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Rigid body modes deflation of the Preconditioned Conjugate Gradient in the solution of discretized structural problems

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ABSTRACT

In the numerical simulation of structural problems, a crucial aspect concern the solution of the linear system arising from the discretization of the governing equations. In fact, ill-conditioned system, related to an unfavorable eigenspectrum, are quite common in several engineering applications. In these cases the Preconditioned Conjugate Gradient enhanced with the deflation technique seems to be a very promising approach in particular because an effective deflation space is already at hand. In fact, it is possible to utilize rigid body motions of the system, that can be calculated easily and cheaply, and only the knowledge of the geometry of problem is required. This paper investigates the advantages of using a Rigid Body Modes Deflated Conjugate Gradient in the solution of challenging systems arising from structural problems. Two different situations are analyzed: the ill-conditioning caused by low constraining is addressed deflating the total rigid body modes, while the one concerning the heterogeneity of the problem by using the rigid body modes of separate components. Moreover, the implemented method is highly parallel and therefore suitable for High Performance Computing. Numerical results show how both approaches performed successfully in reducing the overall system solution time cost and iterations required for convergence.

1. Introduction

The efficient solution to linear systems of equations is a key issue in the numerical simulation of engineering problems [1–5]. Considering a generic system of partial differential equations (PDEs), it is usually solved through a discretization method, such as for instance the Finite Element Method (FEM), in order to approximate the continuous solution and represent it in a discrete way, i.e. by an algebraic system of linear equations. In this way the PDE system can be solved by means of linear algebra tools.

It is well known that, most of times, the solution of such linear systems is the most time consuming part of the entire solution process, hence many different techniques were developed in the last decades to accelerate this process. Nowadays *Krylov Subspaces Methods* are considered among the most effective approaches. These iterative techniques are suitable for linear systems whose dimension may be very large (even billions of unknowns) and whose structure is characterized by high sparsity and irregularity. In this paper we will restrict our analysis to Symmetric Positive Definite systems (SPD), which arise from the FEM discretization of the structural problems examined. The best suited, and probably most famous, Krylov strategy utilized for SPD systems is the Conjugate Gradient (CG).

To be effective, as any other Krylov method, CG convergence is accelerated by means of a *preconditioner*, thus giving rise to the Preconditioned Conjugate Gradient (PCG). Generally speaking, a preconditioner is a matrix which, multiplied by the original system matrix, is able to significantly improve convergence.

Unfortunately, for the solution of some categories of structural mechanics problems the application of a preconditioning matrix alone generally leads to poor results. These problems are all characterized by an eigenspectrum in which a limited number of eigenvalues has a value significantly smaller than the others (several orders of magnitude). This heterogeneity in the spectrum results in a strongly oscillating behavior of the residual during CG iterations and therefore slows down noticeably the overall convergence. Two typical examples characterized by such ill-conditioned behavior of the residual will be addressed in this paper: solids which have a low degree of constraints and heterogeneous

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materials whose components differ significantly in stiffnesses, thus leading to a matrix with high contrasts in the coefficients. For the sake of completeness, a third source for ill-conditioning of the stiffness matrix may be due to a high aspect ratio of elements. This is the case when for example rough meshing methods are used on complex geometries, and/or when the elements during deformation become highly distorted [6,7]. This aspect has been not considered in this paper and will be investigated in future works.

A strategy to solve these ill-conditioned systems may be to draw back to direct solution methods that have been traditionally the only way to cope with highly ill-conditioned systems. The two major drawbacks of direct methods are memory consumption and scalability on large HPC system, two issues recently addressed by the work of Koric adn Gupta [8] and Gupta et al. [9].

Going back to iterative solvers, for these ill-conditioned systems a different approach is developed, and the traditional preconditioning matrix is used in conjunction with an other preconditioning technique known as *deflation*. The latter is a projection method that can annihilate the influence of the slowly converging components of the residual, thus improving the CG performance noticeably. It is known that these components correspond to the eigenvectors associated to the small eigenvalues. Therefore, a limit of the strategy is that computation of eigenvectors is a rather expensive procedure.

A very interesting fact concerning the use of the deflation technique in structural problems is that an effective approximation of slowly converging components, whose computation is mandatory for the application of deflation, is known a priori and can be evaluated cheaply. The idea, illustrated in [10] and here recalled, is to utilize the rigid body modes of the system, whose computation is trivial and requires only the geometry of the structural system as input. For the sake of clearness, note that explicit FEA (Explicit Dynamics) don't have any issues with rigid body modes considered in this paper, which focuses on static solution of FEM problems.

In [10] rigid body modes deflation is utilized to improve the solution of problems concerning heterogeneous materials. In this paper we further exploit this approach and apply the same idea also to poorly constrained structural problems, whose strong ill-conditioning also represent an obstacle in engineering applications. Moreover, a fully parallel implementation of the method is here presented, which allows its efficient use on the modern High Performance Computing (HPC) systems. To ensure parallelizability of the entire algorithm, we adopt an efficient preconditioning matrix suitable for parallel computations known as Factored Sparse Approximate Inverse (FSAI) [11]. Preconditioners usually utilized in PCG are generally based on incomplete factorizations, as the well known Incomplete Cholesky (IC), and are mostly sequential, thus compromising the quality of the overall parallel implementation. FSAI instead is inherently parallel and we include in our code the open source FSAIPACK software package that allows one to compute easily an efficient preconditioner tailored for the problem at hand. This fully parallel implementation of the method is, at the best of our knowledge, rather new and has not been previously used in conjunction with deflation.

Deflation was firstly proposed by Nicolaides [12] and Dostàl [13], who both developed a deflated version of the Conjugate Gradient. Moreover Nicolaides showed how this projective method can be used efficiently in conjunction with a preconditioning matrix as well. In [14] Mansfield shows interesting applications of the deflated version of the CG in different engineering fields. Since that pioneering work many other authors used the strategy in several applications, combining the method with other preconditioning strategies available. Approaches similar to the one developed by Nicolaides are the algorithms proposed by Kolotilina [15] and Saad [16]. The deflated CG presented in this contribution, however, is slightly different and follows the one illustrated in [17] by Vuik et al. Deflation was also implemented in conjunction with other Krylov strategies such as GMRES [18,19]. We remark that deflation is a very general strategy and that it may be virtually utilized with every Krylov method. This is well explained in [20], where Gutknecht illustrates a theoretical framework for Krylov methods enhanced with deflation and augmentation techniques, focusing mainly on GMRES, MinRES and QMR. In [21] Gaul et al. develop this subject presenting a common framework for deflated and augmented Krylov strategies. A complete overview concerning the state of the art of the deflation technique is reported in [22] and in Section 9 of [23]. Deflation presents similarities with other preconditioning techniques based on subspace corrections. This group of preconditioners is often defined as *projective preconditioners* and include methods such as deflation, augmentation, Multi-Grid (MG) and Domain Decomposition (DD). The use of a projective preconditioner in conjunction with a preconditioning matrix is common and the resulting algorithms are called *two-level preconditioners*. A detailed analysis on different two-level approaches involving PCG is presented in [24], where the deflation method appear to be quite an efficient strategy. Interesting comparisons between deflation and other types of projective preconditioners deriving from MG and DD approaches are reported also in [25–27]. Deflation technique has been utilized in several applications concerning different fields of engineering. In [12] Nicolaides shows how the needed eigenvectors may be approximated using a piecewise constant interpolation over subdomains selected on the discretized grid, and applied this strategy on a system resulting from the FEM discretization of the Poisson's equation. This approach, known as *subdomain deflation* has many similarities with MG and DD approaches and is further analyzed in [22], where Frank and Vuik utilize it in many practical examples and find interesting bounds for the spectrum of the projected matrix. Generally speaking, the choice of the deflation space may be done considering physical aspects of the analyzed problem, as in our case, or may be based on algebraic characteristics of the matrix. In [28], for instance, Moutafis et al. utilize suitable partition algorithms for selecting such space in deflating a preconditioned version of GMRES. Other authors calculate approximate eigenvectors (see for example [16]).

The idea of approximating the needed eigenvectors with an a priori chosen deflation subspace has been exploited by several others authors. In [29], for instance, deflation method is used in FEM simulations concerning a magnetic field and in [17] Frank and Vuik show an effective way to approximate eigenvectors in diffusion problems characterized by high contrasts in the coefficients. Finally in [10] rigid body modes are used as approximated eigenvectors for the deflation method, that is the approach further exploited in the present algorithm.

The first part of this paper is dedicated to the exploitation of the main theoretical aspects on which the deflation method is based and to the resulting algorithm. Subsequently some aspects of the numerical implementation are illustrated. Finally extensive numerical results are presented. Starting from a very simple example, more realistic applications are illustrated. The efficient parallelization of the proposed method is confirmed by the results of scalability tests.

2. Accelerating the Conjugate Gradient through deflation

Consider the solution of a symmetric positive definite (SPD) linear system of equations:

$$Ax = b \tag{1}$$

by means of the Conjugate Gradient method (CG). The convergence rate of CG strictly depends on the spectrum $\sigma(A)$ of the system