55

Reuse of Krylov Spaces in the Solution of Large-scale Nonlinear Elasticity Problems

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1 Introduction

We present the Generalized Krylov Correction, an acceleration technique for the solution to a series of symmetric linear problems with several right-hand sides and matrices, and with its efficiency on an industrial three-dimensional nonlinear elasticity problem. Such a technique is based upon the reuse of Krylov spaces.

Nonlinear elasticity problems are a category of problems often encountered in the field of solid and structural mechanics. The techniques the most generally used for their solution are Newton-type methods [Kel83]. These mainly consist in the construction of a series of linear problems, the solutions of which converge towards the solution to the considered problem. Note that the parent matrices of those linear problems are symmetric positive definite for the type of mechanical problems we consider [Rey94]. The use of non-overlapping domain decomposition methods (primal [LeT94] or dual [FR94] approach) coupled with a conjugate gradient algorithm provides a particularly well-adapted solution for parallel computation for the solution to those symmetric linear problems. However, the numerical efficiency of the conjugate gradient algorithm depends upon the construction of Krylov spaces of the solution to the associated problems. In order to significantly speed up the resolutions of the succession of symmetric linear problems, we developed a technique, well-adapted to an implementation on parallel computers, known as the Generalized Krylov Correction [RDL95] [Rey96]. This method relies upon an efficient utilisation of descent directions calculated in the course of the resolution of previous systems so as to correct the new descent directions. Besides, it can be interpreted as a generalization of the iterative solution of symmetric systems with multiple right-hand sides but with an invariant matrix previously addressed in [Par80], [Saa93] and [FCR94]. This technique is tested on an industrial three-dimensional example (see Fig. 1), a steel-elastomer structure.

Such structures are increasingly used and developed in industry to produce efficient elastic supports. But their numerical computation using the finite element method

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implies a number of difficulties linked to the great heterogeneousness of the structure, and to the nonlinear behavior of rubber layers. We demonstrate, using this ill-conditioned three-dimensional example, the efficiency of the Generalized Krylov Correction from a numerical point of view and from the point of view of its implementation on parallel computers. We also outline the validity domain of this correction vis-à-vis the evolution of matrices of the various symmetric linear systems. Then, after briefly recollecting of the solution to nonlinear elasticity problems with a Newton-type method, we describe the Generalized Krylov Correction. In the last section, we study the results obtained for the elastic support.

2 Solution to Nonlinear Elasticity Problems

In order to model bodies made up of compressible or quasi-incompressible hyperelastic materials and undergoing large deformations, we choose the Lagrangian formulation. All variables are thus defined and retained in a reference configuration. The equilibrium equations may be written in a weak form as follows :

$$\text{Find } u \text{ such that } \int_\Omega \frac{\partial \Phi}{\partial F}(u) : \nabla v \, d\Omega = \int_\Omega f.v \, d\Omega + \int_{\partial\Omega} g.v \, d\Gamma \qquad \forall v \tag{2.1}$$

where, $v(x)$, is any admissible displacement field in the reference configuration, $u(x)$, is the displacement field, $f(x)$ and $g(x)$ are the density of body forces and surface tractions respectively, $F(x) = Id + \nabla u(x)$, is the deformation gradient, Φ, is the specific internal elastic energy, and $(:)$, stands for the double-contractor operator.

The problem (2.1) is usually discretized through a finite element method [Cia78] and leads to the solution to a nonlinear problem in the form $G(u) = 0$. Methods classically used for the solution to such problems are Newton-type methods. The simplest method, Newton-Raphson, consists in iteratively replacing in the equation $G(u) = 0$ the function G with its first-order expansion around the point (u). It then iteratively solves the series of linear problems thus obtained.

A first variant of this method (Quasi Newton) consists of reactualizing the linear system matrix only every p nonlinear iterations. However, depending on the stiffness of the problem to be solved, we will use stronger variants, such as that of the Newton Incremental (which consists in incrementing the loading) or even better the so-called bordering algorithm [Kel83]. But whatever the chosen method may be, all the methods come down to the solution to a succession of linear problems, the right-hand sides and matrices of which are to be reactualized.

Refer to Ciarlet [Cia86] for a complete presentation of the formulation of nonlinear elasticity problems and to Keller [Kel83] or Le Tallec [LeT90] for Newton-type nonlinear solvers.

3 Solution to a Succession of Linear Problems

The use of direct solvers for the resolution of such a succession of symmetric linear problems requires huge memory space and is extremely time-consuming when carrying out calculations, particularly for large-scale three-dimensional elasticity problems. Moreover they are not suited for an implementation on parallel computers. This is all the more the case as the matrices of the various problems are to be reactualized.

Domain decomposition methods (primal [LeT94] or dual approach [FR94])), coupled with a conjugate gradient algorithm, make it possible, by condensing problems on the interface of subdomains, to solve the following succession of condensed symmetric linear systems, the parent matrices of which are symmetric, positive definite.

$$C^k \lambda^k = b^k \quad \text{for } k = 1, 2, ..., N \tag{3.2}$$

where C^k is the matrix of Schur complement in dual or primal form according to the approach chosen and b^k the associated condensed right-hand side.

Principle and Initialisation of the Conjugate Gradient

The resolution of the k^{th} of these symmetric linear systems by the algorithm of the conjugate gradient, preconditioned by the matrix M^k generates the following $K(C^k)$ Krylov space, constructed in the course of iterations using descent directions w_i^k [TL87]:

$$K(C^k) = \text{Vect}(w_1^k, ..., w_p^k). \tag{3.3}$$

The λ_p^k p-rank approximation of the solution that minimizes $g = C^k \lambda_p^k - b^k$ residual over the $\{\lambda_0^k\} + K(C^k)$ space (where λ_0^k is a given initial field) for the dot product associated with the C^k matrix is then given by :

$$\lambda_p^k = \lambda_0^k + P(C^k)(b^k - C^k \lambda_0^k) \quad \text{with} \quad P(C^k)(\lambda) = \sum_{i=1}^{p} \frac{(\lambda, w_i^k)}{(C^k w_i^k, w_i^k)} w_i^k \tag{3.4}$$

The approximation may then define a correct initialization for the resolution of a linear system with the same matrix (the initialization is optimal provided that it is used to restart the resolution of the same linear problem). Moreover, these condensed systems are small in comparison to the dimensions of the global problem; we can therefore keep the information obtained following their resolution using the conjugate gradient method; this approach does not however entail high additional costs (in terms of memory capacity). We may therefore use them in order to speed up the resolution of the following systems.

The Generalized Krylov Correction

A good preconditioner of the k^{th} linear system is the matrix M such that $C^k M g = g$. We propose a g^* approximation [Rey96] of the g^{opt} optimal correction term defined

by the relation, $C^k(M^k g + g^{opt}) = g$, being the orthogonal projection (3.4) associated with the C^{k-1} matrix of the g^{app} solution to the system, $C^{k-1}g^{app} = g - C^{k-1}M^k g$, in the $K(C^{k-1})$ p-dimension Krylov space.
According to (3.4), the g^* correction term may be written :

$$g^* = P(C^{k-1})(g - C^{k-1}M^k g) = P(C^{k-1})(g) - \sum_{i=1}^{p} \frac{(M^k g,\, C^{k-1}w_i^{k-1})}{(C^{k-1}w_i^{k-1},\, w_i^{k-1})} w_i^{k-1} \tag{3.5}$$

This expression underlines that the calculation of the correction term does not require the computation of the $C^{k-1}(M^k g)$ matrix-vector product. The calculation time of this correction therefore has a cost comparable to that of a complete reorthogonalization procedure and consequently remains limited.

However, this correction only requires one Krylov space. So as to extend this first Krylov correction to the previous $k-1$ Krylov spaces, we proceed by successive corrections. On each iteration of the conjugate gradient, the correction term is calculated as follows :

Initialization
  State $z = M^k$ g
  For $i = 1$, to $k-1$ do
    Compute the correction $g^* = P(C^i)(g - C^i z)$
    State $z = z + g^*$
  End of Loop
Compute the new descent direction $w = z - \frac{(z, C^k w)}{(C^k w, w)} w$

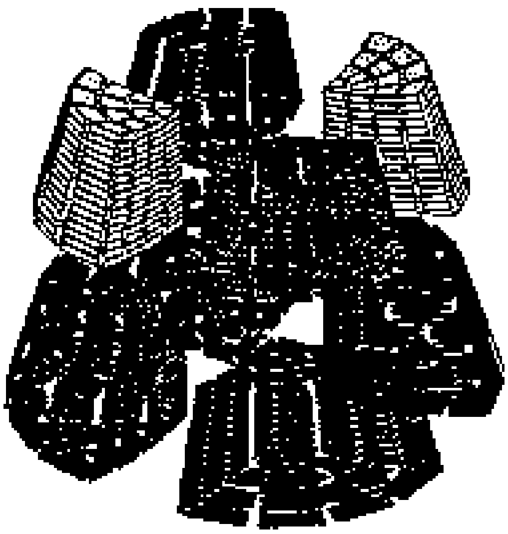
We finally associate to the Krylov correction a complete reorthogonalization procedure [Rou91] of descent directions so as to ensure the correct convergence of the conjugate gradient method.

4 Application

So as to evaluate the efficiency and the validity domain of this technique, we apply it to the resolution of an industrial problem : a steel-elastomer laminated structure (see Fig. 1) subject to an axial compression loading with an imposed displacement. Material behaviors are modelled by the Ciarlet-Geymonat [CG82] specific internal energy Φ. See [Rey94] for a full presentation of the industrial problem.

The problem thus considered is highly nonlinear, and discretized by hexahedral finite elements (Q1 element). The mesh consists of a total of 6435 degrees of freedom and is decomposed into 8 sub-domains (Fig. 1). The domain decomposition method, known as the Dual Schur Complement Method [FR94] coupled with the conjugate gradient algorithm and preconditioned by local rigidity matrices is chosen for the resolution of linear systems. The stopping criterion of this iterative solver is 10^{-3} whereas the stopping criterion of nonlinear iterations (Newton iterations) is 10^{-6}. The difference is justified by the quadratic convergence of the Newton method and by the fact that the solution to linear problems only consists in an intermediate step in the resolution

Figure 1 Decomposition into 8 sub-domains of an elastic support



of the overall problem.

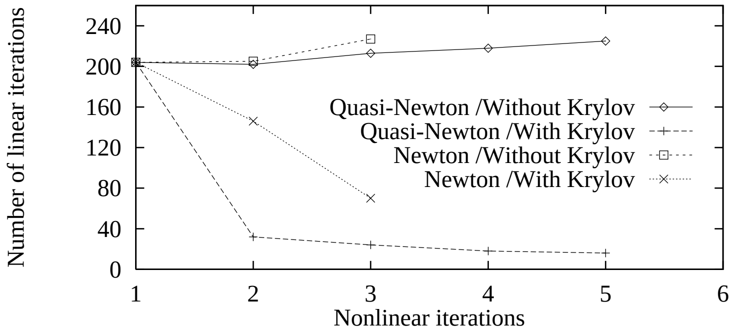
Case where Matrices are not Reactualized

The first case studied is when the nonlinear problem is solved using the Quasi-Newton method without any matrix reactualization. The algorithm then converges in 5 iterations. The number of iterations of the conjugate gradient on each iteration of the Quasi-Newton with or without the addition of the Generalized Krylov correction term (and the initialization introduced in (3.4)) is described in Fig. 2 (Quasi-Newton / Without or With Krylov). It may be observed that introducing the Krylov correction term coupled with the initialization implies a highly significant decrease in the number of iterations. It may thus be observed that this iterative approach corresponds to a semi-direct method which requires only a projection of the solution in Krylov spaces, with a very limited (or even nil) number of the conjugate gradient iterations.

Case of Reactualized Matrices

The nonlinear problem is now solved by the Newton-Raphson method with systematic reactualization of the matrix. The algorithm then converges in 3 iterations. The results obtained with or without the addition of the Generalized Krylov correction term are shown in Fig. 2 (Newton / Without or With Krylov). The decrease in the number of iterations however is smaller than in the previous case but remains significant.

Figure 2 Newton with or Without Generalized Krylov Correction

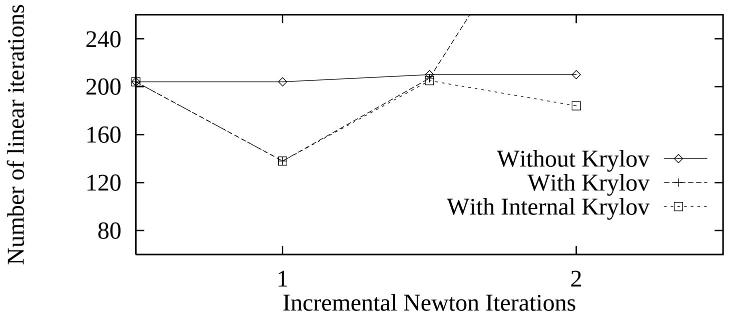


Case of the Incremental Newton Method

In the present section, the problem is solved by the Incremental Newton for a partitioning of the loading into two equal increments. The solution is thus reached after 2 Newton-Raphson iterations for each of the two considered increments. Fig. 3 describes the results obtained in the three following cases :

- without the Generalized Krylov Correction,
- with the Generalized Krylov Correction for the solution of each linear system,
- with the Generalized Krylov Correction only within an Incremental Newton iteration (Internal Krylov).

Figure 3 Incremental Newton with or Without Generalized Krylov Correction



It should be noted that, in the case of the Incremental Newton method, the Krylov Correction fails when it is used for the resolution of each linear system. Indeed, the taking account of the new load increment (here with imposed displacement) implies a very significant evolution of the linear system matrix to be solved and in particularly its spectrum. This explains the loss of efficiency of the Krylov Correction which relies upon the construction of an approximation of the inverse of the linear system matrix. On the other hand, a significant gain may be observed again if the technique is used only for the resolution of nonlinear problems of each load increment (Internal Krylov).

However, its use may be automated when introducing a criterion, which, in the case of a too slow convergence, starts the iteration again without the correction.

5 Conclusion

The introduction of the Generalized Krylov Correction in Domain Decomposition Methods for the resolution of nonlinear elasticity problems may lead to a significant reduction in the number of iterations of the conjugate Gradient. Furthermore, as shown in its expression (3.5), the calculation procedure of the Krylov Correction associated to a Krylov sub-space can be compared to that of a reorthogonalization. It is therefore well suited to an implementation on parallel computers.

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