

APPLICATION OF THE BOUNDARY ELEMENT METHOD FOR ORTHOTROPIC DIFFUSIVE PROBLEMS

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Abstract. *Notwithstanding the most realistic rheological models are based on continuum mechanics, research involving oil extraction in rocks has emphasized a simpler approach using hydraulic diffusivity models, based on Darcy's Equation to simulation of the fluid flow. The constitutive medium, in turn, besides a number of important properties, is presented as a non-isotropic material. Thus, the governing equation in these conditions can be given as a special case of the Generalized Scalar Field Equation. On the other hand, the Boundary Element Method (BEM) is a technique that adapts easily to non regular regions and has a high accuracy in simulation problems in which the mathematical field is scalar, particularly models involving the Darcy's Equation. However, the non-isotropic BEM model has not found highlighting in oil extraction applications, confining itself commonly to a limited set of applications in dams. The BEM should be used more ostensibly, since it is particularly suitable to model non regular domains. Aiming future applications in reservoir engineering, this paper presents the mathematical modelling and the implementation of the BEM in orthotropic problems using the classical formulation that uses a correlate non-isotropic fundamental solution. Numerical tests are implemented in problems with known analytical solution and their results are also compared with solutions achieved by the Finite Element Method (FEM), for a better performance evaluation.*

Keywords: *Boundary Element Method, Orthotropic problems, Darcy's model, Finite Element Method, Scalar Field Problems.*

1. INTRODUCTION

The diffusion problems comprise an important range of situations with practical interest for engineering, involving many physical phenomena, such as heat transfer, electromagnetism, and pressure on fluid flow, among others. Regarding the mathematical models, the most known is the Laplace equation, in which the field of variables is time stationary, depending only on their spatial position in the domain.

In many engineering applications, the material properties cannot be assumed isotropic. The commonest examples occur in non-crystalline substances such as sedimentary rocks and wood or as a result of manufacturing of materials such as a rolling or deep-drawing process. Nowadays, there is the example of composite structures, whose are made from two or more constituent materials that, when combined, produce a material with significantly different physical or chemical properties. In important practical cases, the goal is to achieve a suitable balance between the strength and the thermal conductivity.

Other modern and important application concerns oil extraction in rocks. Many mathematical models use hydraulic diffusivity models based on Darcy's Equation to simulation of the fluid flow (Brebbia and Chang, 1979; Vanalli, 2004). The constitutive medium, in turn, besides a number of important properties, is assumed as a non-isotropic constitutive material. In these problems, a rheological approach in which the constitutive properties are based on the Scalar Field Equation can be used to achieve a simpler, but effective numerical solution.

The Boundary Element Method (BEM) is a technique that has a successful retrospective in applications to the Scalar Field problems that include the approach of Darcy's Equation (Chang et al., 1973). Robust formulations have been improved to solve competitively especial cases, such as: physically non homogeneous problems (Divo et al., n.d.), slender problems and Poisson's problems (Wang et al., 2005). The same effort should to be applied to the BEM orthotropic model that curiously has not found highlight in context of researches. Some exceptions concern the work of Zhou et al. (2015) and certain BEM techniques in which the governing equation is changed to the Poisson (Perez and Wrobel, 1992) or Helmholtz Equations (Partridge, 1999). However, these transformations require the solution of domain integrals by approximation techniques that commonly use radial basis functions (Buhmann, 2003) and the Dual Reciprocity approach (Partridge et al., 1992). Thus, in general, there is an absence of comprehensive and recent bibliography in this sense.

Aiming to take advantages of important BEM features, particularly related to approach of non regular regions in applications to reservoir modeling, this paper presents the BEM mathematical fundamentals and performs the numerical solution, compared to the Finite Element Method (FEM) solution, of two basic problems using non isotropic fundamental solution in problems with known analytical solution.

2. BASIC EQUATIONS

Consider homogeneous domains in steady state situation, without sinks or sources. In these simplified conditions, the Generalized Scalar Field Equation (Loeffler, 1992) is given by:

$$\nabla \cdot [\mathbf{K}\nabla u(\mathbf{X})] = 0 \quad (1)$$

In Equation (1), ∇ means the Nabla operator, $u(\mathbf{X})$ is the basic variable or potential; $\mathbf{X} = \mathbf{X}(x_j)$ are coordinates of field points and \mathbf{K} is a dyadic that represents the constitutive properties of physical medium. In two dimensions, matrix representation of \mathbf{K} has four distinct coefficients that concern an anisotropic material (Carlaw and Jaegger, 1959):

$$\mathbf{K} = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix} \quad (2)$$

It is important to use the Cartesian coordinate system in coincidence with the physical crystallographic directions, since it can simplify the mathematical formulation in situations where exist a constitutive symmetry. Indeed, some materials present simpler crystallographic arrangement, such as the monoclinic arrangement, where the dyadic \mathbf{K} is symmetric. However, the most important situation is the orthorhombic arrangement, since the matrix \mathbf{K} is diagonal. For this last case, Eq. 2 is simplified, that is:

$$k_1 \frac{\partial^2 u}{\partial x_1^2} + k_2 \frac{\partial^2 u}{\partial x_2^2} = 0 \quad (3)$$

Figure 1 illustrates the situation described by Eq. 3 and also some significant features of the orthotropic physical model.

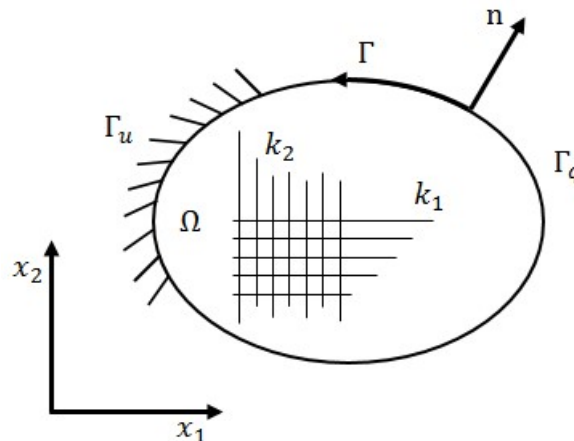


Figure 1. An example of a coordinate system to represent an orthotropic domain.

The essential or Dirichlet boundary condition is those in which the potential $u(\mathbf{X})$ is prescribed. Otherwise, if its derivative $q(\mathbf{X})$ with respect to the outward normal is prescribed, is named natural or Neumann boundary condition. Both types of conditions are respectively exposed the in following equations:

$$u(\mathbf{X}) = \bar{u}(\mathbf{X}) \text{ on } \Gamma_u \quad (4)$$

$$\frac{\partial u(\mathbf{X})}{\partial n} = \bar{q}(\mathbf{X}) \text{ on } \Gamma_q \quad (5)$$

In Equation (5) n is the external unitary normal vector in the point of coordinates \mathbf{X} and Γ_u and Γ_q are parts of the complete boundary $\Gamma(\mathbf{X})$, as shown in Fig. 1.

3. BOUNDARY ELEMENT INTEGRAL EQUATION

Deduction of Boundary Element Integral equation can be done considering fundamentals of the Theory of Integral Equations (Raisinghania, 2011) or then the principles of the Weighted Residuals Methods, such as presented by Brebbia (1978). Considering the first way for convenience, BEM formulation begin taken a strong integral form associated to the governing differential equation (Brebbia et al., 1984), that is:

$$\int_{\Omega} \left(k_1 \frac{\partial^2 u(\mathbf{X})}{\partial x_1^2} u^*(\xi; \mathbf{X}) + k_2 \frac{\partial^2 u(\mathbf{X})}{\partial x_2^2} u^*(\xi; \mathbf{X}) \right) d\Omega(\xi; \mathbf{X}) = 0 \quad (6)$$

In Equation (6) $u^*(\xi; \mathbf{X})$ is an auxiliary function, which in the boundary element method is the fundamental solution. It corresponds to a known solution of a correlated problem, with infinite domain, in which a concentrated source is applied in an arbitrary point ξ , named source point.

The operators that make up the kernel of Eq. (6) are self-adjoint (Brebbia and Walker, 1980), so that it can be applied twice the derivative product rule in the kernel and use the divergence theorem in two of the domain integrals, so as to obtain the following integral equation, commonly called the inverse integral form:

$$\int_{\Gamma} \left[-u \left(k_1 \frac{\partial u^*}{\partial x_1} n_{x_1} + k_2 \frac{\partial u^*}{\partial x_2} n_{x_2} \right) + u^* \left(k_1 \frac{\partial u}{\partial x_1} n_{x_1} + k_2 \frac{\partial u}{\partial x_2} n_{x_2} \right) \right] d\Gamma + \int_{\Omega} u \left(k_1 \frac{\partial^2 u^*}{\partial x_1^2} + k_2 \frac{\partial^2 u^*}{\partial x_2^2} \right) d\Omega = 0 \quad (7)$$

For sake of simplicity:

$$q = k_1 \frac{\partial u}{\partial x_1} n_{x_1} + k_2 \frac{\partial u}{\partial x_2} n_{x_2} \quad (8)$$

In the same way:

$$q^* = k_1 \frac{\partial u^*}{\partial x_1} n_{x_1} + k_2 \frac{\partial u^*}{\partial x_2} n_{x_2} \quad (9)$$

Substituting the Eq. (8) and (9) into Eq. (7), the following equation is obtained:

$$\int_{\Gamma} (-uq^* + u^*q) d\Gamma + \int_{\Omega} u \left(k_1 \frac{\partial^2 u^*}{\partial x_1^2} + k_2 \frac{\partial^2 u^*}{\partial x_2^2} \right) d\Omega = 0 \quad (10)$$

For elimination of the last domain integral in Eq. (10) is taken account the features of the fundamental problem, given by:

$$k_1 \frac{\partial^2 u^*}{\partial x_1^2} + k_2 \frac{\partial^2 u^*}{\partial x_2^2} = -\Delta(\xi; \mathbf{X}) \quad (11)$$

Thus, substituting Eq. (11) into Eq. (10) and applying the properties of the Dirac Delta function, it is possible to achieve the following boundary equation:

$$c(\xi)u(\xi) + \int_{\Gamma} (uq^* - u^*q) d\Gamma = 0 \quad (12)$$

The coefficient $c(\xi)$ depends on the position of its argument, named source point, in relation to the physical domain $\Omega(\mathbf{X}) + \Gamma(\mathbf{X})$. Considering the important situation where the source point is located on the boundary $\Gamma(\mathbf{X})$, its value depends on smoothness of the boundary. (Brebbia et al., 1984).

4. ORTHOTROPIC FUNDAMENTAL SOLUTION

The focal point in the BEM model for orthotropic problems is the determination of the fundamental solution. Thus, it is shown hereinafter in detail. The first step is to operate the following change of coordinates:

$$z_i = \frac{x_i}{\sqrt{k_i}} \quad (13)$$

The substitution of Eq. (13) into Eq. (11), the follow equation is obtained:

$$\frac{\partial^2 u^*}{\partial z_1^2} + \frac{\partial^2 u^*}{\partial z_2^2} = \nabla^2 u^* = -\Delta(\xi; \mathbf{X}) \quad (14)$$

This equation is similar to the Laplace's fundamental problem. Therefore, the radius r , that means the Euclidian distance between the source points and field points \mathbf{X} , now is given by:

$$r = \left[\frac{x_1^2}{k_1} + \frac{x_2^2}{k_2} \right]^{1/2} = [z_1^2 + z_2^2]^{1/2} \quad (15)$$

In Equation (15) z_1 e z_2 represent the directional components of distance between the source point and Field points considered. In two dimensions, the concentrated source $\Delta(\xi; \mathbf{X})$ is written as follows in a new coordinates system (Raisinghania, 2011):

$$\Delta(\xi; \mathbf{X}) = \Delta(\xi; x_1)\Delta(\xi; x_2) = \Delta(\xi; z_1\sqrt{k_1})\Delta(\xi; z_2\sqrt{k_2}) \quad (16)$$

Mathematically, it is possible the substitution of an external singular source by an equivalent natural boundary condition q^* applied uniformly on a circular boundary located around it. Considering the equilibrium condition on this circular boundary with radius r and substituting the Eq. (16) into Eq. (14), this last written suitably in polar coordinates, we have:

$$\int_{\Gamma} q^* d\Gamma = \int_0^{2\pi} \frac{du^*}{dn} r d\theta = - \int_0^{2\pi} \frac{du^*}{dr} r d\theta = \int_{\Omega} \Delta(\xi; z_1\sqrt{k_1})\Delta(\xi; z_2\sqrt{k_2}) d\Omega = \frac{1}{\sqrt{k_1 k_2}} \quad (17)$$

Since the source was replaced by an equivalent natural boundary condition and the angular symmetry exists, the differential equation of fundamental problem becomes simpler, it is given by:

$$\frac{d^2 u^*}{dr^2} + \frac{1}{r} \frac{du^*}{dr} = \frac{\partial}{\partial r} \left(r \frac{\partial u^*}{\partial r} \right) = 0 \quad (18)$$

Making a first integration:

$$\frac{du^*}{dr} = \frac{C_1}{r} \quad (19)$$

Integrating again:

$$u^* = C_1 \ln r + C_2 \quad (20)$$

Substituting the Eq. (19) into Eq. (17), the following equation is obtained:

$$- \int_0^{2\pi} \frac{C_1}{r} r d\theta = \frac{1}{\sqrt{k_1 k_2}} \quad (21)$$

Solving the last integral:

$$C_1 = \frac{-1}{2\pi\sqrt{k_1 k_2}} \quad (22)$$

Integrating again and imposing arbitrarily at $r = 1$ the essential condition equal to zero, the constant C_2 is determined. Thus, in accordance with the original coordinates x_j , we have:

$$u^* = \frac{1}{2\pi\sqrt{k_1 k_2}} \ln \frac{1}{\left[\frac{x_1^2}{k_1} + \frac{x_2^2}{k_2} \right]^{1/2}} \quad (23)$$

The next step is the boundary discretization, wherein it is divided into an arbitrary number of elements, whose definition of the function that describes the field variables along them and the geometric shape of the element is done. In this work, linear isoparametric boundary elements are chosen. Thus, potential and its normal derivative both vary linearly along the straight boundary elements with two nodes located in its extremities.

After the discretization process, the field points \mathbf{X} are used as reference to generate the nodal points, at which the $u(\mathbf{X})$ potential and normal derivative $q(\mathbf{X})$ are calculated or prescribed. For each source point ξ , a scanning related to the integration along the boundary elements is performed, generating a system of algebraic equations that can be written in following standard matrix form:

$$\mathbf{H}\mathbf{u} = \mathbf{G}\mathbf{q} \quad (24)$$

5. NUMERICAL TESTS

In order to verify the capability of BEM formulation to solve orthotropic problems, the examples chosen for numerical simulations have analytical solution. These solutions were obtained by the Separation of Variables Method. BEM results also are compared with the FEM that uses similarly linear functions to interpolate the field variables. This comparison is included, in order to demonstrate the technique effectiveness of BEM in this type of application.

Meshes with different number of nodes are used with both BEM and FEM in the numerical simulations performed. Potential values in internal points with same coordinates are chosen for comparison with analytical values so that a suitable evaluation of the accuracy could be done. In calculating of the average percentage relative error, it was considered the highest analytical value of the potential as the denominator.

5.1 First example

A square domain with unitary sides is subjected to boundary conditions as shown in Fig. 2. Physically, this problem can be interpreted in various ways, depending on the convenience. It can be regarded as a plate in which a temperature field is prescribed in outline but could also be interpreted as a physical domain or porous region, subjected to a potential profile or different piezometric potentials.

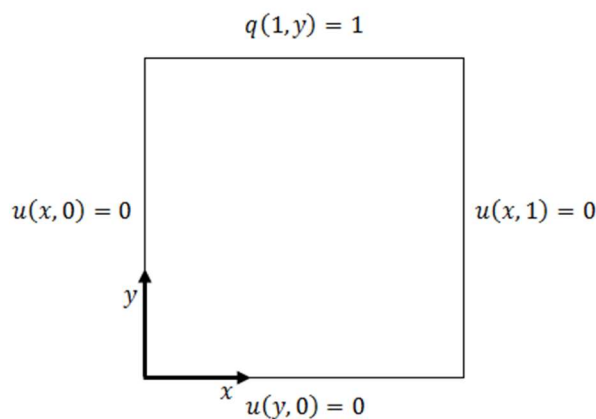


Figure 2. Square plate subjected to both potential such as fluxes prescribed on the boundaries.

The analytical solution for the temperatures in this problem, calculated in a rectangular domain with dimensions $(0, a) \times (0, b)$ using the Variable Separation Method, is given as follows:

$$u(x, y) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1} + 1}{n} \sin\left(\frac{n\pi x}{a}\right) \frac{\sinh\left(\frac{n\pi y}{a} \sqrt{\frac{k_x}{k_y}}\right)}{\left(\frac{n\pi}{a} \sqrt{\frac{k_x}{k_y}}\right) \cosh\left(\frac{n\pi b}{a} \sqrt{\frac{k_x}{k_y}}\right)} \quad (25)$$

A physical interpretation of this example is helpful. The flows coming through all the edges in which the uniform potential is prescribed and go out along the edge where the normal derivative of potential is prescribed. Thus, there is a greater concentration of fluxes in regions near of the vertical superior line.

For convenience, the preliminary BEM results are obtained considering isotropic properties. Subsequently, the properties will be modified in order to emphasize differences caused by the orthotropic properties for each coordinate direction in the numerical model. Particularly, the values of the diffusivity were assumed distinct from real situations, for convenience only, because the goal here is to evaluate the performance of the numerical method. However, in problems

governed by the Laplace equation, only the relationship between the diffusivity properties is important to calculate the potential.

Figure 3 shows the average percentage relative error for the isotropic case with $k_x = k_y = 1$, that represents the Laplace's problem. It can be seen that the results are very good and the values of error are decrease monotonically with the mesh refinement.

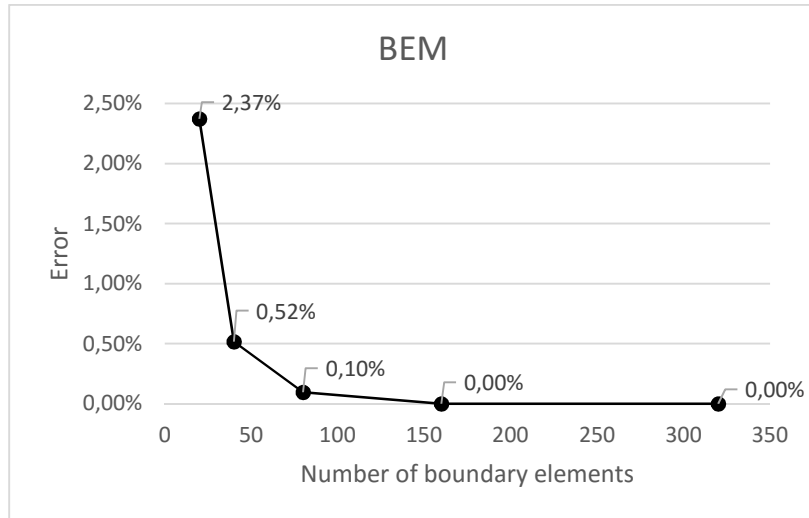


Figure 3. BEM results for the first example considering $k_x = k_y = 1$.

Aiming to demonstrate the capability of the BEM model, results obtained using the FEM are presented in Fig. 4 for better comparison. FEM results of potential were calculated in points with the same coordinates used to the BEM simulations.

It is observed in this case a clear advantage of BEM model, reaching levels much smaller error than the FEM for meshes with much less number of nodal points. It is noteworthy, particularly the reduced error value already achieved with coarser meshes.

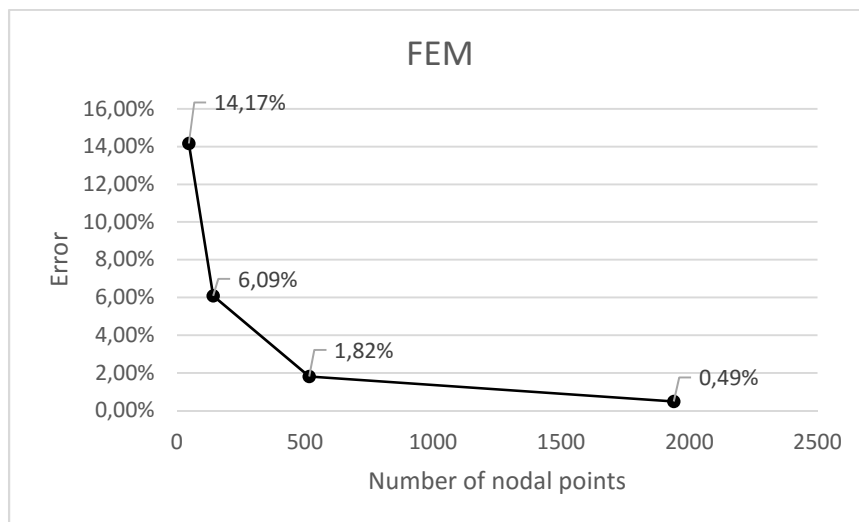


Figure 4. FEM results for the first example considering $k_x = k_y = 1$.

In a second test, the values of the diffusivities are changed to $k_x = k_y = 0.5$. Thus, the problem is still isotropic, but the intention here is to assess the transformation of variables effect, given by Eq. (13), since the distance from the source point to the integration points on the boundary is reduced. Particularly, the values of the diffusivity were assumed distinct from real situations, for convenience only, because the goal here is to evaluate the performance of the numerical method. However, in problems governed by the Laplace equation, only the relationship between the diffusivity properties is important to calculate the potential.

Figure 5 presents the results and, in fact, the errors in all meshes were increased and particularly the accuracy in the coarse mesh was severely reduced.

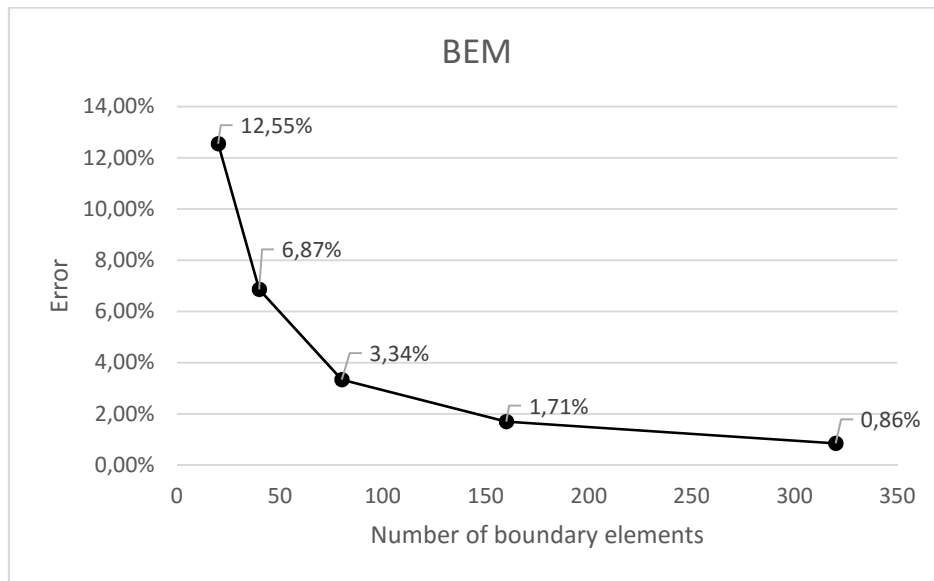


Figure 5. BEM results for the first example considering $k_x = k_y = 0.5$.

Initially, this behavior suggests numerical integration problems, that occur when internal points are positioned very close to the field point on the boundary elements, being necessary to implement an appropriate scheme for numerical integrations, called quasi-singular, which was not implemented in computational code used here. Indeed, the quotient given by Eq. (13) would make a similar effect as locate the points closer, for values of properties smaller than one. For better evaluation concerning the cause of this problem, two easy tests are implemented in this research.

First, the number of points in Gaussian Quadrature was increased in twice, but results do not present any change, indicating that the numerical problems actually are not related to integration problems.

In a second experience, the properties are changed to values that enlarge the distance in fundamental solution given by Eq. (23). Comparisons between results achieved for a mesh with 44 boundary nodes show that the results are sensible to changes occurred in the Euclidian radial distance used to fundamental solution and its normal derivative, as shown in Fig. 6. Making a mesh refinement, both curves converge to the analytical solution with the mesh refinement; however, the way of convergence is different, one of them approaches from below, the other above.

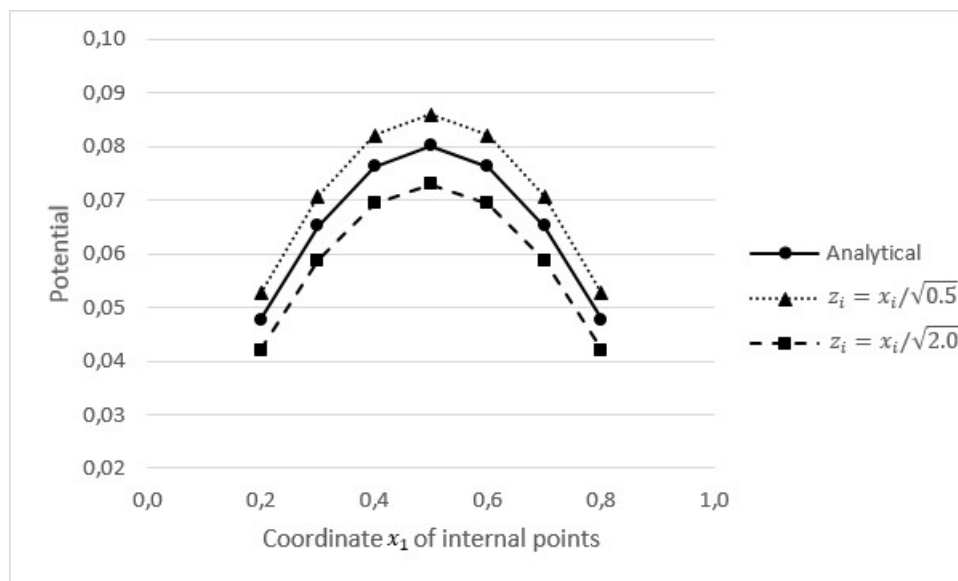


Figure 6. Effect of changed coordinates in BEM results.

In the next simulation, the values of diffusivity are arbitrated as $k_x = 2$ and $k_y = 0.5$. In practical problems, the quotient between orthogonal properties does not overcome this range. The results achieved in the solution of this orthotropic situation are shown in Fig. 7.

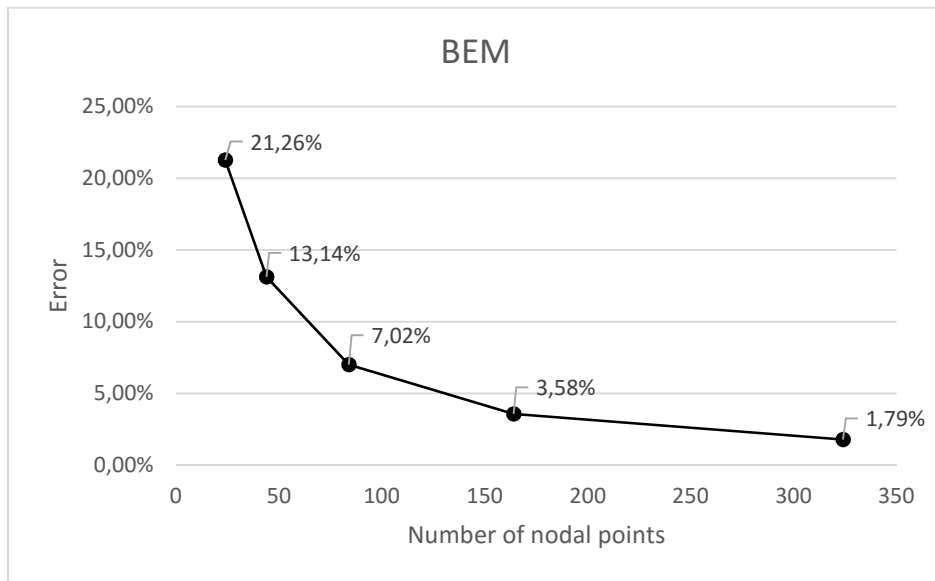


Figure 7. BEM results for the first example considering $k_x = 2$ and $k_y = 0.5$.

Concerning the previous simulation, a significant loss of accuracy is observed in all meshes used, although the level of error is still quite good, particularly in finer meshes. As demonstrated, one cannot attribute this deterioration in performance to the different values of the integration radius. Despite this, the mesh refinement keeps reducing the values of percentage error monotonically, confirming the convergence of the method. By the way, numerical results achieved with the FEM have similar accuracy, as shown in Fig. 8. Concerning the solution of isotropic case shown previously, the FEM performance was improved, if compared to the BEM.

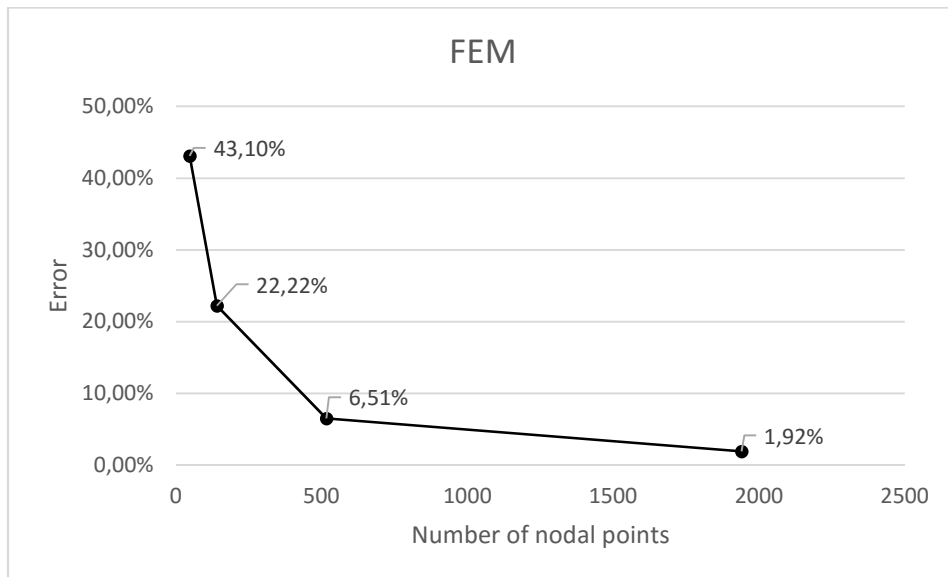


Figure 8. FEM results for the first example considering $k_x = 2$ and $k_y = 0.5$.

5.2 Second example

The same square domain using in previous example is now submitted exclusively to the Dirichlet boundary conditions, according is shown in Fig. 9.

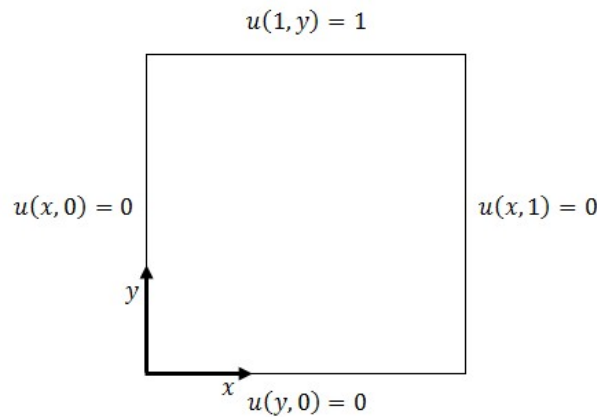


Figure 9. Square plate subjected exclusively to prescribed potentials on the boundaries.

The analytical solution for the temperatures in this problem, calculated in a rectangular domain with dimensions $(0, a) \times (0, b)$ using the Variable Separation Method, is given as follows:

$$u(x, y) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1} + 1}{n} \sin\left(\frac{n\pi x}{a}\right) \frac{\sinh\left(\frac{n\pi y}{a} \sqrt{\frac{k_x}{k_y}}\right)}{\sinh\left(\frac{n\pi b}{a} \sqrt{\frac{k_x}{k_y}}\right)} \quad (26)$$

There is a discontinuity in the potential field, so that the heat fluxes are very intense in these regions, relative to the upper corners. This situation is unrealistic in practice, but serves particularly to test the robustness of the BEM, which deals with the discontinuous values in your system of equations, since it is a mixed method, dealing with potential and its normal derivative together. Already the FEM, by its mathematical formulation eliminates the rows and columns of the matrix system that are related to prescribed potential conditions, mitigating the effect of discontinuities in this variable.

Despite these discontinuities – that would generate in matrix system two equal lines, requiring the changing of coordinates of double nodes in the corner – good results were achieved for finer meshes for this simulation, as shown in Figure 10, taking the constitutive properties $k_x = 2$ and $k_y = 0.5$.

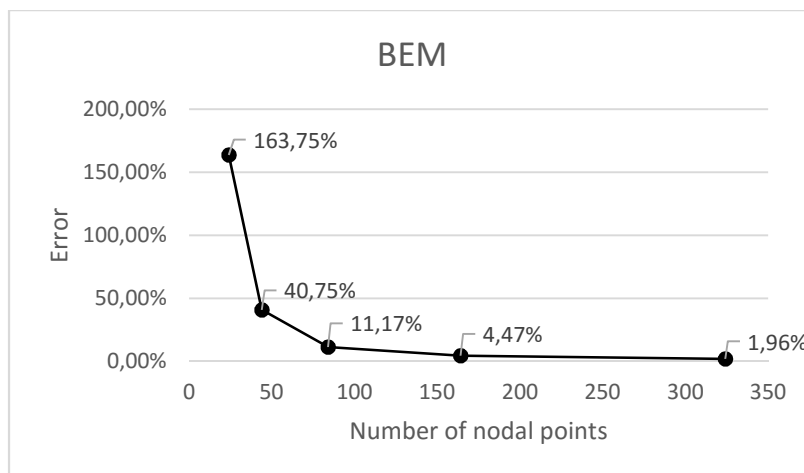


Figure 10. BEM results for the second example considering $k_x = 2$ and $k_y = 0.5$.

It is noteworthy that k_y being four times smaller than k_x and being heat flows directed in the vertical direction, the problem becomes numerically still more difficult. This justifies the high error achieved for coarse meshes. However, the BEM absorbed well as the discontinuity, since the error curve of BEM has been presented monotonicity and the percentage error was reduced continually with the mesh refinement.

For better evaluation, results achieved with the FEM are shown in Fig. 11. It can be observed a slightly superiority of FEM in this case, since for the same number of nodal points its results are in near of 1,5%.

It is noteworthy that in BEM model, values of potentials within the domain are calculated on the basis of boundary nodal values of potential and normal derivatives, previously calculated. As stated earlier, the discontinuities generate extremely high fluxes on the boundary, which contribute to the relative loss in accuracy of BEM results.

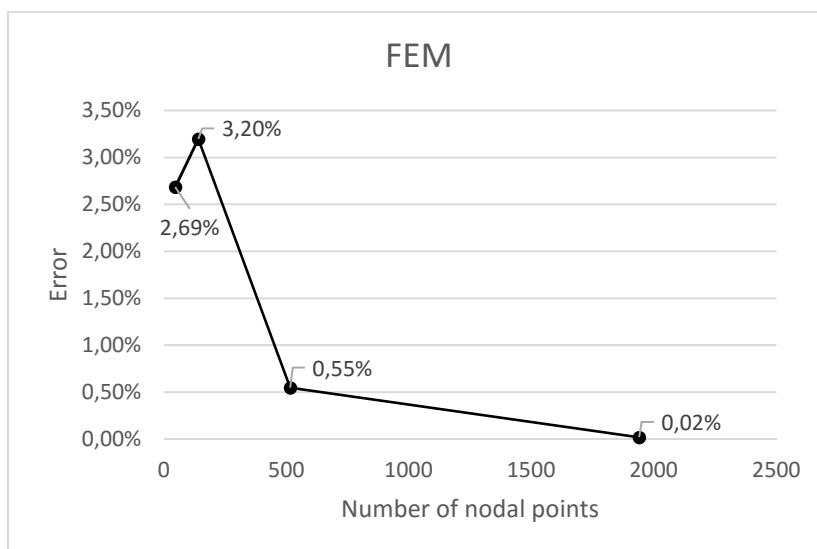


Figure 11. FEM results for the second example considering $k_x = 2$ and $k_y = 0.5$.

5. CONCLUSIONS

Being a technique that discretizes just the boundary, the BEM presents suitable features to model non regular domains, that is a topic that has been object of many researches involving numerical methods applied in engineering. However, its orthotropic models have not been widely researched, despite the interest of these problems and optimal performance of BEM in other scalar field problems.

Thus, the purpose of this paper was to examine the application and potentiality of the BEM in this kind of problem in two dimensions. Two simulations were performed in detail, to examine the particularities of BEM for different relations between constitutive properties. Results were compared with available analytical solutions and the FEM. The performance was satisfactory, since the percentage average error always decrease monotonically with the mesh refinement, reaching small values that are suitable regarding to usual engineering applications.

However, it was observed that the degree of orthotropy affects the BEM results. It is due to the mathematical procedure used for transform the orthotropic problem in an equivalent isotropic one, in which is done by a change in coordinates. This alters the Euclidian distance that characterizes the fundamental solution and its normal derivative in a proportion given by the quotient given by the orthotropic properties. This effect is more sensible in coarse meshes; despite the final errors also increase more slightly for finer meshes. Since that in problems governed by Laplace's Equation with two-dimensions just the quotient between properties is important, a more suitable BEM performance is achieved avoiding that one Cartesian coordinate is more affected than other.

It must be highlighted that the orthotropy also affected the performance of the FEM, as shown in comparisons performed.

Lastly, is possible to conclude that the BEM performance was higher than that presented by FEM in the case where Neumann and Dirichlet conditions appeared together, which represents the practical engineering problems. In the case where there were discontinuities resulting from the exclusive application of Dirichlet conditions, the BEM had lower performance than the FEM. The reason is due the BEM internal values are obtained from the combination of potential and flows calculated on the boundary. However, even this test, purposely addressed to evaluate its numerical robustness, the BEM showed continuous reduction of errors and quite acceptable results.

6. ACKNOWLEDGEMENTS

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