

Analysis of Multiple Inclusion Potential Problems by the Adaptive Cross Approximation Method

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Abstract: Over recent years the rapid evolution of the computational power has motivated the development of new numerical techniques to account for engineering solutions. The Boundary Element Method (BEM) has shown to be a powerful numeric tool for the analysis and solution of many physical and engineering problems. However, BEM fully populated and non-symmetric system matrices implies in higher memory requirements and solution times. This work analyze the application of hierarchical matrices and low rank approximations, applying the Adaptive Cross Approximation - ACA, to multiple inclusion potential problems. The use of hierarchical format is aimed at reducing the storage requirement and the computational complexity arising in the BEM. First, the use of hierarchical matrices and low rank approximation on multidomain potential problems is depicted. Finally, a numerical example is performed to show the applicability of using ACA in large-scale multidomain problems. Moreover, the application of ACA to multidomain problems showed to be an important option in future multiscale problem analyses.

Keywords: Adaptive Cross Approximation, Boundary Element Method, Hierarchical Matrices, Multidomain problems.

1 Introduction

Over recent years, the boundary element method (BEM) has demonstrated to be a powerful numerical tool for the analysis and solution of many physical and engineering problems [Aliabadi (2002)]. However, one of the big disadvantages of BEM when compared with the finite element method (FEM) is the fully populated and non symmetric system matrices, implying in higher memory requirements and solution times. Many research studies have focused in improving the BEM, such as block-based solvers [Crotty (1982); Rigby and Aliabadi (1995)], the lumping technique [Kane, Kumar, and Saigal (1990)] or iterative solvers [Mansur, Araujo, and

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Malaghini (1992)]. A complete review of these methods is available in [Benedetti, Aliabadi, and Davi (2008)]. Many investigations have been carried out to speed up the solution process. One of the most famous methods is the Fast Multipole Method [Rokhlin (1985)]. However, the main disadvantage of this method is the necessity of the harmonic expansion of the kernels. From the algebraic point of view however, the integration of a degenerate kernel over a cluster of suitably selected boundary elements corresponds to the approximation of the related matrix block by a low rank block [Bebendorf (2000)]. As a consequence, it is possible to use purely algebraic algorithms to generate the approximation of suitable blocks of the collocation matrix, using only few entries of the original blocks [Bebendorf and Rjasanow (2003)]. This technique is referred to as the Adaptive Cross Approximation (ACA). [Brancati, Aliabadi, and Milazzo (2011)] presents and improve (ACA) approach developed in conjunction with Hierarchical format matrix and GMRES solver applied for sound absorbent materials, another work presented by [Brancati, Aliabadi, and Benedetti (2009)] used a Hierarchical GMRES solver and the (ACA) for 3D acoustic problems. Analogously to FMMs, the use of the hierarchical format is aimed at reducing the storage requirement and the computational complexity arising in the BEM. After representing the coefficient matrix in hierarchical format, the solution of the system can be obtained either directly, by inverting the matrix in hierarchical format, or indirectly, by using iterative schemes with or without preconditioners [Grasedyck (2005); Bebendorf (2005); Benedetti, Aliabadi, and Davi (2008)].

In this paper the application of hierarchical matrices and ACA in multiple inclusion potential problems is illustrated. First, the use of hierarchical matrices and ACA is discussed. Then, the application of ACA to multidomain potential problems is depicted. Next, a brief formulation of homogenization in regular and random composites is reviewed. Finally, Numerical examples, results and conclusions are shown.

2 Hierarchical Matrices

The objective of hierarchical matrices is to reduce the storage requirements as well as to speed up the time required to complete all matrix operations. In this method the matrix is represented as a collection of blocks, some of which admit a particular approximated representation that can be obtained by computing only few entries from the original blocks. These special blocks are called low rank blocks. Blocks that cannot be represented in this way must be computed and stored entirely and are called full rank blocks [Benedetti, Aliabadi, and Davi (2008); Benedetti, Milazzo, and Aliabadi (2009)]. The formal definition and description of hierarchical matrices can be also found in [Hackbusch (1999); Hackbusch and Nowak (2000)].

Low rank blocks constitute an approximation of suitably selected blocks of the discrete integral operator based, from the analytical point of view, on a suitable expansion of the kernel of the continuous integral operator [Bebendorf (2000); Bebendorf and Rjasanow (2003)]. This expansion, and consequently the existence of low rank approximants, is based on the asymptotic smoothness of the kernel functions, i.e., on the fact that kernels U_{ij}^* and T_{ij}^* are singular only when $x = y$ [Bebendorf (2000); Bebendorf and Rjasanow (2003); Grasedyck (2005)]. This represents a sufficient condition for the existence of low rank approximants and it does not exclude strongly or hyper-singular kernels like those appearing in the traction boundary integral equation. A low rank block M of size $m \times n$ has the following representation

$$M_k = \sum_{i=1}^k a_i \cdot b_i^T = A \cdot B^T \tag{1}$$

where A is a matrix of size $m \times k$ and B is a matrix of size $n \times k$. For admissible blocks, k is low and the representation showed in Eq.(1) requires the storage of $(m + n)k$ real numbers instead of the of the $m \times n$ original block. It is moreover apparent how it speeds up the matrix-vector product of the corresponding block. For a detailed analysis of the memory savings as well as the speed-up the allowed the reader could be referred to Borm, Grasedick, and Hackbusch (2003); Grasedyck and Hackbusch (2003).

A hierarchical approximation of large dense matrices arising from some generating function having diagonal singularity consist of three steps [Kurz, Rain, and Rjasanow (2007)]: (1) construction of clusters, (2) finding of possible admissible blocks and (3) low rank approximation of admissible blocks

The construction of clusters was implemented based on the algorithm showed in [Kurz, Rain, and Rjasanow (2007)]. First, the mass and center of each cluster are stored, then, the covariance matrix of the cluster is obtained by equation (2)

$$C = \sum_{k=1}^n g_k (x_k - X)(x_k - X)^T \tag{2}$$

where n is the number of elements of the cluster, g_k is the element length and X is the center of the cluster.

Then, the largest eigenvalue of C shows in the direction of the longest extension of the cluster. The separation line (plane in 3D) $\{x \in \mathfrak{R}^2 : (x - X, v_1) = 0\}$ goes through the center X of the cluster and is orthogonal to the eigenvector v_1 . This algorithm will be applied recursively to the sons until they contain less than or equal

to some prescribed number n_{min} of elements. Next, cluster pairs which are geometrically well separated are identified. They will be regarded as admissible cluster pairs. An appropriate admissibility criterion is the following simple geometrical condition. A pair of clusters (Cl_x, Cl_y) with $n_x > n_{min}$ and $m_y > n_{min}$ elements is admissible if

$$\min(\text{diam}(Cl_x), \text{diam}(Cl_y)) \leq \eta \text{dist}(Cl_x, Cl_y), \quad (3)$$

where η is called the admissibility parameter. This parameter influences the number of admissible blocks on one hand and the convergence speed of the adaptive approximation of low rank blocks on the other hand [Borm, Grasedyck, and Hackbusch (2003)]. A full study of this parameter was assessed by Benedetti, Aliabadi, and Davì (2008). They showed that the choice of η directly affects the quality of the ACA-generated matrix and a good choice of this parameter results in a matrix closer to the optimal matrix produced by the coarsening procedure. This fact was also justified by the reduction in the number of blocks. A brief study of this parameter is also shown in the present paper. In the present work, the actual diameters and the distance between two clusters were calculated and no approximation, as suggested by Benedetti, Aliabadi, and Davì (2008); Grasedyck (2005); Gieberman (2001), was made. Approximations are easily computable, however, result in a more rough and restrictive criterion. Once the clusters were defined and all admissible blocks were detected, we use the Adaptive Cross Approximation (ACA) to approximate by low rank these blocks. The original ACA algorithm was proposed by Bebendorf (2000). Three years later was further developed Bebendorf and Rjasanow (2003). Several ACA algorithms and variations, as the so-called ACA+, are available in the literature [Grasedyck (2005); Bebendorf and Grzhibovskis (2006); Kurz, Rain, and Rjasanow (2007)]. The algorithm used in this work for the low rank approximations was the same as showed by Kurz, Rain, and Rjasanow (2007). Results obtained after the low rank approximation of the admissible blocks by ACA, can be further recompressed, taking advantage of the reduced singular value decomposition (SVD) [Grasedyck (2005)], increasing the gain in memory storage. However, the recompression for storage purposes are out of the scope of the present work and was not implemented. Some works related to this topic are shown in [Grasedyck (2005); Benedetti, Aliabadi, and Davì (2008); Hackbusch, Khoromskij, and Kriemann (2004)].

3 Multiple Inclusion Problems

In this section the application of ACA to multidomain potential problems is shown. For this purpose, a small 2x2 inclusion problem is analyzed. Then, homogenization

models applied to regular and random composites are reviewed.

3.1 ACA applied to multiple inclusion potential problems

The *multidomain* or *multizone* BEM approach appear to be a natural choice in the solution of multiple inclusion problems. Through the multidomain approach, potential problems can be solved by applying the BEM separately to each of its subdomains. The reason is that the fundamental solution is valid only for homogeneous domains. After the discretization into subdomains, the coupling can be made considering the continuity of the potential property and of the flux in all the interfaces. Further details can be found in [Kane (1994) and Katsikadelis (2002)]. Fig. 1 shows a multidomain potential problem with four inclusions.

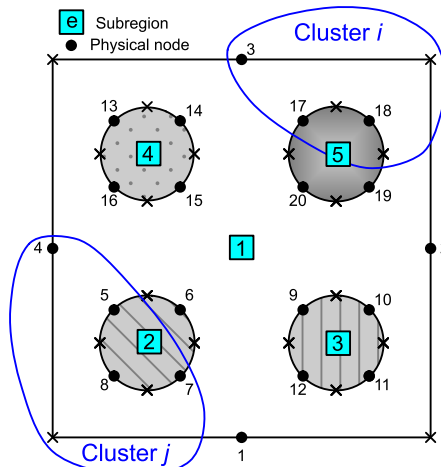


Figure 1: Example for the application of ACA in multidomain problems.

From Fig. 1, it is apparent that subregion one (matrix) has twenty physical nodes and each inclusion (fibers) has four physical nodes. However, the collocation matrix is not a twenty per twenty square matrix. This is because each inclusion physical node has incidence in both the inclusion and the matrix, implying in sixteen (four inclusions per four nodes per inclusion) additional components. Fig. 2 (a) shows the collocation matrix for this example. $[F_{ij}]^e$ and $[G_{ij}]^e$ represent the incidence in matrices $[F]$ and $[G]$ between subregions i and j in the case where quantities are associated to a specific region e . Fig. 2 (b) show real incidences of nodes of Cluster i and Cluster j of Fig. 1. Nodes 3, 17 and 18 of Cluster i represent indeed rows 3, 17, 18, 33 and 34 of the collocation matrix, and, nodes 4, 5, 7 and 8 represent columns 4, 5, 7, 8, 21, 23 and 24 of the collocation matrix, as can be observed

in green from Fig. 2 (b).

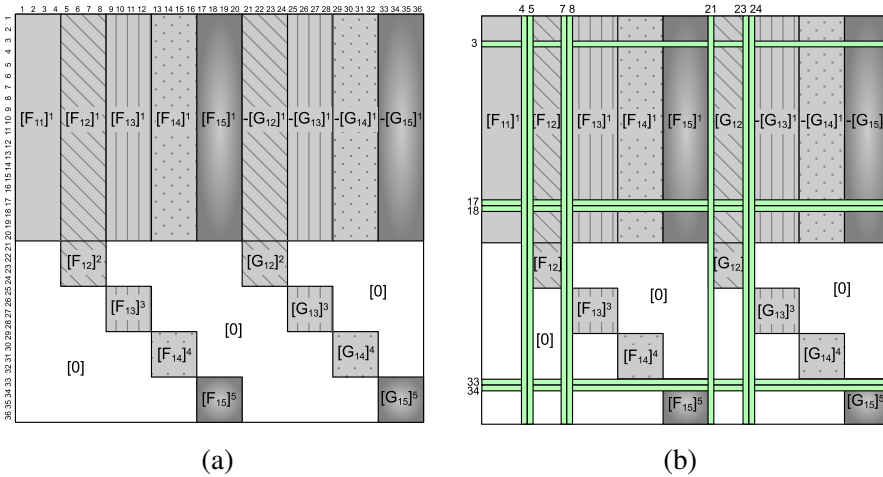


Figure 2: (a) Collocation matrix for the four inclusion example, (b) incidences of physical nodes for the inclusion example

We can conclude that all inclusion physical nodes have double incidence in the collocation matrix. An inclusion node n will have incidence “ n ” and “ $n + \text{total number of inclusion nodes}$ ”. Finally, if Cluster i and Cluster j fulfill an admissibility criterion we can further apply the Adaptive Cross Approximation to this block.

3.2 Homogenization - Shaking-Geometry Composite

The center of each fibre can be randomly deviated within a circle of diameter d whereas these circles themselves form a regular square lattice of the period l . This kind of a microstructure is usually referred as *shaking-geometry* composite [Berlyand and Mityushev (2001), Berlyand and Mityushev (2005)]. As pointed out by Andrianov, Danishevs’kyy, and Weichert (2008) and Kalamkarov, Andrianov, and Danishevs’kyy (2009), the random shaking of the fibers about the periodic lattice could correspond to production or technological reasons. The deviation parameter $\delta = d/l$ describes the *non-regularity rate* of the structure; its maximum value δ_{max} is determined by the case when fibers almost touch each other. Higher values of δ are not allowed since they would lead to penetration of the fibers (percolation). A simple geometrical calculation give:

$$\delta_{max} = 1 - \sqrt{\frac{c}{c_{max}}} \tag{4}$$

where $c = \pi a^2/l^2$ is the volume fraction of the fibers, $c_{max} = \pi/4$ is the maximal volume fraction of the fibers in the case of a perfectly regular material ($\delta = 0$).

Kolzlov (1989) showed for the case of dilute components that a regular lattice possesses the extreme effective properties among the corresponding shaking-geometry random structures. Later, Berlyand and Mityushev (2001), Berlyand and Mityushev (2005) generalized Kozlov’s result for the case of non-dilute components. Therefore, a solution for the perfectly regular lattice can be considered as a lower bound on the effective transport coefficient, [Kalamkarov, Andrianov, and Danishevs’kyy (2009), Andrianov, Danishevs’kyy, and Weichert (2008)]. The upper bound can be obtained using the *security-spheres approach*. Originally created by Keller et al. Keller, Rubinfeld, and Molyneux (1967), in this approach, the upper bound can be obtained by replacing the input non-regular assembly of fibers of radius a by the regular lattice of fibers of radius $a + d/2$, as shown in Fig. 3 (b). Further details of the *security-spheres approach* can be found in [Rubinfeld and Keller (1969), Torquato and Rubinshtein (1991) and Torquato (2002)]. Moreover, alternative approaches for inclusions, voids and cracks modeling can be seen in [Dong and Atluri (2012), Dong and Atluri (2013) and Dong, Gamal, and Atluri (2013)].

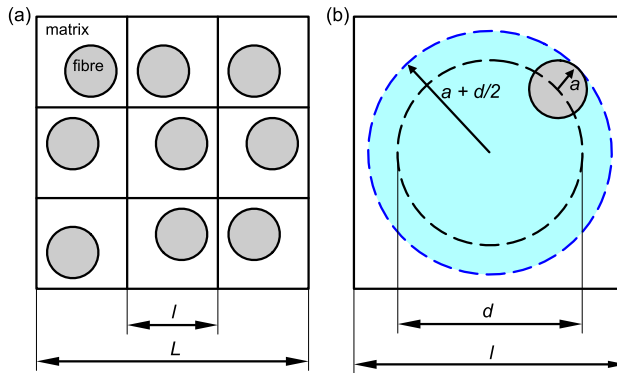


Figure 3: (a) Shaking-Geometry Composite, (b) deviation of the fibers about the regular square lattice.

Introducing lower K_1 and upper K_2 bounds for $\langle k \rangle$ such that $K_1 \leq \langle k \rangle \leq K_2$, and let us denote the conductivity of the perfectly regular material as a function K_0 of the fiber volume fraction c . Then, the lower bound K_1 is given by the solution in the perfectly regular case at $\delta = 0$, [Berlyand and Mityushev (2001), Berlyand and Mityushev (2005) and Kolzlov (1989)].

$$K_1 = \langle k \rangle|_{\delta=0} \tag{5}$$

For the regular case we used the formulation proposed by Perrins, McKenzie, and McPhedran (1979). Several models for the regular case are implemented and studied by Kalamkarov, Andrianov, and Danishevs'kyy (2009) and Andrianov, Danishevs'kyy, and Weichert (2008). The analytic expression for the conductivity, as defined by Perrins, McKenzie, and McPhedran (1979), is:

$$\langle k \rangle|_{\delta=0} = K_1 = \frac{1 - 2c}{\left[T + c - \frac{0.305827c^4T}{T^2 - 1.402958c^8} - \frac{0.013362c^8}{T} \right]} \tag{6}$$

where $T = \frac{1+k_f/k_m}{1-k_f/k_m}$.

To obtain the upper bound K_2 , the original non-regular assembly of fibers of radius a is replaced by a regular lattice of fibers of radius $a + d/2$. This estimation yields

$$K_2 = \langle k \rangle|_{\delta=0}(c = c + 2\delta\sqrt{cc_{\max}} + \delta^2c_{\max}) \tag{7}$$

We should note that the percolation threshold is reached at the maximum volume fraction $c_{\max} \approx 0.41$, [Molchanov (1991)].

4 Numerical results

To test the efficiency of the presented method in terms of the solution time and accuracy of the homogenization method, two configurations are analyzed. In the first part, ACA is applied to regular lattice composites. We analyzed six cases with different inclusion configurations: 14x14, 18x18, 21x21, 24x24, 26x26 and 28x28 inclusions are modeled in a 1x1 plate. The plate is modeled with 2D constant elements. The inner and upper sides are clamped (Flux is equal to zero), and the left and right sides have zero and one degrees, respectively. An illustrative figure with 10x10 inclusions is shown in Fig. 4 (a) to show boundary conditions considered for all cases. The fiber volume fraction c is equal to 12.57%, the matrix conductivity k_m is equal to 1 and the fiber conductivity k_f is equal to 0.1.

The Fig. 5 shows the block-wise representation of the collocation matrix for $\eta = 0.6, 0.8, 1.0, \sqrt{2.0}$ and 2.0. Every block is colored showing the ratio between the

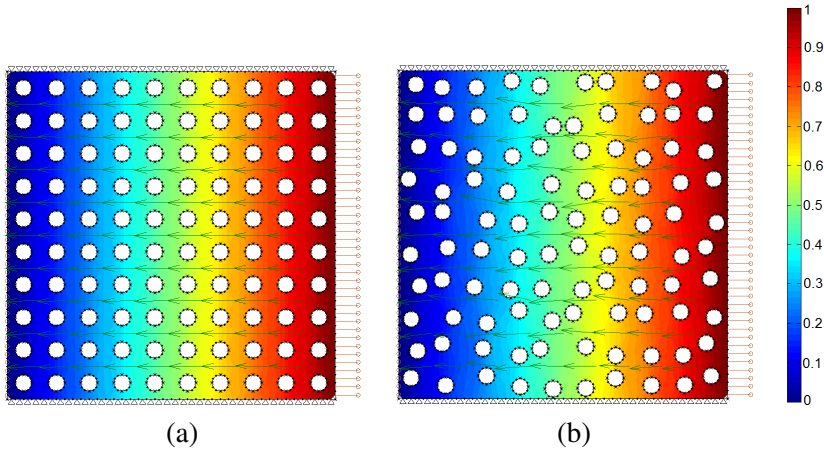


Figure 4: Illustrative figure showing the regular lattice (a), and the shaking-geometry configuration (b).

memory required for low rank representation and the memory in full rank format. The red color (ratio = 1), means that the block was generated as full rank. A helpful colorbar is also shown in Fig. 4.

The Tab. 1 shows speed-up ratios and the quantity of blocks generated by the hierarchical method for each case.

It is worth to point out that due to the sparsity generated by the multidomain method the solution of the system has been obtained using the solver PARDISO, included in the Intel Math Kernel Library (MKL). The selected ACA accuracy for all cases was 10^{-5} . A node by node check of the solution confirmed, that, for a selected accuracy, the average errors are to the order of $0.1 \pm 1.0\%$. Bigger percentage errors can occur for degrees of freedom whose standard solution values are smaller than the requested accuracy. This consideration suggests that it is advisable to set the accuracy at the same order of magnitude as that of the smaller quantities of interest in the analysis, [Benedetti, Aliabadi, and Davì (2008)].

The Fig. 6 shows the Speed-up ratio as a function of the number of elements (a), and as a function of the admissibility parameter η . It is important to notice that the speed-up ratio is less than one beyond a combination of the number of elements and η . That means, that, the method works better in these cases. For our numerical example the method works better for a number of elements greater than 10,000 and just for the cases where η is lower or equal to one.

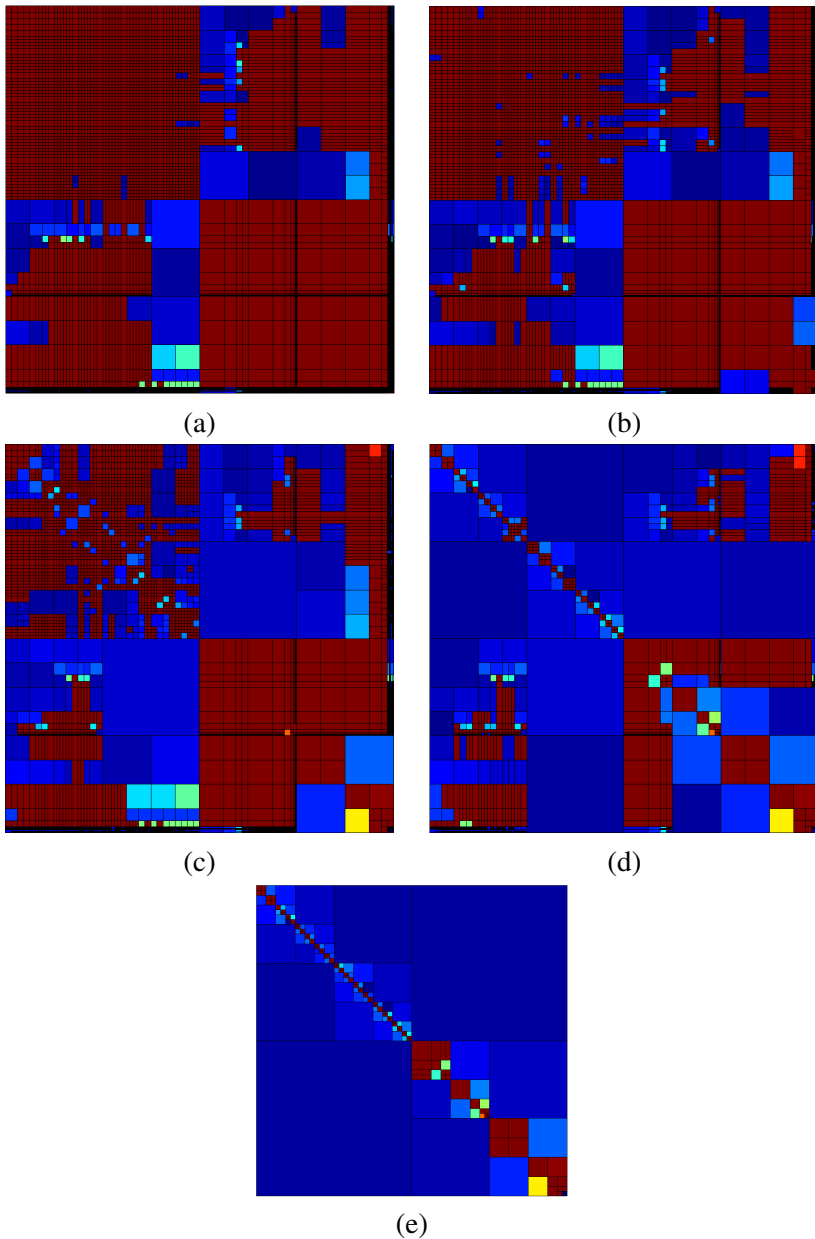
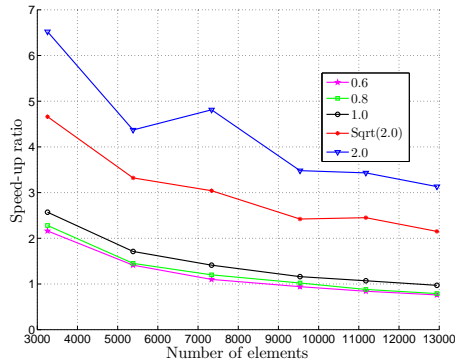


Figure 5: Block-wise representation of the collocation matrix for different admissibility parameters (η): (a) $\eta = 0.6$, (b) $\eta = 0.8$, (c) $\eta = 1.0$, (d) $\eta = \sqrt{2.0}$ and (e) $\eta = 2.0$.

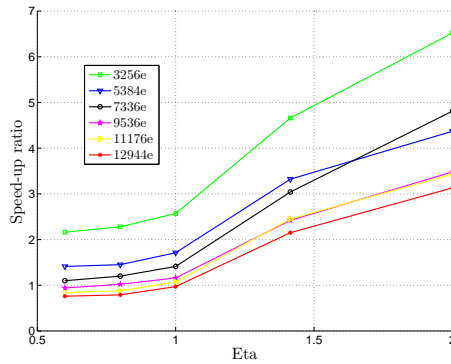
Table 1: Speed-up ratios for each case

Case	Eta (η)	Blocks	Admiss. Pairs	Speed-up ratio	Conventional BEM time (s)
Case 1 - 3256e	0.6	11058	300	2.16	1.89
	0.8	10402	410	2.28	
	1.0	8424	572	2.57	
	$\sqrt{2.0}$	2334	394	4.66	
	2.0	368	140	6.52	
Case 2 - 5384e	0.6	11338	256	1.41	7.63
	0.8	10584	460	1.45	
	1.0	8746	624	1.71	
	$\sqrt{2.0}$	2406	402	3.32	
	2.0	378	148	4.37	
Case 3 - 7336e	0.6	11778	250	1.10	18.16
	0.8	10848	470	1.20	
	1.0	9062	658	1.41	
	$\sqrt{2.0}$	2424	402	3.04	
	2.0	388	148	4.81	
Case 4 - 9536e	0.6	11248	278	0.94	39.07
	0.8	10554	438	1.02	
	1.0	9062	658	1.41	
	$\sqrt{2.0}$	2424	402	3.04	
	2.0	388	148	4.81	
Case 5 - 11176e	0.6	11685	196	0.84	62.80
	0.8	11047	352	0.88	
	1.0	8989	562	1.07	
	$\sqrt{2.0}$	2465	392	2.45	
	2.0	337	138	3.43	
Case 6 - 12944e	0.6	11902	242	0.76	95.73
	0.8	10916	422	0.79	
	1.0	9090	610	0.97	
	$\sqrt{2.0}$	2517	406	2.15	
	2.0	344	136	3.13	

Finally, the effective conductivity of the plate containing the shaking-geometry, Fig. 4 (b), is analyzed by using the ACA. The effective conductivity shown in Tab. 2 is calculated applying Fourier law to the entire plate. Results are compared with



(a)



(b)

Figure 6: (a) Speed-up ratio as a function of the number of elements, (b) Speed-up ratio as a function of η .

Table 2: Computed effective conductivity for each case

Case	No of Inclusions	Total DOFs	No of Elements	Effective Conductivity
1	14 x 14	6392	3256	0.8152
2	18 x 18	10568	5384	0.8151
3	21 x 21	14392	7336	0.8150
4	24 x 24	18752	9536	0.8148
5	26 x 26	21992	11176	0.8150
6	28 x 28	25488	12944	0.8150
Analytical estimates (Eqs. 6, 7):			k = [0.4954 - 0.8135]	

the analytical formulation showed previously. The Tab. 2 shows the compatibility between the implemented ACA model for random composites and the analytical formulation.

5 Conclusions

In this work, the use of hierarchical matrices and low-rank approximations applied to multiple inclusion potential problems has been presented. Low rank approximations were accomplished by the use of ACA. This method is suitable for memory and time savings, especially in the case of large-scale problems. The admissibility parameter η demonstrated to affect directly the quality of the ACA-generated matrix, as well as, the speed-up ratio. As the parameter decreases, the quantity of generated blocks increases, this is mainly because the admissibility criterion becomes less restrictive. The ACA works better for the cases when the admissibility parameter is less than one, and when the number of elements are greater than 10,000. Additionally, the ACA was applied to a shaking-geometry inclusion configuration for the comparison of the effective conductivity. Results were in accordance with analytical homogenization models.

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