ARAS2 Preconditioning Technique for CFD Industrial Cases

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1 Introduction

The convergence rate of a Krylov method such as the Generalized Conjugate Residual (GCR) [6] method, to solve a linear system $Au = f, A = (a_{ij}) \in \mathbb{R}^{m\times m}, u \in \mathbb{R}^m, f \in \mathbb{R}^m$, decreases with increasing condition number $\kappa_2(A) = ||A||_2||A^{-1}||_2$ of the non singular matrix A. Left preconditioning techniques consist of solving $M^{-1}Au = M^{-1}f$ such that $\kappa_2(M^{-1}A) << \kappa_2(A)$. The Additive Schwarz (AS) preconditioning is built from the adjacency graph $G = (W,E)$ of A, where $W = \{1,2,\ldots,m\}$ and $E = \{(i, j) : a_{ij} \neq 0\}$ are the edges and vertices of G. Starting with a non-overlapping partition $W = \cup_{i=1}^{p} W_{i,0}$ and $\delta \geq 0$ given, the overlapping partition $\{W_{i,\delta}\}$ is obtained defining p partitions $W_{i,\delta} \supset W_{i,\delta-1}$ by including all the immediate neighboring vertices of the vertices in the partition $W_{i,\delta-1}$. Then the restriction operator $R_{i,\delta}$ from W to $W_{i,\delta}$ defines the local operator $A_{i,\delta} = R_{i,\delta}AR^T_{i,\delta}, A_{i,\delta} \in \mathbb{R}^{m_{i,\delta}\times m_{i,\delta}}$ on $W_{i,\delta}$. The AS preconditioning writes: $M^{-1}_{AS,\delta} = \sum_{i=1}^{p} R^T_{i,\delta}A^{-1}_{i,\delta}R_{i,\delta}$. Introducing $\tilde{R}_{i,\delta}$ the restriction matrix on a non-overlapping subdomain $W_{i,0}$, the Restricted Additive Schwarz (RAS) iterative process [2] writes:

$$u^k = u^{k-1} + M^{-1}_{RAS,\delta}\left(f - Au^{k-1}\right), \text{ with } M^{-1}_{RAS,\delta} = \sum_{i=1}^{p} \tilde{R}^T_{i,\delta}A^{-1}_{i,\delta}R_{i,\delta} \tag{1}$$

The RAS exhibits a faster convergence than the AS, as shown in [5], leading to a better preconditioning that depends of the number of subdomains. When it is applied to linear problems, the RAS has a pure linear rate of convergence/divergence that can be enhanced with optimized boundary conditions giving the ORAS method of [11]. The RAS method's linear convergence allows its acceleration of the convergence by the Aitken's process as done in [8] for the Schwarz method.

In [4] the present authors designed the ARAS2 preconditioning technique based on the Aitken's acceleration of the convergence technique. This paper presents an approach to solve linear systems coming from CFD industrial cases. The choice of an

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approximation space based on the Singular Value Decomposition of the interface's solutions of the RAS iterative process presented in [14] is done. This provides a preconditioning technique that depends on the Right Hand Side but with a very low computational time and totally algebraic.

2 The ARAS2 Preconditioning Method

In what follows, we write the Aitken Restricted Additive Schwarz (ARAS) iterative process and the associated preconditioner. This preconditioner belongs to the family of the two-level preconditioner techniques (see [10, 13] and references) but the coarse grid operator uses only parts of the artificial interfaces contrary to the patch substructuring method of [7]. In this way, it can be seen as similar as the SchurRAS method of [9] but it differs because the discrete Steklov-Poincaré operator connects the coarse artificial interfaces of all the subdomains.

2.1 The ARAS and ARAS2 Preconditioner's Formulation

Let $\Gamma_i = W_{i,\delta+1} \setminus W_{i,\delta}$ be the interface associated to $W_{i,\delta}$ and $\Gamma = \cup_{i=1}^{p} \Gamma_i$ be the global interface. Then $u_{|\Gamma} \in \mathbb{R}^n$ is the restriction of the solution $u \in \mathbb{R}^m$ on the Γ interface and $e^k_{|\Gamma} = u^k_{|\Gamma} - u^\infty_{|\Gamma}$ is the error of (1) at the interface Γ. Taking into account that there exists a matrix $P \in \mathbb{R}^{n\times n}$ independent of the iterate k such that $e^k_{|\Gamma} = P e^{k-1}_{|\Gamma}$, we can apply the Aitken's acceleration of the convergence process [8] (if $||P|| < 1$ to ensure existence of $(I_n - P)^{-1}$ for example) as follows:

$$u^\infty_{|\Gamma} = (I_n - P)^{-1}\left(u^k_{|\Gamma} - P u^{k-1}_{|\Gamma}\right). \tag{2}$$

P can be computed analytically or numerically for a separable operator on separable geometry [8] or numerically approximated in other cases [14]. Using this property on the RAS method, we would like to write a preconditioner which includes the Aitken's acceleration process. We introduce a restriction operator $R_\Gamma \in \mathbb{R}^{n\times m}$ from W to the global artificial interface Γ, with $R_\Gamma R_\Gamma^T = I_n$.

The Aitken Restricted Additive Schwarz (ARAS) must generate a sequence of solutions on the interface Γ, and accelerate the convergence of the Schwarz process from this original sequence. Then the accelerated solution on the interface replaces the last one. This could be written combining an AS or RAS process Eq. (3a) with the Aitken process written in $\mathbb{R}^{m\times m}$ Eq. (3b) and substracting the Schwarz solution which is not extrapolated on Γ Eq. (3c). We can write the following approximation u^* of the solution u:

$$u^* = u^{k-1} + M^{-1}_{RAS,\delta}(f - Au^{k-1}) \tag{3a}$$

$$+ R_\Gamma^T (I_n - P)^{-1}\left(u^k_{|\Gamma} - P u^{k-1}_{|\Gamma}\right) \tag{3b}$$

$$- R_\Gamma^T I_n R_\Gamma \left(u^{k-1} + M^{-1}_{RAS,\delta}(f - Au^{k-1})\right) \tag{3c}$$

We would like to write u^* as an iterated solution derived from an iterative process of the form $u^* = u^{k-1} + M^{-1}_{ARAS,\delta}\left(f - Au^{k-1}\right)$, where $M^{-1}_{ARAS,\delta}$ is the Aitken-RAS preconditioner.

Hence the formulation Eq. (3) leads to an expression of an iterated solution u^*:

$$u^* = u^{k-1} + \left(I_m + R_\Gamma^T\left((I_n - P)^{-1} - I_n\right)R_\Gamma\right)M^{-1}_{RAS,\delta}\left(f - Au^{k-1}\right)$$

This iterated solution u^* can be seen as an accelerated solution of the RAS iterative process. Drawing our inspiration from the Stephensen's method, we build a new sequence of iterates from the solutions accelerated by the Aitken's acceleration method. Such a process is done in [12]. Then, one considers u^* as a new u^k and writes the following ARAS iterative process:

$$u^k = u^{k-1} + \left(I_m + R_\Gamma^T\left((I_n - P)^{-1} - I_n\right)R_\Gamma\right)M^{-1}_{RAS,\delta}\left(f - Au^{k-1}\right) \tag{4}$$

Then we defined the ARAS preconditioner as

$$M^{-1}_{ARAS,\delta} = \left(I_m + R_\Gamma^T\left((I_n - P)^{-1} - I_n\right)R_\Gamma\right)\sum_{i=1}^{p}\tilde{R}^T_{i,\delta}A^{-1}_{i,\delta}R_{i,\delta} \tag{5}$$

If P is known exactly, the ARAS process written in Eq. (4) needs two steps to converge to the solution u with an initial guess $u^0 = 0$. Then we have:

Proposition 1. *If P is known exactly then we have* $A^{-1} = \left(2M^{-1}_{ARAS,\delta} - M^{-1}_{ARAS,\delta}AM^{-1}_{ARAS,\delta}\right)$ *that leads* $\left(I - M^{-1}_{ARAS,\delta}A\right)$ *to be a nilpotent matrix of degree 2.*

The previous proposition leads to an approximation of A^{-1} written from the 2 first iterations of the ARAS iterative process (4). Those 2 iterations compute the Schwarz solutions sequence on the interface needed in order to accelerate the Schwarz method by the Aitken's acceleration. We now write 2 iterations of the ARAS iterative process (4) for any initial guess and for all $u^{k-1} \in \mathbb{R}^m$.

$$u^{k+1} = u^{k-1} + \left(2M^{-1}_{ARAS,\delta} - M^{-1}_{ARAS,\delta}AM^{-1}_{ARAS,\delta}\right)\left(f - Au^{k-1}\right)$$

Then we defined the ARAS2 preconditioner as

$$M^{-1}_{ARAS2,\delta} = 2M^{-1}_{ARAS,\delta} - M^{-1}_{ARAS,\delta}AM^{-1}_{ARAS,\delta} \tag{6}$$

Hence, if P is known exactly there is no need to use ARAS as a preconditioning technique. Nevertheless, when P is approximated, the Aitken's acceleration of the convergence depends on the local domain solving accuracy, and the cost of the building of an exact P depends on the size n. This is why P is numerically approximated by $P_{\mathbb{U}_q}$, defining $q \leq n$ orthogonal vectors $\mathbb{U}_q \in R^{n\times q}$, that are able to approximate most of the solution at the interface Γ. Then ARAS($\mathbb{U}_q$) and ARAS2($\mathbb{U}_q$) can be defined as:

$$M^{-1}_{ARAS(\mathbb{U}_q),\delta} = \left(I_m + R_\Gamma^T \mathbb{U}_q \left(\left(I_q - P_{\mathbb{U}_q}\right)^{-1} - I_q\right) \mathbb{U}_q^T R_\Gamma\right) \sum_{i=1}^{p} \tilde{R}^T_{i,\delta} A^{-1}_{i,\delta} R_{i,\delta} \tag{7}$$

and

$$M^{-1}_{ARAS2(\mathbb{U}_q),\delta} = 2M^{-1}_{ARAS(\mathbb{U}_q),\delta} - M^{-1}_{ARAS(\mathbb{U}_q),\delta} A M^{-1}_{ARAS(\mathbb{U}_q),\delta} \tag{8}$$

As the basis $\mathbb{U}_q$ can only give an approximation of the searched solution at the interface, it make sense to use $M^{-1}_{ARAS(\mathbb{U}_q),\delta}$ and $M^{-1}_{ARAS2(\mathbb{U}_q),\delta}$ as preconditioners.

2.2 Orthogonal Basis $\mathbb{U}_q$ Arising from SVD of the Interface's Solutions of Richardson Process

The objective is to compute $P_{\mathbb{U}_q}$ saving as much computing as possible. The singular value decomposition offers a tool to concentrate the effort only on the main parts of the solution. A singular-value decomposition of a real $n \times q$ $(n > q)$ matrix Y is its factorization into the product of three matrices $Y = \mathbb{U}_q \Sigma \mathbb{V}^*$, where $\mathbb{U}_q = [U_1, \ldots, U_q]$ is an $n \times q$ matrix with orthonormal columns, Σ is an $n \times q$ nonnegative diagonal matrix with $\Sigma_{ii} = \sigma_i$, $1 \le i \le q$ and the $q \times q$ matrix $\mathbb{V} = [V_1, \ldots, V_q]$ is orthogonal. The left $\mathbb{U}_q$ and right $\mathbb{V}$ singular vectors are the eigenvectors of YY^* and Y^*Y respectively. It readily follows that $Av_i = \sigma_i u_i$, $1 \le i \le q$. We are going to recall some properties of the SVD. Assume that the $\sigma_i, 1 \le i \le q$ are ordered in decreasing order and there exists an r such that $\sigma_r > 0$ while $\sigma_r + 1 = 0$. Then A can be decomposed in a dyadic decomposition:

$$Y = \sigma_1 U_1 V_1^* + \sigma_2 U_2 V_2^* + \ldots + \sigma_r U_r V_r^*. \tag{9}$$

This means that SVD provides a way to find optimal lower dimensional approximations of a given series of data. More precisely, it produces an orthonormal basis for representing the data series in a certain least squares optimal sense.

The orthogonal "basis" $\mathbb{U}_q$ is obtained as follows. q iterations of the Richardson process $u^k = u^{k-1} + M^{-1}_{RAS,\delta}(f - Au^{k-1})$ are performed and $R_\Gamma u^k \in \mathbb{R}^n, 1 \le k \le q$ belonging to the interface Γ are stored in a matrix $Y \in \mathbb{R}^{n \times q}$. Then the SVD of Y is computed to obtain the matrix $\mathbb{U}_q$ with an arithmetic cost less than the one of a local solution. It leads to efficiency and low computational cost as illustrated in [1]. Nevertheless, the preconditioner ARAS2($\mathbb{U}_q$) obtained is solution dependent.

2.3 Building of the $P_{\mathbb{U}_q}$ Matrix

The matrix $P_{\mathbb{U}_q}$ can be computed as follows keeping the $q+1$ first singular values of the SVD greater than a set tolerance, we writes:

$$\mathbf{Y}_{1:q,1:q+1} = \Sigma_{1:q,1:q} \mathbb{V}^T_{1:q,1:q+1} \tag{10}$$

$$\mathbf{E}_{1:q,1:q+1} = \mathbf{Y}_{1:q,2:q+1} - \mathbf{Y}_{1:q,1:q} \tag{11}$$

$$\text{If } \mathbf{E}_{1:q,1:q} \text{ is invertible then} \tag{12}$$

$$P_{\mathbb{U}_q} = \mathbf{E}_{1:q,2:q+1}\, \mathbf{E}^{-1}_{1:q,1:q} \tag{13}$$

The previous building requires the inversion of the matrix $\mathbf{E}_{1:q,1:q}$ which can be ill conditioned. It is why the second building of matrix $P_{\mathbb{U}_q}$ that follows is prefered. Selecting the q first singular values of the SVD greater than a set tolerance, one iteration of the RAS algorithm is applied on the q the homogeneous problems where $U^i, 1 \leq i \leq q$ is set as boundary condition on the interface Γ. The result of this RAS iterate with $M^{-1}_{RAS,\delta}$ on the boundary Γ is the column of $P_{\mathbb{U}_q}$ associated with the component U_i of the basis. Let us notice that this q computing can be made in the same time considering the q right hand sides in a matrix form.

3 Numerical Experiments on 2D and 3D Industrial Problems from Navier-Stokes Equations

In this section we focus on solving linear systems coming from industrial problems with the ARAS2 preconditioning technique. The sparse matrices correspond to the assemblage of all the elementary Jacobian matrices resulting from the partial first-order derivations with respect to the conservative fluid variables of the discrete steady (real) Reynolds-averaged Navier-Stokes equations. We note here that the Jacobian matrix is non-symmetric and is non positive definite.

Table 1 summarizes the main features of the linear systems from the two cases solved. Those cases are available in the sparse matrix collection [3]. Turbulence is considered in the 2D and 3D cases. We partition the system with PARMETIS into p subdomains. We must notice that for such problems with non-elliptic operators, the ILU factorization is hazardous. Then, the preconditioner is computed from exact factorization of local operators.

Figure 1 presents for the case PR02 the convergence behaviour of the Richardson and the GMRES preconditioned by the ARAS2 preconditioner where the $P_{\mathbb{U}_q}$ is approximated by SVD. For this matrix the RAS Richardson process diverges. If the number of singular values kept is not sufficient, the ARAS2 process diverges as well. If we used 60 iterates of RAS Richardson process then the "full" $P_{\mathbb{U}_q}$ makes the ARAS2 Richardson process converge in one iterate. Nevertheless ARAS2 works quite well in both cases as a preconditioner of the GMRES method. We must notice that here we have an effective gain to use the ARAS2 instead of RAS as Richardson process. The same behavior is also retrieved when ARAS2 is used as preconditioner.

For a 3D case the number of non-zero and the band profile increase. Then solving local problems by LU factorization begins to be expensive in terms of memory. A better approach consists of solving subproblems by an iterative method. For the case RM07, we choose to solve subproblems by a GMRES preconditioned by ILU. The idea to save computational time is to approximate the Aitken's acceleration with the basis arising from SVD and solving subproblems with less accuracy for the computing of the preconditioner. Table 2 shows the good strong numerical scalability of the ARAS2 preconditioning compare to the RAS.

case ID	*order*	*dim*	*nn*	*nnz*
PR02	161 070	2*D*	23 010	8 185 136
RM07	381 689	3*D*	54 527	37 464 962

Table 1. Main features of the linear systems with *order* the size of the matrix with real coefficients, *dim* the dimension of the problem, *nn* is the number of mesh nodes, *nnz* is the number of non-zero elements in the matrix

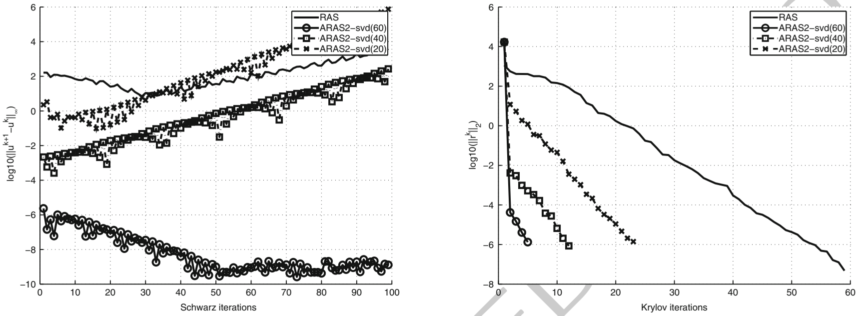

Fig. 1. Solving 2D Navier Stokes equation with turbulence (CASE PR02), PARMETIS partitioning, $p = 4$, overlap 2, ARAS2 is built with a SVD basis, (*left*) Convergence of Iterative Schwarz Process, (*right*) convergence of GMRES method preconditioned by RAS and ARAS2

p	RAS	ARAS(36)	ARAS2(36)
3	87 (1.)	77 (1.1299)	53 (1.6415)
6	112 (1.)	93 (1.2043)	63 (1.7778)
12	171 (1.)	124 (1.3790)	84 (2.0357)

Table 2. CASE RM07 : Number of GMRES iterations (ratio of iterations with RAS over iterations with ARAS or ARAS2) for a tolerance 1e-10, overlap 1.

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