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EFFICIENCY INCREMENT IN 3D MULTI-ZONE BOUNDARY ELEMENT ALGORITHMS BY USE OF ITERATIVE SOLVERS

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ABSTRACT

In this work general aspects of developing efficient generic multi-zone BEM algorithms are discussed, focusing specifically on three-dimensional formulations. The main idea followed in the article for coupling a certain number of subregions discretized with boundary elements is that the global sparse matrix of the coupled system is implicitly considered, without condensing the problem quantities into the interface variables and also without manipulating any of the zero blocks appearing in the system matrix. Thereby an algorithm, optimum in respect to storage requirements, is developed. Also, the performance of the proposed coupling algorithm is further increased by making use of iterative solvers. Recently reported research emphasising the efficiency of such solvers in comparison with direct ones and the results obtained in this paper for a simple 3D elasticity problem are used to show the efficiency of the multi-zone BEM strategy presented.

I. INTRODUCTION

Boundary element formulations based on subregion techniques are commonly used for treating problems defined in nonhomogeneous domains and also for simulating domain cracks, thin barriers, etc. In order to develop such formulations, it is necessary to idealise the whole definition domain of the problem as an assemblage of a series of homogeneous parts (subregions or zones) to which the boundary integral equation of the physical problem being considered can then be applied (Brebbia *et al.*, 1984; Brebbia and Dominguez, 1989). An algebraic system of equations for each subregion can then be derived, and with further considerations of coupling conditions on the interfaces between the subdomains, the approximated response of the problem in each subdomain is obtained.

As multi-zone BE algorithms originate coupled system matrices exhibiting a great deal of blockmatrices with zero coefficients, some researches has been developed in recent years in order to get optimised boundary element algorithms (Bialeck *et al.*, 1996; Kane *et al.*, 1990; Santiago and Telles, 1997) concerning the storage and manipulation techniques of the matrix coefficients. The ideas adopted for developing such optimised algorithms consist mainly in making use of special node renumbering schemes for each subregion, such that an optimum arrangement of the final coefficient matrix, i.e. an arrangement minimizing the *fill-in* effects (Kane *et al.*, 1990; Rigby and Aliabadi, 1995), is obtained;

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furthermore, direct solvers e.g. the Gaussian elimination, possibly restricted to the non-zero blocks, have usually been employed for solving the resulting system of algebraic equations (Bialecki *et al.*, 1996; Santiago and Telles, 1997). Nevertheless, by analysing problems consisting of various coupled subregions with a direct-solver-based BE multi-zone algorithm, the originally zero blocks are normally filled with non-zero entries along the coefficient transformations of the direct procedure - the so-called *fill-in* phenomenon - so that such a class of coupling algorithms cannot be properly classified as an ideal multidomain BEM strategy.

In this work an algorithm for coupling a generic number of subregions based on the implicit consideration of the global sparse matrix of the coupled system is presented. Special characteristics of this algorithm are that no condensing of the problem quantities into the interface variables (common surfaces between the subdomains) is carried out and also none of the many blockmatrices with zero coefficients appearing in the coupled system is considered. The use of iterative techniques for handling the resulting system of equations makes possible only blockmatrices with non-zero coefficients being stored and manipulated during the analysis process, because by applying iterative solution schemes the coefficient matrix remains unchanged through the whole solution process, whereas by using direct solvers it is altered (transformed). The way in which the blockmatrices are organised and stored in the coupled system for further manipulation in the solution phase is also discussed. The efficiency of the algorithm also depends on this fact.

By means of research developed in the last ten years it was possible to establish reliable iterative solvers for treatment of BEM unsymmetric systems of equations (see Araújo and Mansur (1989), Araujo *et al.* (1990), Kane *et al.* (1991), Mansur *et al.* (1992), Barra *et al.* (1992) and Prasad *et al.* (1994). The results reported in these articles hint that if the verified iterative procedures are used together with good preconditioning matrices (Araújo and Mansur, 1989; Araújo *et al.*, 1990; Barra *et al.*, 1992; Mansur *et al.*, 1992; Prasad *et al.*, 1994), e.g. the Jacobi (or diagonal) preconditioner, the lack of convergence normally found in anterior works concerning iterative techniques (Bettess, 1983; 1987; Mullen and Rencis, 1987), can be completely avoided for normal Engineering systems (non-singular or non-quasi-singular ones). Specifically the study done in this work focuses the performance of a 3D multidomain BE algorithm based on the iterative Lanczos process with and without Jacobi preconditioning (Araújo and Mansur, 1989; Araújo *et al.*, 1990; Mansur *et al.*, 1992); however, the ideas followed in this article are naturally applicable to other iterative procedures as well. Details of the formulation and a brief convergence analysis of the iterative process are presented.

A simple 3D elastostatic problem discretized with diverse subregions is used to observe the performance of the proposed multi-zone BEM strategy. With the aid of the results obtained in this paper (in terms of CPU times, required storage room and accuracy), the authors endeavour, concretely, to show the efficiency of the proposed coupling algorithm.

II. MULTI-ZONE STRATEGY

As is well-known, direct BEM formulations are derived for general stationary physical problems from a boundary integral equation of the following aspect:

$$c_{ik}(\xi)u_k(\xi) + \int_\Gamma p^*_{ik}(x;\xi)u_k(x)d\Gamma(x)$$

$$= \int_\Gamma u^*_{ik}(x;\xi)p_k(x)d\Gamma(x) + \int_\Omega u^*_{ik}(x;\xi)b_k(x)d\Omega(x), \qquad (1)$$

where p^*_{ik} and u^*_k are the fundamental kernels and c_{ik} is the integral-free term dependent upon the boundary geometry in ξ. Details of the physical problem will not be given further attention here, solely the coupled geometric definition of the problem domain will be highlighted. But, naturally, the ideas in this work are equally applicable to general physical situations (also transient ones).

Concerning the proper multi-zone algorithm proposed in this work, just two points should be commented, namely, (1) how the coefficient blocks of each subregion in the coupled system (whether condensed or not) should be organised and (2) how they should be ideally stored. Defining a *coefficient block* as the submatrix of the coefficient matrix of a certain subregion that corresponds only to degrees of freedom of the external boundary or only to degrees of freedom of the intersections of the subregions with each other (common surfaces) or, simultaneously, two, three or more others (curves and points), the points above can then be discussed. In respect to the first point, the option adopted was not to condense the field quantities in variable blocks, but to allocate them in a global sparse matrix involving all the system unknowns. Thereby, the necessary inversions of submatrices that were necessary in order to get the condensed coupled system are avoided. The second point - concerning the way in which the coefficients should be stored - was then treated by storing, exclusively, the non-zero blocks in a work vector, beginning with the first column of the first non-zero block of the first subregion, and so on, column by column, block by block, subregion by subregion.

Some details on the storing procedure are that the coefficient blocks (in terms of global node numbering pertaining to them) are determined during the mesh generation in the pre-processing module of the computer code and, furthermore, two variables indicating the position of each block in the coupled sparse matrix of the whole system (in terms of its initial and final lines and columns) and one other variable pointing the position of the first element of each block in the work vector are used.

In order to give a more concrete idea of the multi-zone algorithm, the domain of Fig. 1 with three substructures will be considered[1]. By writing Eq. (1) in algebraic form (after discretizing it with boundary elements) for each substructure of the body in Fig. 1 and by introducing the equilibrium and compatibility conditions in points of common variable blocks (not pertaining to the external boundary), the following coupled system, organised in terms of the block variables in a non-condensed form, is obtained:

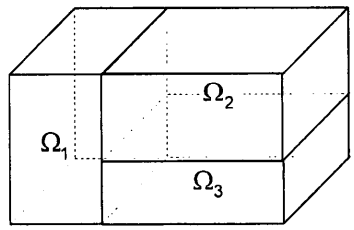

Fig. 1 Body with substructures

no further discussion about numbering schemes being necessary, as will be seen.

III. ITERATIVE SOLVERS

There are nowadays some important works emphasising the efficiency of iterative solvers (Araújo and Mansur, 1989; Araújo *et al.*, 1990; Barra *et al.*, 1992; Davey and Rosindale, 1994; Kane *et al.*, 1991; Mansur *et al.*, 1992; Prasad *et al.*, 1994; Urekew and

$$\begin{bmatrix} H^1 & H^{1,2}-G^{1,2} & H^{1,3}-G^{1,3} & H^{1,2,3}-G^{1,2,3} & 0 & 0 & 0 & 0 \\ 0 & H^{2,1} & G^{2,1} & 0 & 0 & H^{2,1,3} & G^{2,1,3} & H^2 \; H^{2,3}-G^{2,3} \; 0 \\ 0 & 0 & 0 & H^{3,1} & G^{3,1} & H^{3,1,2} & G^{3,1,2} & 0 \; H^{3,2} \; G^{3,2} \; H^3 \end{bmatrix} \begin{Bmatrix} u^1 \\ u^{1,2} \\ p^{1,2} \\ u^{1,3} \\ p^{1,3} \\ u^{1,2,3} \\ p^{1,2,3} \\ u^2 \\ u^{2,3} \\ p^{2,3} \\ u^3 \end{Bmatrix} = \begin{bmatrix} G^1 & 0 & 0 \\ 0 & G^2 & 0 \\ 0 & 0 & G^3 \end{bmatrix} \begin{Bmatrix} p^1 \\ p^2 \\ p^3 \end{Bmatrix}. \tag{2}$$

The superscripts in Eq. (2) indicate the subregion or subregions to which the degrees of freedom pertain. After introducing the boundary conditions of the subdomains, a system of equations of the form

$$Ax=b, \tag{3}$$

usual in the Boundary Element Method, then results. Though, implicitly, the matrix A of the coupled system is treated as the matrix on the left-hand side of Eq. (2), explicitly this matrix is the work vector commented on above. The coupling formulation of a generic number of subregions is therefore concluded, Rencis, 1993; 1994; Walker and Lee, 1997). In this study only the solution scheme based on the Lanczos tridiagonalization algorithm is considered (Wilkinson, 1965).

In order to apply the Lanczos algorithm for solving algebraic systems of equations the iterative formula

$$u^{n+1}=\rho_{n+1}\gamma_{n+1}r^n+\rho_{n+1}u^n+(1-\rho_{n+1})u^{n-1}, \tag{4}$$

which gives the system solution at iteration $n+1$, is adopted, the corresponding residue at this iteration, r^{n+1}, (obtained by $r^{n+1}=b-Au^{n+1}$) being consequently

[1] A domain with any number of substructures could naturally be taken into account. In the computer code the subregions and all their variable blocks are established in the data pre-processing module.

Table 1 Storage and CPU timing results

Mesh	Work vector (Mbytes)	Preconditioner	Iterations	CPU time (s)	
				Matrix assemblage	Solver
I	2.396	none	24	56.3	3.2
II	2.144	none	30	64.3	4.8
I	2.396	Jacobi	20	56.3	2.9
II	2.144	Jacobi	25	64.3	3.9

$$\boldsymbol{r}^{n+1}=\rho_{n+1}(-\gamma_{n+1}\boldsymbol{A}\boldsymbol{r}^{n}+\boldsymbol{r}^{n})+(1-\rho_{n+1})\boldsymbol{r}^{n-1}. \tag{5}$$

The residue vector (5) has the aspect of the vectors derived from the $\boldsymbol{A}$-matrix by the Lanczos algorithm. This fact hints the consideration of vectors $\overline{\boldsymbol{r}}^{n+1}$ associated with $\boldsymbol{A}^T$ of the form

$$\overline{\boldsymbol{r}}^{n+1}=\overline{\rho}_{n+1}(-\overline{\gamma}_{n+1}\boldsymbol{A}^{T}\overline{\boldsymbol{r}}^{n}+\overline{\boldsymbol{r}}^{n})+(1-\overline{\rho}_{n+1})\overline{\boldsymbol{r}}^{n+1}. \tag{6}$$

By proposing now that vectors $\boldsymbol{r}^{n+1}$ and $\overline{\boldsymbol{r}}^{n+1}$ are in fact Lanczos vectors, expressions for the parameters in iterative formulae (4), (5) and (6) can then be obtained. It results in:

$$\gamma_{n+1}=\overline{\gamma}_{n+1}=\frac{\overline{\boldsymbol{r}}^{n,T}\boldsymbol{r}^{n}}{\overline{\boldsymbol{r}}^{n,T}\boldsymbol{A}\boldsymbol{r}^{n}} \text{ and}$$

$$\rho_{n+1}=\overline{\rho}_{n+1}=[1-\frac{\gamma_{n+1}}{\gamma_n}\cdot\frac{\overline{\boldsymbol{r}}^{n,T}\boldsymbol{r}^{n}}{\overline{\boldsymbol{r}}^{n-1,T}\boldsymbol{r}^{n-1}}\cdot\frac{1}{\rho_n}]^{-1}, \tag{7}$$

with $\rho_1=1$ and $\boldsymbol{r}^1=\overline{\boldsymbol{r}}^1$. With these expressions two vector sets $\boldsymbol{r}^1$, $\boldsymbol{r}^2$, ... and $\overline{\boldsymbol{r}}^1$, $\overline{\boldsymbol{r}}^2$, ... are then generated for which the orthogonality property

$$(\boldsymbol{r}^i, \overline{\boldsymbol{r}}^j)=0 \text{ if } i\neq j \tag{8}$$

is verified; this property makes such iterative schemes very attractive, then the generated set $\overline{\boldsymbol{r}}^1$, $\overline{\boldsymbol{r}}^2$, ... being linearly independent (see Wilkinson (1965)) and the residue vector $\boldsymbol{r}^n$ pertaining to the N-dimensional Euclidean space R^N, where N is the system order, so it must be found that $\boldsymbol{r}^{N+1}=\boldsymbol{0}$. Naturally, as a consequence of errors introduced in the data processing in the computer, it may happen that convergence is not reached for $n\leq N$, mainly for ill-conditioned systems. This eventual lack of convergence has then been avoided by considering preconditioning matrices in the iterative schemes (Araújo and Mansur, 1989; Barra *et al.*, 1992; Kane *et al.*, 1991; Mansur *et al.*, 1992; Prasad *et al.*, 1994). It should be also observed that there is no difficulty in avoiding the manipulation of all zero blocks, as the most complex operation in the Lanczos algorithm is a matrix-vector multiplication. In Araújo (1989) the complete derivation of all expressions involved in the Lanczos solution scheme is given.

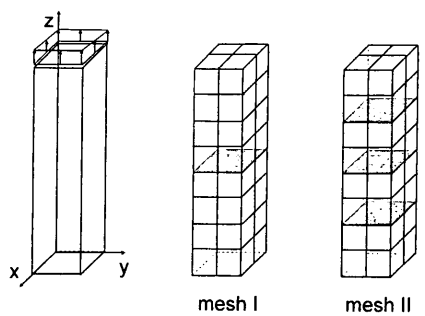

Fig. 2 Prismatic bar and adopted BE discretization meshes

IV. APPLICATIONS

The performance of the multi-zone algorithm with the Lanczos-based iterative solver (preconditioned and non-preconditioned) is observed by analysing the prismatic bar depicted in Fig. 2 with length of 20 m and square cross section of side 5.0 m long. The material constants are $E=21\times10^5$ tf/m^2 and $\nu=0.15$, and the boundary conditions are the load of $p_z=1.0$ tf/m^2, uniformly distributed at the upper end, and displacement restriction in direction z at the lower end and in directions x and y normal to two of the faces along the bar length, such that rigid body displacement is constrained, but free deformation of the bar is possible. The hatched surfaces in Fig. 2 indicate the separation between subregions.

In the analysis a pentium II computer with 300 MHz processor and 64 MBytes of RAM under Microsoft-FORTRAN 90 compiler (Power Station) was used. The results for the problem (in terms of storage room, number of iterations and CPU times) obtained with stop criterion $\frac{\|\delta^n\|}{\|b\|}\leq tol=10^{-6}$, where $\delta^n=\boldsymbol{u}^n-\boldsymbol{u}^{n-1}$, are shown in Table 1. Mesh I contains 2 subregions, 76 boundary elements and 244 nodes (system order N=732) and mesh II, 4 subregions, 84 elements and 296 nodes (system order N=888).

V. CONCLUSIONS

As expected, the use of the Lanczos iterative

technique for treatment of the coupled systems originated from the bar had a quite good performance, which can be concluded, though no direct comparison what a direct solver could be done, by observing the relation between the system order and the number of iterations necessary for reaching the convergence (N/n). By adopting mesh I (N=732 equations) convergence was obtained with n=24 iterations (without preconditioner) and with n=20 iterations (with preconditioner), and for mesh II (N=888 equations) 30 and 25 iterations were needed for obtaining convergence with the non-preconditioned and preconditioned solver respectively. In such cases of relation N/n the iterative scheme has surely superior performance to the direct schemes (see results given by Araújo and Mansur (1989), Araújo *et al.* (1990), Kane *et al.* (1991), Mansur *et al.* (1992)), especially if a pivotal search must be conducted in order to ensure numerical stability of the direct solver. It should be furthermore mentioned that in the multi-zone strategy presented here the CPU time per iteration is smaller than in those cases for which systems of equivalent order are originated from single domain discretizations, as no manipulation of zero blocks is carried out in the resulting sparse coupled systems here.

Concerning storage saving, it should be observed that if the matrices for meshes I and II were *fully* stored, it would be necessary to have 4.088 MBytes and 6.016 MBytes storage room instead of the 2.396 and 2.144 MBytes respectively (see Table 1). This corresponds to storage saving of about 41 % for mesh I and 64 % for mesh II. It is also worth mentioning that for mesh II, which has more subregions than mesh I, the number of elements and nodes is consequently bigger, but also the matrix sparsity increases, as is shown through the significant storage saving pointed out above, and it should be also pointed out that the matrix sparsity is also important for increasing the performance of the iterative scheme.

The numerical results (in terms of displacements and stresses) for the simple elasticity problem analysed, which coincided quite well with the analytical ones for both meshes, are not reported. Finally, one can also observe that there was no considerable difference between the performance of the Lanczos solver with and without precondioner, this fact being explained by the possibly well-conditioned matrices resulting in both cases.

NOMENCLATURE

$\boldsymbol{A}$	BE coefficient matrix after introduction of the boundary conditions
$\boldsymbol{b}$	right-hand side vector
b_k	body force vector
c_{ik}	integral free term of the boundary integral
$\boldsymbol{H}$, $\boldsymbol{G}$	BE coefficient matrices originated from the traction and displacement fundamental kernels respectively
i, k	indexes assuming values 1, 2 and 3
p^*_{ik}	fundamental tractions
$\boldsymbol{p}$	boundary tractions
$\boldsymbol{r}^n$, $\overline{\boldsymbol{r}}^n$	residue vectors at the nth iteration associated with $\boldsymbol{A}$ and $\boldsymbol{A}^T$ respectively
u^*_{ik}	fundamental displacements
$\boldsymbol{u}$	displacement vector before and unknowns (solution) vector after introducing the boundary conditions
$\boldsymbol{u}^n$	solution at iteration n
$\boldsymbol{x}$	field point
δ^n	solution difference between iterations n and $n-1$
γ_n, $\overline{\gamma}_n$	parameters of the Lanczos iterative procedure
Γ	domain boundary
Ω	problem domain
ρ_n, $\overline{\rho}_n$	parameters of the Lanczos iterative procedure
ξ	source point

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三維多重區域之邊界元素疊代演算法

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摘 要

本文探討高效率多重區域之邊界元素演算法，著重於三維的計算公式。主要構想是以邊界元素分割幾個次區域，可考慮整體耦合系統的大域稀疏矩陣，並免於濃縮物理量到界面變數上，亦不需處理在系統矩陣中大量出現的零區塊。因此本演算法發展出最佳的儲存效果。換句話說，本演算法在疊代過程中更能發揮其功能。本文和過往的一些研究就三維彈力問題以多區域邊界元素法的分析結果作比較，驗證本研究之高效率。

關鍵詞：多重區域邊界元素程序，迭代求解，三維問題。