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Influence of iterated Gram–Schmidt orthonormalization in the asymptotic numerical method

Rédouane Jamai, Noureddine Damil

Laboratoire de calcul scientifique en mécanique, faculté des sciences Ben M'Sik, av. Cdt Driss El Harti, BP 7955, Casablanca, Morocco

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Abstract

In this paper we discuss the influence of Gram–Schmidt orthonormalization for the computation of the rational representation in the asymptotic numerical method. Classical, modified and iterated Gram–Schmidt algorithms are compared using the ordinary and the mass scalar products. The accuracy of the proposed algorithms are tested on elastic shells. ***To cite this article: R. Jamai, N. Damil, C. R. Mecanique 331 (2003).***

Résumé

Influence de l'orthonormalisation itérative de Gram–Schmidt dans la méthode asymptotique numérique. Dans ce travail, on discute l'influence de l'orthonormalisation de Gram–Schmidt sur le calcul de la représentation rationnelle dans la méthode asymptotique numérique. Les algorithmes classique, modifié et itératif de Gram–Schmidt sont comparés en utilisant les produits scalaires ordinaire et masse. Les précisions des algorithmes proposés sont illustrées sur des exemples de coques élastiques. ***Pour citer cet article : R. Jamai, N. Damil, C. R. Mecanique 331 (2003).***

Keywords: Solids and structures; Asymptotic numerical method; Finite element; Nonlinear elasticity; Padé approximant; Gram–Schmidt orthonormalization

Mots-clés : Solides et structures ; Méthode asymptotique numérique ; Élément fini ; Élasticité non-linéaire ; Approximant de Padé ; Orthonormalisation de Gram–Schmidt

1. Introduction

Within the asymptotic numerical method (ANM), the basic idea is to search a parametric representation of the solution path $\mathbf{U}$ of a nonlinear problem in the form of integro-power series [1]. For instance, the unknown is represented as follows:

$$\mathbf{U}(a) = \mathbf{U}_0 + a\mathbf{U}_1 + a^2\mathbf{U}_2 + \cdots + a^p\mathbf{U}_p \tag{1}$$

E-mail address: n.damil@univh2m.ac.ma (N. Damil).

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where p is the order of truncature. The vectors fields $(\mathbf{U}_i)_{1\leqslant i\leqslant p}$ are the solutions of a recurrent sequence of linear problems, with a single tangent operator to be inverted. These linear problems are solved by the finite element method. Of course the domain of validity of the representation (1) is limited by the radius of convergence of the series. In order to extend the domain of validity of the representation (1), we have used in [1] and [2] a rational representation called Padé approximant [3].

As the representation (1) is not a scalar series, we have first, used the Gram–Schmidt procedure, which is the most known method in linear algebra, to compute an orthonormal basis $\mathbf{U}_1^*, \ldots, \mathbf{U}_p^*$ for the space spanned by the vectors $\mathbf{U}_1, \ldots, \mathbf{U}_p$ in the following manner:

$$\begin{aligned}
&\alpha_{1,1}\mathbf{U}_1^* = \mathbf{U}_1 \\
&\alpha_{i,i}\mathbf{U}_i^* = \mathbf{U}_i - \sum_{j=1}^{i-1} \alpha_{i,j}\mathbf{U}_j^* \\
&\left\langle \mathbf{U}_i^*, \mathbf{U}_j^* \right\rangle = \delta_{i,j} \quad (i, j = 1, \ldots, p)
\end{aligned} \tag{2}$$

The coefficients $\alpha_{i,j}$ of the Gram–Schmidt procedure are then used to compute a set of $p-1$ coefficients $d_1, d_2, \ldots, d_{p-1}$ and $p-1$ polynomials D_i defined by:

$$d_i = -\frac{1}{\alpha_{p-i,p-i}}\left(\alpha_{p,p-i} + \sum_{k=1}^{i-1} d_k \alpha_{p-k,p-i}\right) \tag{3}$$

$$D_i(a) = 1 + d_1 a + d_2 a^2 + \cdots + d_i a^i \tag{4}$$

After some rearrangement, we obtain the following rational representation [2] of the solution:

$$\mathbf{U}(a) = \mathbf{U}_0 + a\frac{D_{p-2}(a)}{D_{p-1}(a)}\mathbf{U}_1 + \cdots + a^{p-2}\frac{D_1(a)}{D_{p-1}(a)}\mathbf{U}_{p-2} + a^{p-1}\frac{1}{D_{p-1}(a)}\mathbf{U}_{p-1} \tag{5}$$

In the ANM, we must be able to compute accurately the coefficients $\alpha_{i,j}$. Let's recall that a process of orthonormalization is a numerical instability source [4]. These instabilities observed in the ANM for the calculation of $\alpha_{i,j}$ change all the coefficients d_i. This point have been discussed in [2] and [5] in the case of an elastic beam subjected to a bending force. The comparison between the exact coefficients of Gram–Schmidt procedure using a symbolic software (MAPLE) and those obtained by finite elements shows that numerical errors are accumulated and that the new vectors $\mathbf{U}_i^*$ are completely false beyond a certain order. Results in [5] clearly show the influence of the orthonormalization without establishing if instabilities are due to the orthonormalization or something else as the calculation of the vectors themselves. One can also note that these instabilities don't prevent a better solution quality than the series nor a good evalutation of the smallest pole, that is assimilated to the radius of convergence [6]. But one has also observed, especially in iterative algorithm, that the curves residual-order had a bizarre behavior at large orders, that let suppose a harmful numerical instability effect. What practical drawbacks do these instabilities drag? Is one able to reduce them while only changing the technique of orthonormalization or the scalar product? Does that improve the ANM?

In this paper, we show that the numerical stability of Gram–Schmidt procedures can be vastly improved by applying the procedure iteratively. This so-called iterated Gram–Schmidt procedure has been used in [7]. In a recent paper [4], LINGEN shows how this algorithm can be implemented on a parallel computer. In this paper we will compare the numerical accuracy and stability of the three versions of Gram–Schmidt algorithm in the ANM. Two examples of cylindrical shells will be used to show that the ANM using iterated Gram–Schmidt orthonormalization leads to a stable algorithm with respect to the scalar product contrary to modified Gram–Schmidt algorithms.

Table 1
The classical (CGS), modified (MGS) and iterated (IGS) Gram–Schmidt algorithms

Tableau 1
Algorithmes classique (CGS), modifié (MGS) et itératif de Gram–Schmidt

CGS	MGS	IGS

for $i = 1, \ldots, p$ do
for $j = 1, \ldots, i-1$
$\alpha_{i,j} = \langle \mathbf{U}_i, \mathbf{U}_j^* \rangle$
enddo
$\mathbf{q}_i = \mathbf{U}_i - \sum_{j=1}^{i-1} \alpha_{i,j} \mathbf{U}_j^*$
$\mathbf{U}_i^* = \mathbf{q}_i / \Vert \mathbf{q}_i \Vert$
enddo
	for $i = 1, \ldots, p$ do
	$\mathbf{q}_i = \mathbf{U}_i$
	for $j = 1, \ldots, i-1$
	$\alpha_{i,j} = \langle \mathbf{q}_i, \mathbf{U}_j^* \rangle$
	$\mathbf{q}_i = \mathbf{q}_i - \alpha_{i,j} \mathbf{U}_j^*$
	enddo
	$\mathbf{U}_i^* = \mathbf{q}_i / \Vert \mathbf{q}_i \Vert$
	enddo
		for $i = 1, \ldots, p$ do
		$\mathbf{U}_i^{*0} = \mathbf{U}_i, \alpha_{i,j}^0 = 0$
		for $k = 1, 2, \ldots$ do
		for $j = 1, \ldots, i-1$ do
		$\gamma_{i,j}^k = \langle \mathbf{U}_i^{*k-1}, \mathbf{U}_j^* \rangle$
		$\alpha_{i,j}^k = \alpha_{i,j}^{k-1} + \gamma_{i,j}^k$
		enddo
		$\mathbf{U}_i^{*k} = \mathbf{U}_i^{*k-1} - \sum_{j=1}^{i-1} \gamma_{i,j}^k \mathbf{U}_j^*$
		if ($\Vert \mathbf{U}_i^{*k} \Vert > \beta \Vert \mathbf{U}_i^{*k-1} \Vert$) then
		stop
		endif
		enddo
		$\mathbf{U}_i^* = \mathbf{U}_i^{*k} / \Vert \mathbf{U}_i^{*k} \Vert$
		for $j = 1, \ldots, i-1$ do
		$\alpha_{i,j} = \alpha_{i,j}{}^k$
		enddo
		enddo

2. Gram–Schmidt orthonormalization procedures

The classical Gram–Schmidt algorithm (CGS) is summarized in the first row of the Table 1. We have observed in many tests that using this algorithm, the new vectors $\mathbf{U}_i^*$ are completely false beyond a small order [2]. It is known that the modified Gram–Schmidt algorithm (MGS), which is summarized in the second row of the Table 1, has a better stability.

The accuracy of classical Gram–Schmidt algorithm can be vastly improved by applying it iteratively [4,7]. This algorithm (IGS), which is an iterative version of the classical one, is presented in the third row of the Table 1. Let us notice that with one iteration of IGS, for each vector, we get back the CGS algorithm. The most important part of the algorithm is the stopping criterion $\Vert \mathbf{U}_i^{*k} \Vert > \beta \Vert \mathbf{U}_i^{*k-1} \Vert$ which depends on an arbitrary parameter β. In [7] it has been shown that the IGS algorithm converges within two iterations with $\beta \approx 0.5$. Let us note that the CPU time of two iterations is negligible compared to the CPU time to get one vector of the series (1) and that the vectors and coefficients generated by Gram–Schmidt procedure depends on the choice of the scalar product.

3. Comparison of the three Gram–Schmidt orthonormalizations

To compare the three Gram–Schmidt orthonormalizations, we test two nonlinear elastic problems. These problems depend on a load parameter λ. In the ANM, we replace also this parameter λ by a rational representation analogous to (5) (see [1,2]).

The first example is a cylindrical roof hinged along two opposite sides submitted to a concentrated force at the central point (Fig. 1(a)). Assuming symmetry conditions, only one quarter of the shell is discretized with 200 triangular DKT18 elements for a total number of degrees of freedom 726. The analysis is carried out with two differents values of the thickness: $h_1 = 12.7$ mm, $h_2 = 6.35$ mm. The second example is a cylinder with two diametrically opposite cut out loaded by a uniform compression (Fig. 1(b)). For symmetry reasons, one eight of

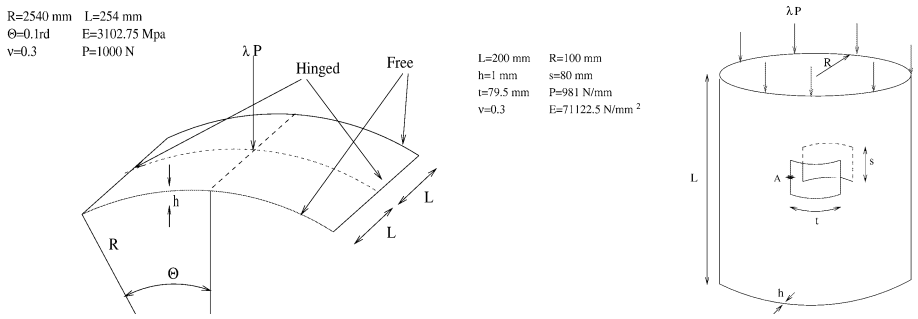


Fig. 1. (a) Cylindrical roof loaded in its center, (b) cut out cylinder with a compressive load.

Fig. 1. (a) Toit cylindrique chargé au centre, (b) cylindre troué avec un chargement en compression.

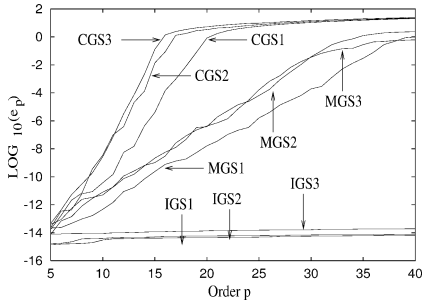


Fig. 2. Precision e_p versus the order p.

Fig. 2. Précision e_p en fonction de l'ordre p.

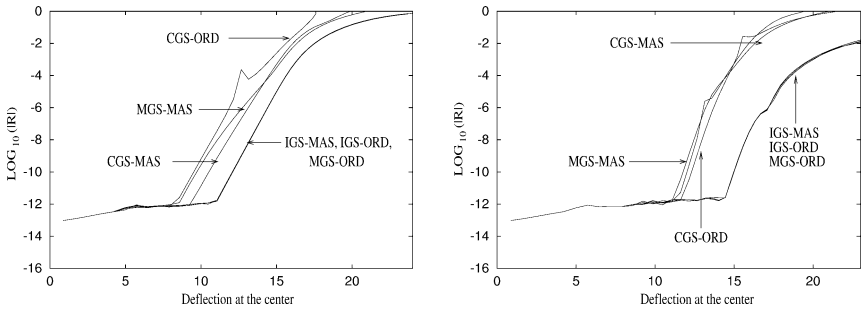
the structure is discretized with 1608 triangular DKT18 elements. The total number of degrees of freedom is 5190. In all this section, we choose $\beta = 0.5$ for the iterated Gram–Schmidt (IGS) algorithm.

To analyse the quality of the Gram–Schmidt algorithms (CGS, MGS and IGS), we consider the criterion e_p defined by:

$$e_p = \left\| \mathbf{Q}_p^{\mathrm{T}} \mathbf{Q}_p - \mathbf{I}_p \right\|_F \tag{6}$$

where the matrix $\mathbf{Q}_p$ is $(\mathbf{U}_1^*, \ldots, \mathbf{U}_{p-1}^*)$, $\mathbf{I}_p$ is the identity matrix and the matrix $[\alpha]$ is a lower triangular one defined by the Gram–Schmidt coefficients $[\alpha] = [\alpha_{i,j}]_{1 \leqslant i,j \leqslant p}$. The notation $\| \cdot \|_F$ is the Frobenius norm which is defined for a matrix $A = [a_{i,j}]$ as $\|A\|_F = \sqrt{\sum_{i,j} a_{i,j}^2}$. The scalar product used, for the three Gram–Schmidt algorithms, is the ordinary scalar product defined by $\langle \mathbf{U}, \mathbf{V} \rangle_{\mathrm{ORD}} = \sum_{k=1}^{N} U_k V_k$ where $\mathbf{U} = (\mathbf{U}_k)_{k=1}^N$ and $\mathbf{V} = (\mathbf{V}_k)_{k=1}^N$. Let us recall that we must have theoretically $(\langle \mathbf{U}_i^*, \mathbf{U}_j^* \rangle)_{1 \leqslant i,j \leqslant p} = \mathbf{I}_p$ and $(\langle \mathbf{U}_i, \mathbf{U}_j \rangle)_{1 \leqslant i,j \leqslant p} = [\alpha][\alpha]^{\mathrm{T}}$. Therefore the precision e_p analyses the quality of the orthogonality of the basis.

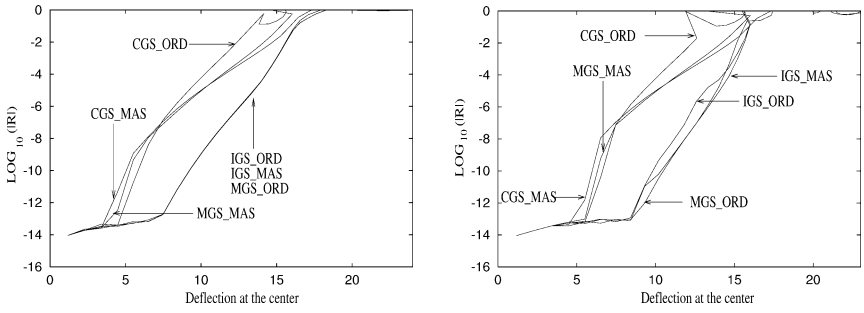
In Fig. 2, we represent the decimal logarithm of the precision e_p versus the order of truncature p. The curves (CGS1, MGS1, IGS1) and (CGS2, MGS2, IGS2) correspond to the cylindrical roof respectively with thickness $h_1 = 12.7$ and $h_2 = 6.35$ and (CGS3, MGS3, IGS3) correspond to the cut out cylinder. In Fig. 2, one can clearly see that the better accuracy is obtained using the IGS algorithm and that the CGS algorithm is the least accurate. The behavior of the curves IGS is stable ($e_p \simeq 10^{-15}$ for IGS1, IGS2 and $e_p \simeq 10^{-14}$ for IGS3) until the order $p = 40$ while the CGS and MGS algorithms loose the precision ($e_p = 10^{-4}$) from respectively the order $p \simeq 14$ for CGS2 and CGS3, $p \simeq 16$ for CGS1, $p \simeq 25$ for CGS2 and CGS3, $p \simeq 30$ for MGS1.



(a) (b)

Fig. 3. Residual curve for the cylindrical roof with $h_1 = 12.7$: (a) order $p = 30$, (b) order $p = 60$.

Fig. 3. Courbe résidu pour le toit cylindrique avec $h_1 = 12.7$: (a) ordre $p = 30$, (b) ordre $p = 60$.



(a) (b)

Fig. 4. Residual curve for the cylindrical roof with $h_2 = 6.35$: (a) order $p = 30$, (b) order $p = 60$.

Fig. 4. Courbe résidu pour le toit cylindrique avec $h_2 = 6.35$: (a) ordre $p = 30$, (b) ordre $p = 60$.

Let us analyse the decimal logarithm of the residual of the rational representation (5). We used for this analysis two sorts of scalar product: the ordinary scalar product (noted $\langle \cdot, \cdot \rangle_{\mathrm{ORD}}$) and the mass scalar product defined by $\langle \mathbf{U}, \mathbf{V} \rangle_{\mathrm{MAS}} = \mathbf{U}^{\mathrm{T}}\mathbf{M}\mathbf{V}$ where $\mathbf{M}$ is the mass matrix. We compare the rational representation (5) for the example of the cylindrical roof with a thickness $h_1 = 12.7$ (Fig. 3) and for the example of the cylindrical roof with a thickness $h_2 = 6.35$ (Fig. 4). The Figs. 3 and 4 give the influence of the choice of scalar product (ORD for ordinary scalar product and MAS for mass scalar product) and the choice of the orthonormalization algorithm (CGS, MGS, IGS). In Figs. 3 and 4 one can see that if we use the IGS algorithm, we obtain the same results for the two scalar products. For the CGS algorithm, we obtain with the two scalar products the same results that are less accurate. The results obtained by using the MGS algorithms (usually used in the ANM) depend on the choice of the scalar product as can be seen in Figs. 3 and 4. The MGS algorithm using the ordinary scalar product give the same results as the IGS algorithm and the MGS algorithm using the mass scalar product give the same results as the CGS algorithm.

We have tested the Gram–Schmidt algorithms in ANM continuation [6], in the case of the cylindrical roof with $h_1 = 12.7$, by using the ordinary scalar product (Fig. 5(a)) and the mass scalar product (Fig. 5(b)). One can see from these figures that using the ordinary scalar product, two ANM steps coupled with IGS are slightly better than two ANM steps coupled with MGS and using the mass scalar product two ANM steps coupled with IGS are slightly lower than three ANM steps coupled with MGS.

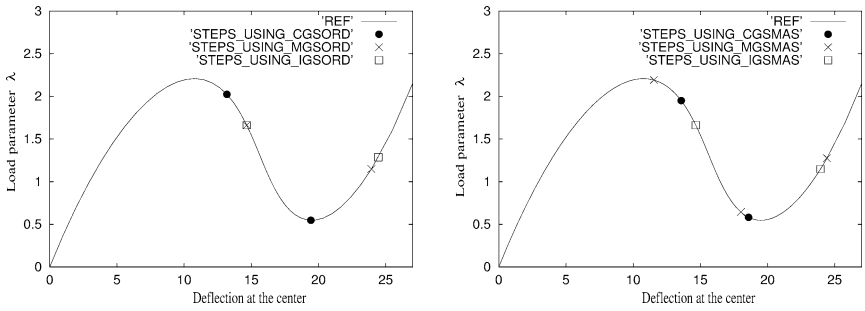


Fig. 5. Load-displacement curves for the cylindrical roof with $h_1 = 12.7$ at the order $p = 28$.

Fig. 5. Courbes charge-déplacement pour le toit cylindrique avec $h_1 = 12.7$ à l'ordre $p = 28$.

4. Conclusion

In this Note, we have compared the classical, modified and iterated Gram–Schmidt orthonormalization by using the ordinary and mass scalar product. The domain of validity obtained using the iterated and modified algorithm is much larger than the domain of validity obtained when we use the classical Gram–Schmidt algorithm. The better results are always obtained by the IGS algorithm and, morever, the efficiency of the IGS algorithm does not depend on the scalar product. That is why it is recommanded to apply the orthogonalization iteratively.

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