES, generalized minimal residual.

TABLE 6 Number of cycles required for convergence of preconditioned matrices using the SLGMRES-E(m, l, d) and A-SLGMRES-E(m_j, l, d) methods

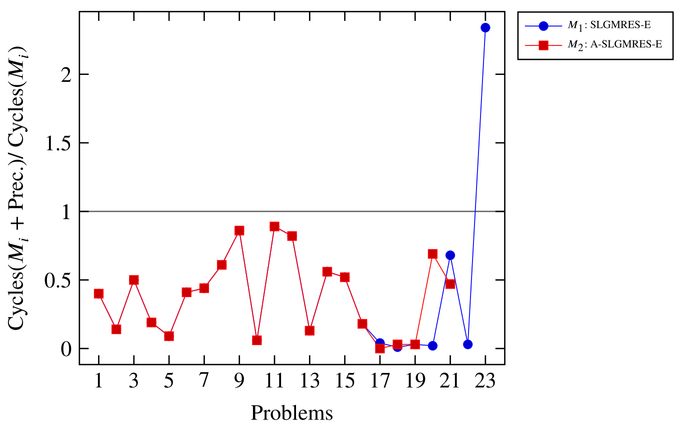


FIGURE 7 A comparison of the cycles required for convergence for Problems of Table 1 using the proposed methods with and without preconditioners

methods require fewer cycles to converge. To the SLGMRES-E, the last two problems (ex40 and wang4) are not considered since this method converges only in its preconditioned form. The only one for which the ratio is more than one is for the wang4 problem. According to Table 6, the best preconditioner for the wang4 problem is the Jacobi. Recall that for the wang4 problem the proposed A-SLGMRES-E and the PD-GMRES[20] are the only ones that converge without a preconditioner and for the Jacobi preconditioner they continue to achieve convergence. It can be said that choosing a more appropriate preconditioner could improve the convergence decreasing the number of cycles, but in general, the selection of an appropriate preconditioner requires some *a priori* knowledge of the problem. It is possible to conclude that for all tested problems the use of a preconditioner improves the rate of convergence when an effective preconditioner is used.

The proposed methods SLGMRES-E and A-SLGMRES-E, are not (in general) a substitute for an effective preconditioner. Experimental results show that preconditioning improves both proposed methods with and without preconditioning, but more importantly, it is the fact that the proposed methods can help when the GMRES(m) stagnates due to a bad selection of the restart parameter m.

5 | CONCLUSIONS

In this article, a hybrid method for improving GMRES(m) by restraining the stagnation and slowdown convergence was introduced. To this end, based on definitions of the literature and control theory the stagnation and the slowdown of convergence was characterized using angles between iterations, cycles of GMRES(m) and the structure of the matrices of the Arnoldi decomposition relationship. A Lyapunov function was used as a sufficient condition for stability. With the characterizations, an adaptive strategy for solving the linear system using a switching convergence approach was introduced. The idea behind the variation of the structure of the GMRES(m) relies on the fact that once either the slowdown of convergence or stagnation is detected, a rule of switching between two strategies chooses the one most appropriate for facing the identified convergence problem. In this step two monotonically decreasing strategies, obtained from the literature, were tested: the LGMRES and the GMRES-E, this results in the switching method denoted as SGMRES-E. The methods were tested using benchmark problems from practical engineering problems.

Both of the methods employed in the switching use the augmentation of the Krylov search subspace. The first method augments the search subspace with some error vectors; which, in turn, introduces part of the information from previous cycles, usually lost during the conventional restarting process. The method speeds up the rate of convergence, but the residual can still stagnate. The second method enriches the search subspace by appending approximate eigenvectors to the Krylov subspace. The approximate eigenvectors are harmonic Ritz vectors associated with the smallest (in magnitude) harmonic Ritz values and approximate the eigenvalues of the matrix A. This method helps to mitigate stagnation behavior, but it is computationally expensive. Hence, once slowdown of convergence or stagnation is detected, the rule switches from one method to another, allowing unnecessary computations to be avoided, and therefore reducing the computational cost. In order to determine when to switch from one strategy to another, a switching threshold ϵ_0 was introduced. Although there are some differences in the running time for the algorithm with respect to the choice of the switching threshold, these differences were not significant. The question of what is the optimal dimension of the subspace for performing the augmentation or enrichment was not focused on this article and the values used were the typical values encountered in the literature.

In some cases, the stagnation is due to structural problems, observed in the Arnoldi decomposition relation, hence the methods (LGMRES and GMRES-E) will not help to improve convergence. In this case, based on the Lyapunov function, a proportional derivative rule was introduced to modify the restarted parameter m. This is done to modify (and in general enlarge) the Krylov subspace, when the information introduced by the augmentation or the enrichment (which is computed using the Krylov subspace of the previous cycle) is not enough to overcome the slowdown of convergence or the stagnation. The method that switches between the LGMRES and the GMRES-E and also can modify the dimension of the Krylov subspace is denoted by A-SLGMRES-E. It is observed that the combination of the three strategies at the appropriate stage improves the rate of convergence even for the most difficult problems, and the combination of the strategies achieves a better trade-off between the number of iterations required to converge to a prespecified tolerance and its computational cost. At the moment the authors are working to explore the use of nonmonotonic methods, as well as to analyze the optimum size for the augmenting and enriching subspaces.

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AUTHOR CONTRIBUTIONS

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CONFLICT OF INTEREST

The authors declare no potential conflict of interests.

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