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Multipreconditioning for nonsymmetric problems: The case of orthomin and biCG

Multipréconditionnement pour les problèmes non symétriques : le cas des solveurs orthomin et biCG

Christophe Bovet [a,c], Pierre Gosselet [b], Nicole Spillane [c]

[a] *Onera – The French Aerospace Lab, 92322 Châtillon, France*
[b] *LMT-Cachan, ENS-Cachan, CNRS, Université Paris-Saclay, 61, av. du Président-Wilson, 94235 Cachan, France*
[c] *CMAP, École polytechnique, CNRS, Université Paris-Saclay, route de Saclay, 91128 Palaiseau cedex, France*

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ABSTRACT

Preconditioned Krylov subspace methods [7] are powerful tools for solving linear systems but sometimes they converge very slowly, and often after a long stagnation. A natural way to fix this is by enlarging the space in which the solution is computed at each iteration. Following this idea, we propose in this note two multipreconditioned algorithms: multipreconditioned orthomin and multipreconditioned biCG, which aim at solving general nonsingular linear systems in a small number of iterations. After describing the algorithms, we illustrate their behaviour on systems arising from the FETI domain decomposition method, where in order to enlarge the search space, each local component in the usual preconditioner is kept as a separate preconditioner.

RÉSUMÉ

Les solveurs de Krylov préconditionnés [7] sont des outils performants pour la résolution de systèmes linéaires. Il arrive cependant qu'ils convergent lentement, souvent après une phase de stagnation. Une manière naturelle de remédier à cette situation est d'agrandir l'espace dans lequel on cherche la solution à chaque itération. En suivant cette idée, nous proposons dans cette note deux algorithmes multipréconditionnés : orthomin multipréconditionné (MPorthomin) et biCG multipréconditionné (MPbiCG) avec l'objectif de résoudre des systèmes linéaires généraux en un petit nombre d'itérations. Après avoir décrit les nouveaux algorithmes, nous illustrons leur comportement sur des systèmes linéaires issus de la méthode de décomposition de domaine FETI, où au lieu d'appliquer le préconditionneur habituel, on fait agir chaque contribution locale au préconditionneur séparément.

E-mail addresses: christophe.bovet@onera.fr (C. Bovet), gosselet@lmt.ens-cachan.fr (P. Gosselet), nicole.spillane@cmap.polytechnique.fr (N. Spillane).

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L'objectif de cette note est de présenter brièvement deux nouveaux algorithmes pour la résolution de systèmes linéaires non symétriques. Ils appartiennent à la famille des solveurs de Krylov multipréconditionnés. Les premiers solveurs de ce type sont le gradient conjugué multipréconditionné (MPCG) [2], FETI simultané (SFETI) [6] et GMRES multipréconditionné (MPGMRES) [5]. Comme nous considérons les problèmes non symétriques, MPCG ne s'applique pas. MPGMRES, dans sa forme originale, conduit à une croissance exponentielle de la taille de l'espace de minimisation. Comme remarqué dans [5], il est possible de se limiter à une croissance linéaire par rapport au nombre d'itérations en ne sélectionnant que certains vecteurs. Ici, nous considérons des solveurs pour lesquels cette croissance linéaire est plus naturelle. En effet, à la différence de GMRES, orthomin et biCG rendent le résidu disponible explicitement à chaque itération, et c'est à celui-ci que l'on applique le (ou les) préconditionneur(s). Ceci explique la croissance linéaire de la taille de l'espace de minimisation.

Nous notons $\mathbf{A}\mathbf{x}_* = \mathbf{b}$ le système linéaire considéré, où $\mathbf{x}_* \in \mathbb{R}^n$ est la solution recherchée, $\mathbf{A}$ est une matrice de taille $n \times n$ inversible et $\mathbf{b}$ est le second membre (source donnée). Une famille de N préconditionneurs (qui sont aussi des matrices inversibles de taille $n \times n$) notée $\{\mathbf{H}^s\}_{s=1,\dots,N}$ est utilisée. Les algorithmes orthomin multipréconditionné (MPorthomin) et biCG multipréconditionné (MPbiCG) sont présentés dans les Algorithmes 1 et 2 respectivement.

Les propriétés qui définissent les coefficients dans MPorthomin sont :

- $(\mathbf{A}^\top\mathbf{A})$-orthogonalité des directions de recherche ($\mathbf{Q}_i^\top\mathbf{Q}_j = \mathbf{0}$ pour tous $j \neq i$).
- $\mathbf{x}_i$ minimise la $\mathbf{A}^\top\mathbf{A}$-norme de l'erreur $\|\mathbf{x}_* - \mathbf{y}\|_{\mathbf{A}^\top\mathbf{A}}$ parmi tous les $\mathbf{y} \in \mathbf{x}_0 + \sum\limits_{k<i} \operatorname{span}(\mathbf{P}_k)$.

Les propriétés qui définissent les coefficients dans MPbiCG sont :

- bi-orthogonalité des directions de recherche ($\hat{\mathbf{P}}_i^\top\mathbf{Q}_j = \mathbf{0}$ si $i \neq j$),
- $\hat{\mathbf{r}}_i^\top\mathbf{P}_j = \mathbf{0}$ et $\mathbf{r}_i{}^\top\hat{\mathbf{P}}_j = \mathbf{0}$ si $j < i$. Ceci n'est pas une propriété de minimisation.

Le multipréconditionnement est particulièrement intéressant dans le cas des méthodes de décomposition de domaine où le préconditionneur usuel possède une structure additive. Il revient alors à améliorer la combinaison des termes du préconditionneur classique, ce qui peut éviter de propager des contributions locales problématiques pour la convergence [4]. Dans le cadre symétrique défini positif, une alternative pour se prémunir contre ces mauvaises contributions est de les détecter préalablement à l'aide de problèmes aux valeurs propres généralisés et de les éliminer par un solveur de Krylov augmenté [10]. C'est une force du multipréconditionnement de se déployer simplement sur des cas plus généraux.

Nous appliquons ces algorithmes à des systèmes linéaires issus de la méthode de décomposition de domaine FETI [3]. Le cas test utilisé est une plaque lamifiée, composée alternativement de plis à comportements élastiques et élastoviscoplastiques non associés [1] (Fig. 1). Les algorithmes multipréconditionnés sont moins sensibles à l'hétérogénéité des matériaux. Ils convergent avec un faible nombre d'itérations, bien que le manque de stabilité de MPbiCG soit observé pour $E_2/E_1 \geqslant 10^4$, et qu'une orthogonalisation de Gram–Schmidt modifiée avec réorthogonalisation soit nécessaire pour MPorthomin (Fig. 2).

1. Introduction

The objective of this note is to present for the first time two algorithms for solving nonsymmetric linear systems. They belong to the family of multipreconditioned Krylov subspace solvers of which MPCG (multipreconditioned CG) [2], SFETI (Simultaneous FETI) [6] and MPGMRES (multipreconditioned GMRES) [5] are the first. Since we consider nonsymmetric problems, MPCG is out of the question. MPGMRES, in its original form, leads to an exponential increase in the size of the minimization space. Although it is pointed out in [5] that this can be decreased to a linear growth by selecting some vectors, we propose to look at methods where this is naturally the case. Indeed, one significant difference between GMRES and both biCG and orthomin is that in the last two methods the residual is readily available at each iteration and the preconditioner (or set of preconditioners) is applied to it. This explains the linear growth of the size of the minimization space with respect to the number of iterations.

Multipreconditioning makes particular sense in domain decomposition approaches where the usual preconditioners possess an additive structure. In that case, multipreconditioning simply amounts to finding, at each iteration, an improved (or even optimal depending on the solver) combination of the terms of the classical preconditioner. It was explained in [4] that such a procedure prevents the propagation of problematic local contributions which are known to penalize convergence. The alternative to prevent these bad contributions is to pre-detect them thanks to localized generalized eigenvalue computations and to remove them by augmenting the Krylov solver [10]. Unfortunately, the theory of pre-detection is currently limited to symmetric positive semi-definite problems; it is one strength of multipreconditioning approaches to extend seamlessly to more general cases.

2. Multipreconditioned orthomin and multipreconditioned biCG

We consider the problem of finding $\mathbf{x}_* \in \mathbb{R}^n$ such that $\mathbf{A}\mathbf{x}_* = \mathbf{b}$ where $\mathbf{A}$ is a nonsingular $n \times n$ matrix and $\mathbf{b}$ is a given right hand side. A family of N preconditioners (also nonsingular $n \times n$ matrices) denoted by $\{\mathbf{H}^s\}_{s=1,\ldots,N}$ is used. The multipreconditioned orthomin (MPorthomin) and multipreconditioned biCG (MPbiCG) algorithms are presented in Algorithms 1 and 2 respectively.

Algorithm 1: Multipreconditioned orthomin (MPorthomin).

```
$\mathbf{x}_0$ given ;                                                          // Initial Guess
$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$;
$\mathbf{Z}_0 = \left[\mathbf{H}^1\mathbf{r}_0 \,|\, \ldots \,|\, \mathbf{H}^N\mathbf{r}_0\right]$;   $\mathbf{P}_0 = \mathbf{Z}_0$;      // Initial search directions
$\mathbf{Q}_0 = \mathbf{A}\mathbf{P}_0$;
for $i = 0, 1, \ldots,$ convergence do
    $\boldsymbol{\alpha}_i = (\mathbf{Q}_i^\top \mathbf{Q}_i)^{-1} (\mathbf{Q}_i{}^\top \mathbf{r}_i)$;
    $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i\boldsymbol{\alpha}_i$;                          // Update approximate solution
    $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i\boldsymbol{\alpha}_i$;                          // Update residual
    $\mathbf{Z}_{i+1} = \left[\mathbf{H}^1\mathbf{r}_{i+1} \,|\, \ldots \,|\, \mathbf{H}^N\mathbf{r}_{i+1}\right]$;                // Multi Precondition
    $\boldsymbol{\beta}_{i,j} = (\mathbf{Q}_j^\top \mathbf{Q}_j)^{-1} (\mathbf{Q}_j^\top (\mathbf{A}\mathbf{Z}_{i+1}))$,   $j = 0, \ldots, i$;
    $\mathbf{P}_{i+1} = \mathbf{Z}_{i+1} - \sum_{j=0}^{i} \mathbf{P}_j\boldsymbol{\beta}_{i,j}$;                 // Orthogonalize
    $\mathbf{Q}_{i+1} = (\mathbf{A}\mathbf{Z}_{i+1}) - \sum_{j=0}^{i} \mathbf{Q}_j\boldsymbol{\beta}_{i,j}$;
end
Return $\mathbf{x}_{i+1}$;
```

Algorithm 2: Multipreconditioned biconjugate gradient algorithm (MPbiCG).

```
$\mathbf{x}_0$ given ;                                                          // Initial Guess
$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ and $\hat{\mathbf{r}}_0 = \mathbf{r}_0$;
$\mathbf{Z}_0 = \left[\mathbf{H}^1\mathbf{r}_0 \,|\, \ldots \,|\, \mathbf{H}^N\mathbf{r}_0\right]$;   $\mathbf{P}_0 = \mathbf{Z}_0$;      // Initial search directions
$\hat{\mathbf{Z}}_0 = \left[\mathbf{H}^{1\top}\hat{\mathbf{r}}_0 \,|\, \ldots \,|\, \mathbf{H}^{N\top}\hat{\mathbf{r}}_0\right]$;   $\hat{\mathbf{P}}_0 = \hat{\mathbf{Z}}_0$;      // Initial conjugate search directions
for $i = 0, 1, \ldots,$ convergence do
    $\mathbf{Q}_i = \mathbf{A}\mathbf{P}_i$ and $\hat{\mathbf{Q}}_i = \mathbf{A}^\top\hat{\mathbf{P}}_i$    ;
    $\boldsymbol{\alpha}_i = (\hat{\mathbf{P}}_i^\top \mathbf{Q}_i)^{-1} (\hat{\mathbf{P}}_i^\top \mathbf{r}_i)$ and $\hat{\boldsymbol{\alpha}}_i = (\mathbf{P}_i{}^\top \hat{\mathbf{Q}}_i)^{-1} (\mathbf{P}_i{}^\top \hat{\mathbf{r}}_i)$;
    $\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{P}_i\boldsymbol{\alpha}_i$;                          // Update approximate solution
    $\mathbf{r}_{i+1} = \mathbf{r}_i - \mathbf{Q}_i\boldsymbol{\alpha}_i$ and $\hat{\mathbf{r}}_{i+1} = \hat{\mathbf{r}}_i - \hat{\mathbf{Q}}_i\hat{\boldsymbol{\alpha}}_i$ ;     // Update residual
    $\mathbf{Z}_{i+1} = \left[\mathbf{H}^1\mathbf{r}_{i+1} \,|\, \ldots \,|\, \mathbf{H}^N\mathbf{r}_{i+1}\right]$ and $\hat{\mathbf{Z}}_{i+1} = \left[\mathbf{H}^{1\top}\hat{\mathbf{r}}_{i+1} \,|\, \ldots \,|\, \mathbf{H}^{N\top}\hat{\mathbf{r}}_{i+1}\right]$;   // Multi Precondition
    $\boldsymbol{\beta}_{i,j} = (\hat{\mathbf{P}}_j^\top \mathbf{Q}_j)^{-1} (\hat{\mathbf{Q}}_j^\top \mathbf{Z}_{i+1})$ and $\hat{\boldsymbol{\beta}}_{i,j} = (\hat{\mathbf{P}}_j^\top \mathbf{Q}_j)^{-T} (\mathbf{Q}_j{}^\top \hat{\mathbf{Z}}_{i+1})$ for $j = 0, \ldots, i$;
    $\mathbf{P}_{i+1} = \mathbf{Z}_{i+1} - \sum_{j=0}^{i} \mathbf{P}_j\boldsymbol{\beta}_{i,j}$ and $\hat{\mathbf{P}}_{i+1} = \hat{\mathbf{Z}}_{i+1} - \sum_{j=0}^{i} \hat{\mathbf{P}}_j\hat{\boldsymbol{\beta}}_{i,j}$;   // Orthogonalize
end
Return $\mathbf{x}_{i+1}$;
```

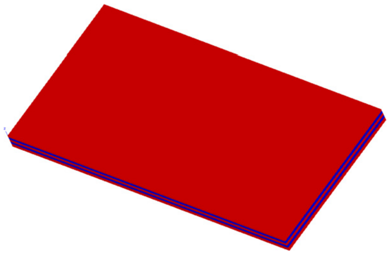
The two properties that define the coefficients in MPorthomin are:

- the $(\mathbf{A}^\top\mathbf{A})$-conjugacy of the search directions (*i.e.*, $\mathbf{Q}_i^\top\mathbf{Q}_j = \mathbf{0}$ for any $j \neq i$).
- the minimization property that $\mathbf{x}_i$ minimizes the $\mathbf{A}^\top\mathbf{A}$-norm of the error $\|\mathbf{x}_* - \mathbf{y}\|_{\mathbf{A}^\top\mathbf{A}}$ over all $\mathbf{y} \in \mathbf{x}_0 + \sum\limits_{k<i} \operatorname{span}(\mathbf{P}_k)$ (*i.e.*, $\mathbf{r}_i^\top\mathbf{Q}_j = 0$ for any $j < i$).

The properties that define the coefficients in MPbiCG are:

- the biconjugacy of search directions (*i.e.*, $\hat{\mathbf{P}}_i^\top\mathbf{Q}_j = \mathbf{0}$ if $i \neq j$),
- $\hat{\mathbf{r}}_i^\top\mathbf{P}_j = \mathbf{0}$ and $\mathbf{r}_i{}^\top\hat{\mathbf{P}}_j = \mathbf{0}$ if $j < i$. Note that this is not a minimization property: with MPbiCG, as with biCG, there is no error norm that is guaranteed to decrease at every iteration.

MPbiCG is expected to inherit the lack of stability of biCG (an issue addressed in biCGstab of which we did not manage to derive a multipreconditioned version), but there exist many configurations were it remains competitive in spite of the need to store twice as many vectors at each iteration. We encountered unexpected poor conditioning of the orthogonalization step of MPorthomin; as a first answer we used a modified Gram–Schmidt method with reorthogonalization which allowed to achieve convergence, at the cost however of more operations and communications per iteration. We also note that the preconditioning step in MPorthomin could have been $\mathbf{Z}_{i+1} = \left[\mathbf{H}^1(\mathbf{Q}_i\boldsymbol{\alpha}_i) \,|\, \ldots \,|\, \mathbf{H}^N(\mathbf{Q}_i\boldsymbol{\alpha}_i)\right]$ leading to an MPorthodir algorithm.



(a) Soft material is in red, stiff material in blue

Soft material

E_1	100	ν	0.3

Stiff material

E_2	ν	K	m	C	D	a
variable	0.3	400	7	6000	100	0.3

(b) Material parameters

Fig. 1. Heterogeneous composite.

3. Numerical results: application to the FETI method

The algorithms presented in the previous sections have been applied to the FETI method [3]. FETI is a domain decomposition-based iterative method: the domain is split into reasonably small subdomains where local solves are performed using direct solvers, and an iterative solver is used to find the Lagrange multipliers that glue all the subdomains together. FETI with multipreconditioned CG was studied in [4] where a trick was proposed to limit extra computations caused by the presence of the coarse problem which globally balances floating subdomains.

The methods have been implemented in the Finite element suite ZSet 8.6 (http://www.zset-software.com). The test case aims at representing a laminated material (a soft material reinforced by a stiffer one): a five-layer plate occupies the domain $\Omega = [0,10] \times [0,5] \times [0,0.5]$. It is clamped on the $x = 0$ side and a displacement is imposed on the opposite side. Stiff layers are made of a nonassociated elastoviscoplastic material (which causes the nonsymmetry of the tangent systems). Soft layers follow a classical linear elastic constitutive law. Small displacements are assumed. The prescribed displacement linearly grows with time, the computation ends at $t = 0.05$. A Newton scheme with a constant time step 0.01 is used. It is small enough for all Newton steps to converge in 1 iteration. The mechanical problem is:

$$\begin{cases} \operatorname{div}(\sigma(\boldsymbol{u})) = \boldsymbol{0} \text{ in } \Omega & \boldsymbol{u} = \dfrac{xt}{10000}\,\boldsymbol{e}_x \text{ for } x \in \{0,10\} \\ \text{constitutive law} & \sigma(\boldsymbol{u}) \cdot \boldsymbol{n} = 0 \text{ on } \partial\Omega \text{ with } x \notin \{0,10\} \end{cases} \tag{1}$$

The soft material follows an isotropic linear elastic constitutive rule characterized by the Young's modulus E and the Poisson's coefficient ν given in Fig. 1b. The nonassociated elastoviscoplastic constitutive law combines a nonsymmetric yield criterion, a Norton flow rule and a Ziegler kinematic hardening [1]. It is defined by (2), where ε^{vp} is the viscoplastic strain tensor, X is the hardening variable, $\dot{p}$ is the viscoplastic multiplier. J, J_2, I_2 are tensor invariants and σ_D is the deviatoric part of σ. All material parameters are given in Fig. 1b. In order to assess the robustness of the solvers, we make the ratio of the Young's moduli vary between 1 and 10^5. Since a prescribed displacement is applied, the increase of the heterogeneity ratio produces more (incompressible) viscoplastic flow inside the stiff layers, which contributes to the bad condition number of the tangent systems.

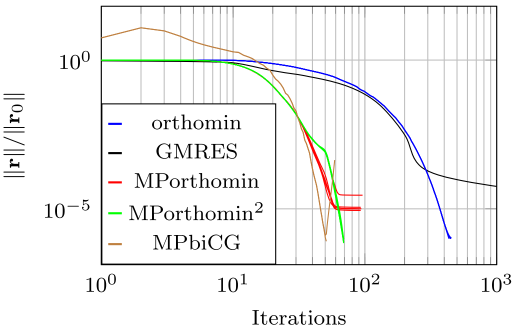
$$\begin{cases} \sigma(\boldsymbol{u}) = \dfrac{E}{1+\nu}(\varepsilon(\boldsymbol{u}) - \varepsilon^{vp}) + \dfrac{\nu E}{(1+\nu)(1-2\nu)}\operatorname{Tr}(\varepsilon(\boldsymbol{u}) - \varepsilon^{vp})I \text{ with } \varepsilon(\boldsymbol{u}) = \dfrac{1}{2}\left(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^{\top}\right) \\ \dot{\varepsilon}^{vp} = \dfrac{3}{2}\dfrac{\sigma_D - X}{J_2(\sigma - X)}\dot{p} \text{ with } \dot{p} = \left(\dfrac{\langle f \rangle}{K}\right)^m \text{ and } f = (1-a)J(\sigma - X) + aTr(\sigma) \\ X = \dfrac{2}{3}C\alpha \text{ and } \dot{\alpha} = \dot{p}\left\{\dfrac{\sigma - X}{I_2(\sigma - X)} - \dfrac{D}{C}X\right\} \end{cases} \tag{2}$$

The problem is discretized into $150 \times 75 \times 15$ regular twenty-node brick elements (c3d20), the problem size is 2,158,068 degrees of freedom (*dofs*). The mesh is split into 64 domains using the Metis automatic graph partitioner. Subdomains are composed on average of 38,000 *dofs* and 2,600 elements. A 10^{-6} relative convergence threshold is used on the Euclidean norm of the residual. All computations use a Dirichlet preconditioner with a k-scaling and symmetric coarse grid projector.

Fig. 2 summarizes all the results. We compare classical GMRES and orthomin with our new algorithms. MPorthomin^2 stands for MPorthomin with a modified Gram–Schmidt with reorthogonalization (see [7] p. 162). In terms of Krylov iterations, all multipreconditioned algorithms are less sensitive to the increase in the heterogeneity. The lack of stability of MPbiCG is however observed for $h \geqslant 10^4$. The poor conditioning of the Orthomin orthogonalization step is visible for $h = 10^4$. Thanks to the reorthogonalization, MPorthomin^2 achieves convergence even for $h = 10^5$. When they converge, GMRES and orthomin remain faster than the multipreconditioned algorithms. This indicates that the best algorithm should mix multipreconditioned iterations (that help with robustness) and usual preconditioned iterations (that are less expensive).

	Total # Krylov iter.					Time to solution (s)				
$h = E_2/E_1$	10^1	10^2	10^3	10^4	10^5	10^1	10^2	10^3	10^4	10^5
GMRES	315	445	825	–	–	165	198	295	–	–
orthomin	305	445	830	2231	–	153	185	265	621	–
MPbiCG	130	185	235	–	–	374	524	684	–	–
MPomin	125	185	240	472	–	221	303	386	870	–
MPomin^2	125	185	240	345	534	251	360	488	803	1565

(a) Performance for various heterogeneity ratios. A dash means that the solver did not converge.



(b) Evolution of the residual for $h = 10^4$. All Newton steps are superposed.

Fig. 2. Heterogeneous composite. MPomin^2 uses a modified Gram–Schmidt orthogonalization with reorthogonalization.

4. Conclusion

We have presented two new multipreconditioned algorithms for possibly nonsymmetric linear systems that rely on the same ideas as the existing ones, and whose complexity only grows linearly with respect to the iteration number. We assessed them in combination with the FETI domain decomposition method on non-associated viscoplasticity problems. The next step is to derive adaptive variants such as [8,9] (developed for MPCG), in order to achieve the best compromise between robustness and efficiency.

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