Extension of the Variational Self-Regular Approach for the Flux Boundary Element Method Formulation

P. A. C. Porto[1], A. B. Jorge[1] and G. O. Ribeiro[2]

Abstract: This work deals with a numerical solution technique for the self-regular gradient form of Green's identity, the flux boundary integral equation (flux-BIE). The required $C^{1,\alpha}$ inter-element continuity conditions for the potential derivatives are imposed in the boundary element method (BEM) code through a non-symmetric variational formulation. In spite of using Lagrangian C^0 elements, accurate numerical results were obtained when applied to heat transfer problems with singular or quasi-singular conditions, like boundary points and interior points which may be arbitrarily close to the boundary. The numerical examples proposed show that the developed algorithm based on the self-regular flux-BIE are highly efficient, and quite straightforward in that no integral transformations are necessary to compute the singular integrals and even a small number of integration Gauss points gives very accurate results. The variational self-regular flux-BIE formulation has improved the results for quadratic elements, while only minor improvements were obtained for higher order elements. The proposed approach is also compared with other formulations showing to be a robust alternative as a BEM approach in heat transfer problems.

keyword: BEM - Boundary Element Methods, Variational Formulation, Self-Regular Formulations, Near-Boundary Heat Transfer.

1 Introduction

The purpose of this work is to extend the non-symmetric variational self-regular traction-BEM formulation recently presented by Jorge, Cruse, Fisher and Ribeiro (2003) to the flux-BIE, demonstrating its application through classical heat transfer examples and problems with quasi-singular conditions (in what follows, 'quasi'

means that an interior or a boundary source point is very close to the element where the integral is being evaluated).

The main disadvantage that has prevented the generalized use of BEM algorithms is the mathematical singularity that appears on the fundamental solutions of the governing equations leading to the use of analytical, semi-analytical or special integrations schemes to prevent the loss of stability and precision, see Sladek and Sladek (1998).

One of the techniques to eliminate the need for special numerical integration procedures for singular integrals is regularization. Several approaches for regularization can be found in the literature, such as for potential, elasticity and fracture mechanics problems, as seen in Bonnet (1999), Cruse and Richardson (2000), and Dominguez, Ariza and Gallego (2000). Most of these approaches require the primary variable to have $C^{1,\alpha}$ smoothness and the unit normal to be continuous, at the collocation point. These continuity requirements ensure that the resultant integrals are convergent, i.e. that the regularization is effective.

According to Krishnasamy, Rizzo and Rudolphi (1992), a sufficient condition for the existence of the hypersingular integral is the $C^{1,\alpha}$ continuity of the density function at the source point. Standard isoparametric boundary elements do not satisfy this requirement and for this reason, approximate solution techniques for solving hypersingular integral equations by means of the BEM require special consideration. One of them is the self-regular formulation proposed by Huang and Cruse (1994) and developed by Cruse and Richardson (2000) and by Jorge, Ribeiro, Cruse and Fisher (2001). This formulation, based on conforming C^0 elements, uses the idea of "relaxed" continuity, as these elements do not comply with the above continuity requirement. Indeed, standard isoparametric boundary elements provide only a piecewise $C^{1,\alpha}$ interpolation, which is the basis for this so-called relaxed continuity approach.

[1] Institute of Mechanical Engineering, UNIFEI - Federal University of Itajubá-MG, BRAZIL.
Email: ariosto.b.jorge@unifei.edu.br
[2] Department of Structural Engineering, UFMG Federal University of Minas Gerais-MG, BRAZIL

In spite of the very successful numerical results reported by Richardson, Cruse and Huang (1997) and Richardson and Cruse (1999) using various forms of these relaxed algorithms combined with piecewise $C^{1,\alpha}$ interpolations, Krishnasamy, Rizzo and Rudophi (1992) and Martin and Rizzo (1996), have concluded that these algorithms could not be theoretically justified. This means that from a strictly mathematical point of view, only boundary element implementations that ensure $C^{0,\alpha}$ or $C^{1,\alpha}$ continuity at each collocation point can be applied in the discretizations of the standard, or the hypersingular boundary integral equations, respectively.

Martin, Rizzo and Cruse (1998) renewed the discussion between the theoretical continuity requirements and the good numerical results reported by Cruse and his co-workers. They reaffirm the smoothness requirements of the density function for the existence of limits to the boundary, which give rise to Cauchy-singular and hypersingular integral equations, and they have pointed out two possibilities for relaxing the theoretical smoothness requirements. The first possibility is the introduction of various apparent or "pseudo-limits" to the boundary, and the second one is the relaxed regularization in which a regularized integral equation, derived rigorously under certain smoothness assumptions, is used when less smoothness is available.

As shown in Martin, Rizzo and Cruse (1998), a BIE under relaxed continuity conditions is related to a pseudo-limit to the boundary. The limit exists, the results are bounded, but there is no theoretical study showing that these results correspond to the unique solution of the original boundary value problem, although some previous numerical results were promising.

Introducing constraints equations into the original system of equations Jorge, Cruse, Fisher and Ribeiro (2003) presented a non-symmetric variational approach. In that paper, $C^{1,\alpha}$ continuity requirement was enforced at inter-element nodes for the self-regular traction-BIE discretized using the relaxed continuity approach with Lagrangian C^0 elements. With this approach, the authors reported impressive improvements.

It should be pointed out that all the aforementioned discussions are related to the collocation approach for the traction-BEM using conforming C^0 elements. Other solutions of the traction-BIE through either global Petrov-Galerkin type BEM (Han and Atluri, 2003) or through the meshless local Petrov-Galerkin methods (Atluri, Han and Shen, 2003) have also being shown very promising, especially for solving elastic problems in which the singularities in any variable are of primary concern.

A non-symmetric variational form for the self-regular flux-BIE is implemented for quadratic and higher order elements in this work. The validity of the relaxed continuity hypothesis in the self-regular flux-BIE implementation is investigated by comparing the numerical results of benchmark problems and quasi-singular heat transfer problems. For comparison purposes, a previously derived local error estimator based on an external formulation for the potential is extended in this work to include also the evaluation of the gradient magnitude at exterior points, and thus two independent measures of the external local error are implemented.

2 Self-regular BEM formulations

2.1 Self-regular flux-BIE for 2-D potential problems

The standard boundary integral equation (BIE) formulations lead to singular integrals for which the computation can be simplified if these formulations are written in a self-regular bounded form. Using the proposed approach applied to Green's identity for 2-D Laplace's equation, a self-regular flux-BIE can be obtained. In this section this formulation is only presented, and further details can be found in Jorge *et al*. (2001) and in Cruse and Richardson (1999).

Green's second identity for Laplace's equation is written as follows, using the 2-D fundamental solutions integrated over the closed boundary plane curve $S = \sum_{i=1}^{m} S_i$, where each S_i curve segment is taken to be smooth in the sense of Liapunov (Kupradze, 1979).

$$2\pi\phi(y) = -\int_{s} \phi(s)\vec{\nabla}\ln\left(\frac{1}{r(s,y)}\right)\cdot\vec{n}(s)\,dS +$$
$$\int_{s} \vec{\nabla}\phi(s)\cdot\vec{n}(s)\ln\left(\frac{1}{r(s,y)}\right)dS \qquad \forall y \in R \tag{1}$$

The boundary S bounds the finite plane region R with outward unit normal vector $\dot{n}(s)$. The points y and s are taken to be the interior free point and the boundary integration point respectively. The fixed boundary point x may be at an intersection of two curved segments. The interior $y \in R$ form of the Green's identity is given by the following combination of double and single layer potentials as in Eq. 1, where the term $\vec{\nabla}\phi(S)$ is the gra-

dient of the potential ϕ evaluated at the boundary point s unless otherwise noted by a subscript.

The potential field $\phi(y)$ satisfies Laplace's equation and the boundary conditions (B.C.) for the finite region. Using the directional derivative definition, then

$$\vec{\nabla} \ln\left(\frac{1}{r(s,y)}\right) \cdot \vec{n}(s) = \frac{d}{dn}\ln\left(\frac{1}{r(s,y)}\right) \tag{2}$$

Equation 2 represents the derivative of the fundamental solution in the outward normal direction defined by $\dot{n}(s)$.

The Green's identity for problems in which the potential field is continuous in the Hölder sense can be regularized (Dominguez *et al.*, 2000). The Hölder continuity condition is denoted as $T(y) \in C^{0,\alpha}$, $\alpha > 0$. The procedure of regularization consists in subtracting and adding back the integral:

$$\phi(x)\int_S \vec{\nabla}\ln\left(\frac{1}{r(s,y)}\right) \cdot \vec{n}(s)\, dS \tag{3}$$

Equation 3 has the value of $\phi(x)(-2\pi)$, as the swept angle integral of the two-dimensional closed boundary is 2π for any $y \in R$. The self-regular form of the potential-BIE is then given by

$$2\pi\phi(y) = 2\pi\phi(x) + \int_S \vec{\nabla}\phi(s) \cdot \vec{n}(s)\ln\left(\frac{1}{r(s,y)}\right) dS$$
$$- \int_S [\phi(s) - \phi(x)]\vec{\nabla}\ln\left(\frac{1}{r(s,y)}\right) \cdot \vec{n}(s)\, dS \tag{4}$$

The first integral in Eq. 4 is regular and bounded for all points, while the second is weakly singular but also bounded. The result is called self-regular in the sense that the mathematical properties of the double-layer potential and the Hölder continuity of the harmonic function as $y \rightarrow s$ are all that is required to modify the original formulation, as discussed in Jorge *et al.* (2001).

Since Eq. 4 is continuous for $y \rightarrow x$, $\forall x \in S$, including at corners, by taking the limit to the boundary, the boundary integral equation is obtained for all boundary points, and is given by

$$0 = -\int_S [\phi(s) - \phi(x)]\frac{d}{dn}\ln\left(\frac{1}{r(s,x)}\right) dS +$$
$$\int_S \frac{d\phi}{dn}\Big|_S \ln\left(\frac{1}{r(s,x)}\right) dS \tag{5}$$

The self-regular form of the flux-BIE is derived by taking the gradient of the integral representation for the potential at the interior point y, followed by subtracting and adding back a linear potential field given by $\phi^L(s) = \phi(x) + \phi_{,i}?_x[x_i(s) - x_i(x)]$. The gradient of this linear field is given by $\nabla\phi^L(s) = \nabla\phi(x)$. This use of a linear field is the analogous operation for the gradient equation as the constant field is for the regular potential representation. The resultant equation is the self-regular form of the potential gradient at an interior point y, which is regular for all interior point limits to the boundary, where the continuity condition $\phi(y) \in C^{1,\alpha}$ is satisfied.

By taking the limits to the boundary, $y \rightarrow x$, at all boundary points satisfying the condition $\phi(y) \in C^{1,\alpha}$, at any given point $s \equiv x$, the following regular boundary integral equation is obtained

$$0 = \int_S [\phi(s) - \phi^L(s)]\ln\left(\frac{1}{r(s,x)}\right)_{,ij} n_j(s)\, dS -$$
$$\int_S [\vec{\nabla}\phi(s) - \vec{\nabla}\phi(x)] \cdot \vec{n}(s)\ln\left(\frac{1}{r(s,x)}\right)_{,i} dS \tag{6}$$

This vector equation is called the gradient-BIE Green's identity for potential theory. This equation is overspecified and it is usual to operate on it with the local normal $n_i(x)$. The resulting scalar equation is called the flux-BIE, and this is the usual scalar form which produces the best numerical results. The flux-BIE is expressed by:

$$0 = n_i(x)\int_S [\phi(s) - \phi^L(s)]\ln\left(\frac{1}{r(s,x)}\right)_{,ij} n_j(s)\, dS -$$
$$n_i(x)\int_S [\vec{\nabla}\phi(s) - \vec{\nabla}\phi(x)] \cdot \vec{n}(s)\ln\left(\frac{1}{r(s,x)}\right)_{,i} dS \tag{7}$$

It is worth noting that the above self-regular formulations, the potential-BIE in Eq. 5 and the flux-BIE in Eq. 7, were obtained through manipulation and limit to the boundary of the integral equations before discretization. The self-regular form of these equations and their limit to the boundary are predicated on the same continuity requirements that went into the derivation of the singular integrals in the original problem, before regularization. Thus, the regularized integrals contain no strong or non-integrable singularity only if the density is sufficiently continuous at the limit as the field point goes to the boundary, as assumed in the derivations.

2.2 Self-regular BEM formulations including domain sources

A very common heat transfer problem arises in the evaluation of the potential field when nonzero interior heat sources are present. In these cases, a contribution term should be added in the right-hand side of Eq. 5 and Eq. 7 as a domain integral. The domain integral to be added to Eq. 5 has the form

$$-\int_{\Omega} \ln\left(\frac{1}{r(p,x)}\right) b(p) dV(p) \tag{8}$$

while the domain term to be added to Eq. 7 corresponds to the gradient form of the term in Eq. 8.

The heat source $b(p)$ can be a laser beam aimed to any point. In this case, the domain point source could be interpreted as a singularity in the potential field at the point source. So, the source can be written as $Q_D*\delta(y,X_D)$, where Q_D is the magnitude of a domain source located at the point X_D and $\delta(y, X_D)$ is the Dirac Delta function. For an interior point $y \neq XD$, then $\delta(y,X_D) = 0$, and the potential field is continuous.

In the case of N_D domain point sources, the integral on the domain is transformed in just the sum of the value of each magnitude Q_D times the fundamental solution at point $p = P_D$. In this case, the self-regular potential-BIE and flux-BIE can be written respectively as (Jorge, Porto e Ribeiro, 2004):

$$0 = -\int_{S} [\phi(s) - \phi(x)] \frac{\partial}{\partial n} \ln\left(\frac{1}{r(s,x)}\right) dS +$$
$$\int_{S} \frac{\partial}{\partial n} \phi(s) \ln\left(\frac{1}{r(s,x)}\right) dS + \sum_{I=1}^{N_D} Q_D(I) \ln\left(\frac{1}{r(P_D,x)}\right) \tag{9}$$

$$0 = n_i(x) \int_{S} [\phi(s) - \phi^L(s)] \ln\left(\frac{1}{r(s,x)}\right)_{,ij} n_j(s) dS -$$
$$n_i(x) \int_{S} [\vec{\nabla}\phi(s) - \vec{\nabla}\phi(x)] \cdot \vec{n}(s) \ln\left(\frac{1}{r(s,x)}\right)_{,i} dS + \tag{10}$$
$$n_i(x) \sum_{I=1}^{N_D} Q_D(I) \vec{\nabla} \ln\left(\frac{1}{r(P_D,x)}\right)$$

For domain points approaching the source point where the singularity is concentrated, numerical difficulties may arise when evaluating the potential field. The singular point is out of the domain where the potential is

defined, so the solution for the potential field at interior points in the vicinity of the point source is also seen as a near-boundary heat transfer problem.

On the other hand, if the domain has one dimension that is much smaller than the other one, then the domain point source will be located very close to some part of the boundary, this can represent a quasi-singularity in the boundary solution at a boundary points close to this domain point source.

Equations 9 and 10 allow the evaluation of the influence of domain sources for the aspect ratio problem and for the near-boundary interior point problem, either problem considered separately or in combination.

3 Variational self-regular BEM formulation for potential problems

The discretization of the self-regular flux-BIE into C^0 elements violates the $C^{1,\alpha}$ continuity requirements for the flux at the interface between adjacent elements. In this section, a non-symmetric variational approach, similar to the one proposed by Jorge *et al*. (2003), is developed for potential problems, leading to a set of subsidiary constraint equations to enforce $C^{1,\alpha}$ continuity on the smooth parts of boundary when discretized using the relaxed continuity.

3.1 $C^{1,\alpha}$ continuity for the potential derivatives at smooth inter-element nodes

By noting $\vec{q} = d\phi/d\vec{n}$, the geometry x_k, the potential ϕ_k and the flux q_k in the above self-regular potential-BIE formulations can be obtained based on a discretization using standard isoparametric functions, N_i:

$$x_k(S) \approx x_k(\xi) = \sum_{i=1}^{m} N_i(\xi) x_k^i$$
$$\phi_k(S) \approx \phi_k(\xi) = \sum_{i=1}^{m} N_i(\xi) \phi_k^i \tag{11}$$
$$q_k(S) \approx q_k(\xi) = \sum_{i=1}^{m} N_i(\xi) q_k^i$$

Using the relaxed continuity approach, the same discretization is applied to the above self-regular flux-BIE formulations.

Considering that the potential derivatives are evaluated independently for each element in terms of nodal potentials and fluxes, a jump discontinuity in the potential

derivatives ($\Delta\phi_{,i}$) as evaluated in the first node ($\xi = -1$) of element *I*, in comparison with its evaluation at the last node ($\xi = 1$) of the previous element $I - 1$ can be defined as:

$$\Delta\phi_{,i}^I = \phi_{,i}^I(\xi = -1) - \phi_{,i}^{I-1}(\xi = 1) \tag{12}$$

The strategy that follows is to introduce constraint equations to enforce the C^0 discretized regularized potential density, $\phi(S) - \phi^L(S)$ in Eq. 7 or Eq. 10, to have zero value and zero derivative at the inter-element source points where the boundary is smooth. In other words, the goal is to eliminate any "jump" discontinuity of the potential derivatives, as defined in Eq. 12, at all the smooth boundary inter-element source points.

For the 2-D case, an inter-element node shares two continuous elements. In this case, the normal unit vector is continuous at the smooth node, leading to a simpler set of equations where only the equations for continuity of derivatives in the tangent direction (noted in what follows as $i = 1$) need to be introduced as constraint equations in the original formulation:

$$\phi_{,1}^I(\xi = -1) = \phi_{,1}^{I-1}(\xi = 1)$$

$$\frac{\phi_{,\xi}^I(\xi = -1)}{J^I(\xi = -1)} = \frac{\phi_{,\xi}^{I-1}(\xi = 1)}{J^{I-1}(\xi = 1)} \tag{13}$$

where $J(\xi)$ is the Jacobian of the transformation between the original boundary element (of coordinate *S*) and the standard element (of coordinate ξ). Also, the potential derivatives, $\phi_{,i}$, are obtained from Eq. 11:

$$\phi_{,i} = \sum_{i=1}^{m} N_i'(\xi)\phi^i \tag{14}$$

The new set of equations to be obtained uses only boundary unknowns evaluated at existing nodes, so no extra variables are added. Writing these constraint equations in matrix notation gives:

$$[Q_{dd}]\{q\} = \{0\} \tag{15}$$

It has to be pointed out that, in this work, only the variational formulation with constraint equations defined at smooth nodes is implemented, adapted from a similar formulation for the elasticity problem presented in Jorge *et al.* (2003). As discussed by the authors in that case, the implementation of an equivalent variational formulation, for the variables in global coordinates at corner nodes, lead to poor numerical results, and thus this corner-node variational formulation is not implemented here.

3.2 *System of equations from minimization of energy functional*

In Brebbia, Telles and Wrobel (1984) it was shown that the total potential energy functional for an elastic system could be written in terms of boundary integrals only. An extension for the potential case could be written as $\Pi = \Pi = (\phi, q)$. Now introducing the approximation of *{ϕ}* and *{q}* using the element shape functions, the potential energy functional Π can be rewritten with respect to nodal boundary variables as $\Pi = \Pi(\phi^n, q^n)$. A non-symmetric system of equations can be obtained by requiring the first variation $\delta\Pi$ to be zero. Because each variation $\delta\phi^n$ and δq^n is arbitrary, a system of equations is obtained.

The boundary solution must satisfy the self-regular flux-BIE a priori. The solution for the system of equations *[A]{x}={b}* obtained from the discretized BIE is unique, provided the appropriate inter-element continuity and boundary conditions are imposed. In the 2*N*-dimensional space for the boundary solution, where *N* is the number of boundary nodes, the solution of the BIE is represented by one point. This boundary solution satisfies exactly the original boundary value problem in the *N* collocation points.

On the other hand, new equations have been added to the problem constraining this boundary solution to satisfy a minimum in the potential energy. The problem is over-constrained because the boundary solution must satisfy both the BIE at a finite number of collocations points and the minimum condition for the energy functional on the entire boundary. When using the collocation approach, the boundary solution is exact at the boundary nodes and approximated everywhere else. Also, the exact solution for the boundary value problem corresponds to the minimum of the potential energy functional. Only in the limiting situation, when the number of collocation points tends to infinity (and the element sizes tend to zero), will both equations represent exactly the same constraint for the boundary variables. For a sufficiently large number

of collocation points, the solution to the discretized BIE is approximately equivalent to the solution of the problem of minimization of the functional Π.

$$\left\{ \begin{array}{cc} \frac{\partial \Pi}{\partial \phi^n} & \frac{\partial \Pi}{\partial q^n} \end{array} \right\} = \{0\} \overset{approx.}{\Leftrightarrow} [A]\{X^n\} = \{B\} \qquad (16)$$

A variation about the original solution can be allowed so that this perturbed solution now is imposed to satisfy a set of modified equations (to include extra degrees of freedom) and a number of subsidiary equations. In this work, the subsidiary equations are given by the inter-element continuity conditions for the temperature derivatives as explained in Section 3.1.

For each new subsidiary equation, one Lagrange multiplier is inserted allowing for a variation of the solution in the form of a set of $\{\lambda_{dd}\}=\{\lambda_\phi \lambda_q\}^T$. For 2-D problems, a set of at most $2N$ equations (depending on the boundary conditions) is added to the original system of $2N$ equations, and the boundary solution is now embedded in an expanded set of variables $\{\phi^n, q^n , \lambda_T, \lambda_q\}^T$ of dimension at most $4N$. In a general case, subsidiary constraint equations and the corresponding degrees of freedom in the form of Lagrange multipliers can be added to a particular BEM formulation obtained from the discretization of the BIE so that extra relations for both the nodal temperatures and fluxes can be enforced. An augmented Lagrangian functional L can be constructed from the original functional $\Pi = \Pi(\phi^n, q^n)$ and the subsidiary constraint equations as

$$L(\phi^n, q^n, \lambda) = \Pi(\phi^n, q^n) + \{\{\phi^n\}^T \{q^n\}^T\}[Q_{dd}]\{\lambda_{dd}\}$$
$$(17)$$

so that the problem of minimization of the functional Π with the constraining subsidiary equations is recast as a problem of finding the stationary point of the augmented Lagrangian L. The first variation of the Lagrangian $\delta L=0$ gives an augmented system of equations for the nonsymmetric variational BEM formulation.

The approximate boundary solution is a perturbation or variation from the original BIE solution. This approximate solution satisfies the modified discretized BIE and the subsidiary constraining equations for the boundary solutions, forming an expanded set of equations. The original problem for minimization of the functional Π is

now transformed into a constrained minimization problem with subsidiary equations.

This approach possesses some similarity to that employed by Mustoe, Volait and Zienkiewicz(1982) for a variational symmetric BEM formulation, except that constraining equations for equilibrium of stresses were enforced in that case, instead of the inter-element continuity equations used here. In this work, the system of equations is non-symmetric and the double integrations to symmetrize the system of equations are not needed. Thus, no extra equations, such as the ones that would be equivalent to the equilibrium of stresses used in the case referenced, are needed to be enforced here as an extra set of constraining equations.

Technically, the implementation of this non-symmetric variational approach simply involves obtaining the augmented system of equations directly from the existing system of equations *[A]{x}={b}* of the discretized BIE, and adding to this system extra columns of the form *[Q]ᵀ{λ}* and extra rows of the form *[Q]{ϕⁿ   uⁿ}ᵀ = 0*. Finally, a boundary solution is obtained by solving the augmented system of equations for this expanded set of variables, now including both the boundary variables and the Lagrange multipliers.

The boundary conditions and the appropriate inter-element continuity conditions for temperature and fluxes are imposed now for the added terms involving the matrices $[Q_{dd}]$ so that the augmented system of equations can be solved. Besides the original $2N$ nodal temperature and flux variables, $2N$ (at most) extra unknowns in the form of Lagrange multipliers $\{\lambda_{dd}\}$ are added to account for the subsidiary equations enforcing the inter-element continuity of the displacement derivatives. By enforcing the boundary conditions, the subsidiary equations are rewritten as in Eq. 15, so that the augmented system of equations is obtained as

$$\left[\begin{array}{cc} [A] & [Q_{dd}]^T \\ [Q_{dd}^{\phi^n} Q_{dd}^{q^n}] & [0] \end{array} \right] \left\{ \begin{array}{c} X \\ \lambda_{dd} \end{array} \right\} = \left\{ \begin{array}{c} B \\ B_{dd} \end{array} \right\} \qquad (18)$$

which is obtained from the original system of equations by adding $2N$ (at most) extra columns and rows to matrix $[A]$. The number of additional equations depends on the boundary conditions. If the potential is prescribed at all nodes in both adjacent elements, then the corresponding constraining equation has no boundary unknowns associ-

ated with it and is a redundant equation. In this case, no constraining equation is added. The added columns and rows represent sparse sub-matrices.

4   Numerical results

Some numerical examples of two-dimensional heat transfer problem problems are performed to evaluate the strategy proposed. In all cases the numerical integrations are performed using eight Gaussian points.

The boundary solution accuracy is analyzed comparing the numerical results either to an analytical solution or using an error estimator. The error estimator proposed herein is an extension of a local and global error estimator derived by Jorge, Ribeiro and Fisher (2001). The essentials of the approach are summarized below.

Boundary integral equation (BIE) formulations are exact representations of boundary value problems (BVP). In spite of that, errors may appear in the discretization process because the BIE is valid only at a finite number of collocation points.

The error estimator is based on the fact that the accuracy in the boundary solution plays an important role on the accuracy on any interior point solution. If exterior points are treated as interior points, i.e. solutions at exterior points are evaluated using the interior point's subroutine, thus the solution at those points will reflect the accuracy on the boundary.

As both the exact potential and the exact gradient magnitude at any external point should be zero, any depart from zero in the numerical solution will be an indication of error. The closer is this external point to some region of the boundary, the more this error indicator is influenced by this part of the boundary. Thus, by positioning this external point at a small distance with regard to an element, most of the contribution to the error will come from this element, giving a local measure of the error (the element error).

On the other hand, because fundamental solutions are functions of the distance between source and field points, the error measure is sensitive to the external point position for non-trivial problems. In this work, a distance of 0.25 of the size of the element closer to the external point is selected, following Jorge *et al.* (2001).

4.1   Square domain

At first, the code is used in a very simple problem of a square domain, with straight line elements, as shown in Fig. 1. The exact density variation is either constant or linear throughout the boundary due to the boundary conditions. Any BEM solution can easily follow this distribution, regardless of the integration order, or the interpolation polynomial used. Thus, this problem could work as an approximate "patch" test.

It should be noted that an exact patch test is taken to be one in which the solution is within computer accuracy, regardless of the order of integration (at least above some low-level integration order).

As stated above, this problem has an analytical solution and according to Fourier's law, the flux and potential are either constant or vary linearly throughout the boundary. Thus, for any interpolation polynomial of order higher or equal than one, there is no error related to the interpolation of these quantities in the boundary. Hence, any errors present in the numerical solution must be due to the formulation itself.
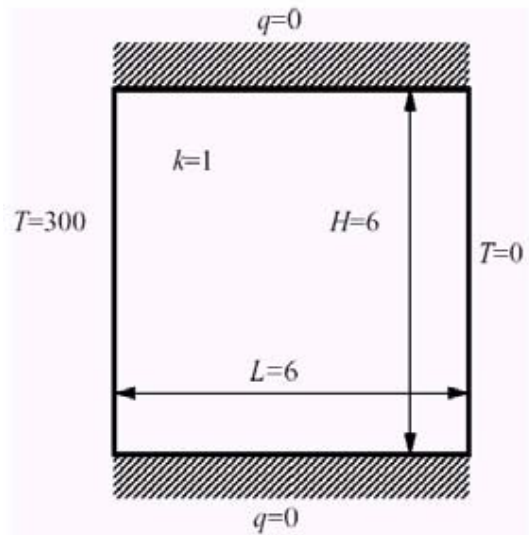

Figure 1 : Square domain

Table 1 summarizes, for four-element meshes, the relative errors for potential and flux obtained with the variational and non-variational approaches of the self-regular flux-BIE. The square domain patch test reveals that, even for a coarse discretization, the variational self-regular flux-BIE produces highly accurate results, which are of the order of machine precision in some cases.

Table 1 : Variational and non-variational flux-BIE

Element	Potential: Magnitude of maximum error (%)	
	Variational	Non- Variational
Quadratic	Mach. precision	$\sim \quad 10^{-14}$
Cubic	Mach. precision	$\sim \quad 10^{-10}$
Quartic	$\sim \quad 10^{-12}$	$\sim \quad 10^{-10}$

Element	Flux: Magnitude of maximum error (%)	
	Variational	Non- Variational
Quadratic	$\sim \quad 10^{-12}$	$\sim \quad 10^{-12}$
Cubic	$\sim \quad 10^{-12}$	$\sim \quad 10^{-10}$
Quartic	$\sim \quad 10^{-11}$	$\sim \quad 10^{-9}$
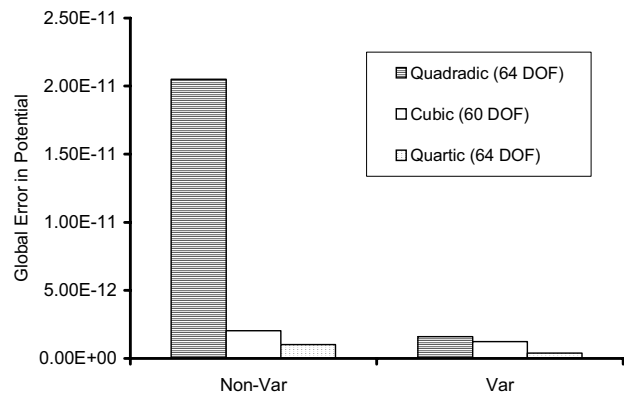
Figure 2 : Square problem: Variational X non-variational flux-BIE . Important improvement for quadratic elements while minor improvement for cubic and quartic elements.

Even in the worst case presented in Table 1, the errors are less than 10^{-9} and no improvement is obtained when increasing the degree of the interpolation polynomial. Instead, due to the greater number of calculations to be performed, round-off errors seemed to become important, and even predominant, so that the results for higher order elements are in fact, poorer than the results for the quadratic interpolation.

Figure 2 presents a comparison of the global error in the flux-BIE for finer meshes, with quadratic, cubic and quartic elements. This figure highlights the important error reduction obtained when using the variational formulation with quadratic elements, whilst only minor improvements in the error are obtained for cubic and quartic elements. The errors in the non-variational form of the flux-BIE are greatly influenced by its non-conformity with the $C^{1,\alpha}$ continuity requirements, and are especially high for quadratic elements. The variational formulation is able to improve the error results, the error reduction being important for quadratic elements, where higher error existed in the non-variational form. On the hand, only a minor error reduction is obtained for cubic and quartic elements, where the errors in the original non-variational formulation are already small.

4.2   Pipe problem

This example is concerned with heat transfer in a cylindrical domain with known analytical solution as well. Due to the symmetry, only a quarter of the circle is ana-

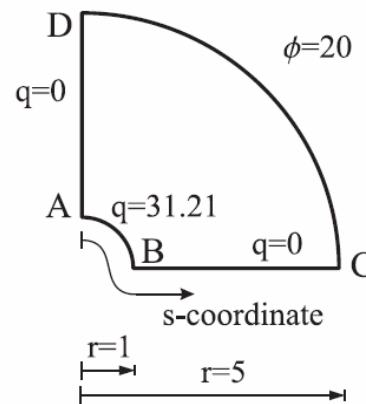lyzed with the geometry and boundary conditions shown in Fig. 3.

Figure 3 : Pipe problem

The influence of the variational formulation in the error behavior for higher order elements is also investigated. Comparisons using the external error estimator are presented in Fig. 4 for discretizations with 156, 160 and 288 nodes. One can note the improvement in the global error when using quadratic elements, while only minor reductions in the error, or even a disadvantage, are obtained for the case of cubic and quartic elements.
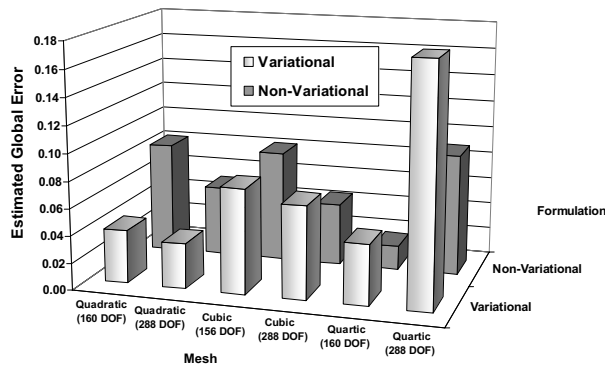
Figure 4 : Pipe problem: Variational X non-variational flux-BIE . A considerable improvement with quadratic elements while minor improvement, or even a disadvantage, for cubic and quartic elements.
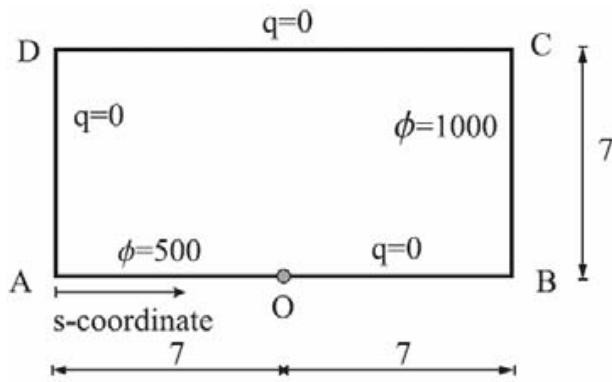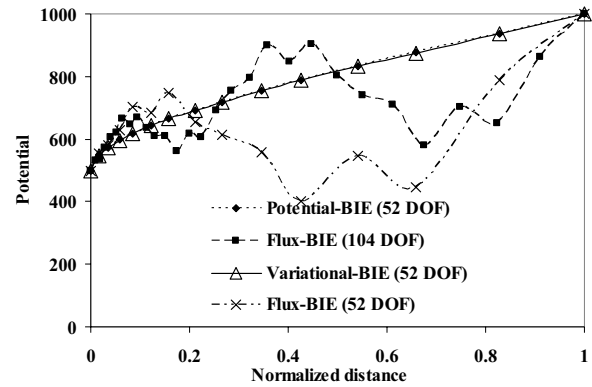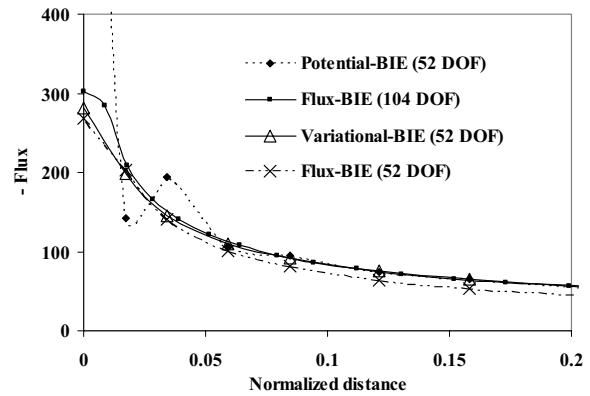

Figure 5 : Motz problem

(a)

(b)

Figure 6 : Motz problem: (a) Equivalence between potential-BIE (non-variational) and variational flux-BIE in potential. (b) Values of the flux close to singular point do not oscillate but are lower than the expected.

4.3 Motz problem

The problem proposed by Motz, as presented in Jaswon and Symm (1977), consists of a rectangular domain, as shown in Fig. 5, in which a singularity exists at the point $O(s = 7)$. The potential (temperature) is prescribed in the element to its left, and the flux equals zero in the element to its right. The flux is singular at point O in the element where the potential is prescribed.

The results for potential and flux in a region close to the singular point in the Motz problem using the 26 quadratic elements (52 DOF) with the self-regular potential-BIE, the self-regular flux-BIE and the proposed variational self-regular flux-BIE formulations are presented in Fig. 6a and Fig. 6b respectively. These results are also compared to those obtained by self-regular flux-BIE using a finer mesh of 52 elements (104 DOF). One can observe that, even with a finer mesh, the oscillations in the potential along the line OB, existing in the flux-BIE (non-variational) still remain, but otherwise, disappear when the variational approach is implemented and the result converges to the values obtained by potential-BIE.

In Fig. 6b, results are obtained for the flux along line *AO*, where the flux is singular at point *O*. These results are very close to each other in a region far away from the singular point. When approaching the singular point, the flux calculated by flux-BIE formulations (variational and non-variational) grows up monotonically, but with values far away from those calculated by the potential-BIE. This might happen due to the inability of the non-singular
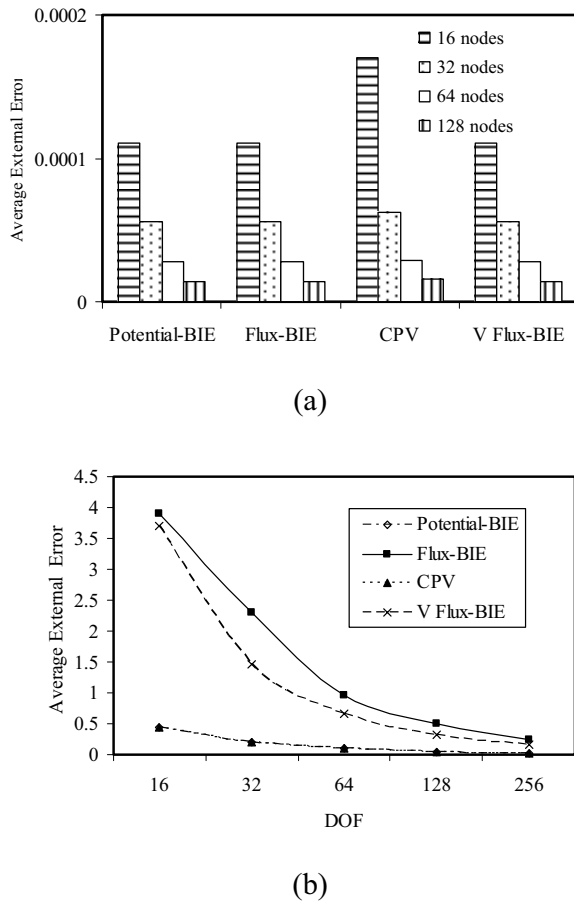
(a)

(b)

Figure 7 : Global error in potential: (a) no domain source; (b) domain source of magnitude $Q = 100$ at the center.

quadratic elements to reflect the singular evolution of the flux. Mesh refinement or singular elements should be implemented to account properly for the singular behavior of the variable.

4.4 Near-boundary heat transfer

The discretized self-regular variational flux-BIE and the external error estimator presented in the previous sections are now used in the study of near boundary heat transfer in a square domain such as that presented in Fig. 1.

The numerical results for the average (global) error from the external formulation are shown in Fig. 7, where part (a) corresponds to the original problem, with no domain source, and part (b) corresponds to a domain source of magnitude $Q_D = 100$ added at the center of the domain.

Starting from a 16-node mesh, refined meshes are obtained in a simple *h*-refinement procedure, by just dividing the element size by two. This means that at every refinement, the distance between the external point and the boundary, is also divided by two. This distance is used for the error measure in the external error estimator procedure described above. Using the potential-external error estimator, the self-regular variational flux-BIE formulation results are then compared with the available results for self-regular potential-BIE, self-regular flux-BIE, and standard Cauchy Principal Value (CPV) formulations, presented in Jorge, Porto and Ribeiro (2004).

In all cases considered, the order of magnitude of the average (global) error estimate decreases with mesh refinement, showing that the finer mesh is acting to decrease the local error. If the exterior point (used to obtain error estimator results) is approximated to the boundary without refining the mesh, the error would increase due to the proximity to the boundary. The self-regular BEM results are slightly better than the corresponding standard-CPV results for most cases, with the best results obtained for the coarse mesh where the results are significantly better than the corresponding standard-CPV results.

Regarding the flux-BIE, it is worth noting that the average error results degrade significantly when a domain source is included, while the variational formulation for the self-regular flux-BEM keeps the error at a level between the other formulations. For this reason, in what follows, only the self-regular potential-BIE and the self-regular variational flux-BIE formulation continue to be compared.

To evaluate the influence of the scaling factors and the near-boundary location of the interior points in the boundary solution accuracy, the heat conduction problem in the square domain is still considered. Regardless of the aspect ratio of the "square", if no domain sources are added, the analytical solution equations for the potential and for the flux are the same, thus allowing for the exact error to be evaluated.

A point is collocated at the center of the square, and then moved to the boundary though three different paths, as shown in Fig. 8. The first path (to left) moves to a smooth part with known potential. The second path (to bottom) also moves to a smooth part of the boundary, in the middle of a side, with no discontinuities in the boundary and with prescribed flux. The third path moves towards a boundary corner, where both discontinuities of the nor-
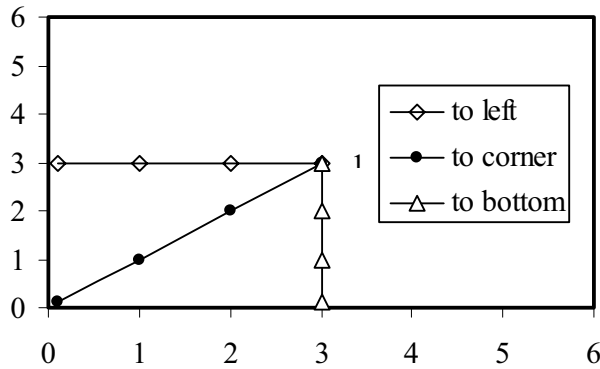
Figure 8 : Near-boundary problem: different paths leading towards boundary regions with different B.C.
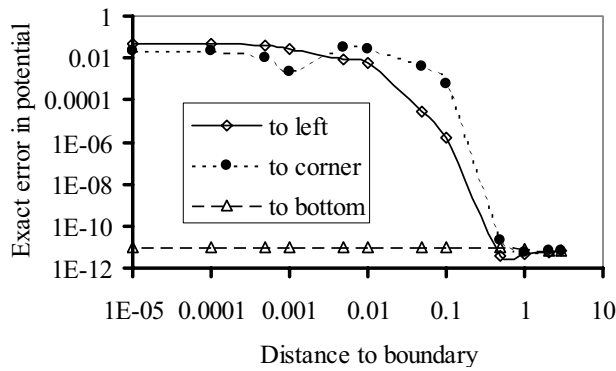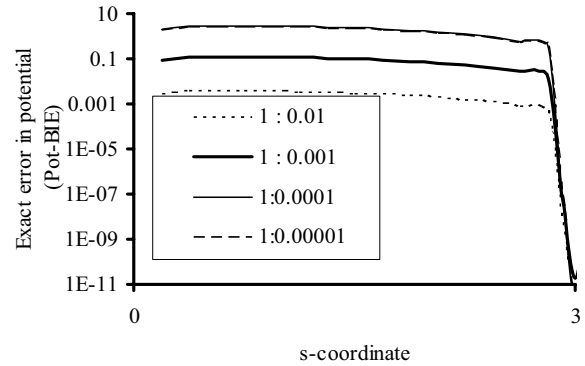

(a)

Figure 9 : Exact local error in potential at interior points approaching the boundary through different paths.

(b)

Figure 10 : Influence of domain aspect ratio, without domain sources: (a) Potential-BIE; (b) Variational flux-BIE.
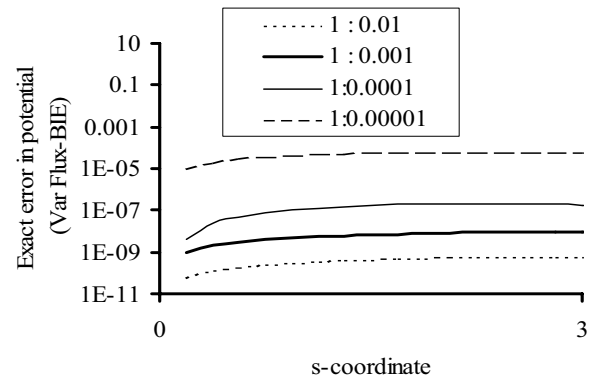
mal vector and of the boundary conditions occurred.

The exact error results for the potential at interior points approximating the boundary following the different paths, using the self-regular variational flux-BIE formulation, are shown in Fig. 9. It is worth noting an insignificant change in the error when approaching the region with prescribed flux, while small errors are obtained even for interior points very close the boundary following the others paths.

The influence of the domain aspect ratio is evaluated by keeping constant the horizontal sides, while shrinking the vertical sides, from the original 1:1 ratio (square problem) to ratios up to 1:0.00001. For the problem discretized with 64 quadratic elements (128 nodes) and with no domain sources, the exact error (error compared with the available exact solution) in the potential in half of the horizontal sides is shown in Fig. 10. The error increases

with shrinking and is higher in the self-regular potential-BIE formulation (Fig. 10a) than in the self-regular variational flux-BIE formulation (Fig. 10b).

5 Conclusions

In this work, a non-symmetric variational approach was derived, to enforce $C^{1,\alpha}$ continuity requirement at inter-element nodes for the self-regular flux-BIE discretized using the relaxed continuity approach. For this purpose, the variational approach has used only Lagrangian C^0 elements and the algorithm only enforced $C^{1,\alpha}$ continuity at smooth inter-element nodes.

The variational formulation for the flux-BIE was implemented in this work for quadratic, cubic and quartic elements for three classical potential problems and for some

near-boundary heat transfer problems.

Comparisons were also made with the potential-BIE, which does not require $C^{1,\alpha}$ continuity for the potential. For all cases considered, the most impressive improvements were obtained in the Motz problem where the non-variational self-regular was unable to give reliable results for the potential variable.

The lack of smoothness of the potential derivatives at inter-element nodes was shown to be an important source of both local and global errors for the flux-BIE formulation, especially for quadratic elements. The accuracy of the boundary solution obtained from the flux-BIE was improved when $C^{1,\alpha}$ continuity was enforced whenever possible, i.e., at the smooth inter-element nodes only. When the degree of the interpolating polynomial increased to cubic and quartic, small improvements or even worse results were obtained.

Local and global measures of the error were obtained by means of a new error estimator based on a recently post-processing error estimator derived by the authors. The estimator proposed here is based on an external formulation combining the potential and the gradient of the potential at external points. Knowledge of the exact solution is not required.

The variational approach was able to demonstrate the influence of the aspect ratio, of the presence of domain sources and of the proximity of interior points to domain boundary in a near-boundary heat transfer example. Higher error values were present when the aspect ratio increased, when a source was added, or when an interior point was moved towards the boundary.

The boundary element method seems to be the most appropriate approach to deal with near-boundary heat transfer problems. Among the different BEM possibilities, the variational self-regular flux-BIE formulations presented in this work seems to offer slightly better – or at least comparable – results than the self-regular potential –BIE and CPV, yet to be confirmed by more exhaustive studies

References

Atluri, S. N.; Han, Z. D.; Shen, S. (2003): Meshless Local Petrov-Galerkin (MLPG) Approaches for Solving the Weakly-Singular Traction & Displacement Boundary Integral Equations, In: *CMES: Computer Modeling In Engineering & Sciences* 4 (5), pp. 507-517.

Bonnet, M. (1999): In: *Boundary Integral Equation Methods for Solids and Fluids*. Wiley, West Sussex.

Brebbia, C. A.; Telles, J. C. F.; Wrobel, L. C. (1984): In: *Boundary Element Techniques.* Springer-Verlag, Berlin.

Cruse, T. A.; Richardson, J. D. (2000): Self-regularized hypersingular BEM for Laplace's equation. In: Bonnet, M., Sändig, A. -M., & Wendland W. L. (ed), *Mathematical Aspects of Boundary Element Methods*, Chapman & Hall / CRC, Boca Raton, FL.

Dominguez, J.; Ariza, M. P.; Gallego, R. (2000): Flux and traction boundary elements without hypersingular or strongly singular integrals. In: *International Journal for Numerical Methods in Engineering*, vol. 48, n. 1, pp. 111–135.

Han, Z. D.; Atluri, S. N. (2003): On Simple Formulations of Weakly-Singular Traction & Displacement BIE and Their Solutions Through Petrov-Galerkin Approaches, In: *CMES:Computer Modeling In Engineering & Sciences* 4 (1), pp. 5-20.

Huang Q. P.; Cruse T. A. (1994): On the nonsingular traction-BIE in elasticity. In: *International Journal for Numerical Methods in Engineering*, vol. 37: pp. 2041–2072

Jaswon M. A., Symm G. T. (1977): Integral Equation Methods In: *Potential Theory and Elastostatics*, Academic Press, London-UK.

Jorge, A. B.; Ribeiro, G. O.; Cruse, T. A.; Fisher, T. S. (2001): Self-Regular Boundary Integral Equation Formulations for Laplace's Equation in 2-D. In: *International Journal for Numerical Methods in Engineering*, vol. 51, n. 1, pp. 1–29.

Jorge, A. B.; Ribeiro, G. O.; Fisher, T. S. (2003): New Approaches for Error Estimation and Adaptivity for 2-D Potential Boundary Element Methods, In: *International Journal for Numerical Methods in Engineering*, vol. 56, n. 1, pp. 117-144.

Jorge, A. B.; Cruse, T. A.; Fisher, T. S.; Ribeiro, G. O. (2003): A new variational self-regular traction-BEM

formulation for inter-element continuity of displacement derivatives. In: *Computational Mechanics*, vol. 32, n. 4-6, pp. 401–414.

Jorge, A. B.; Porto, P. A. C.; Ribeiro, G. O. (2004): Near-boundary heat transfer using a self-regular boundary element method formulation. In: Aliabadi, M. H. & Leitão, V. M. A. (ed), *Advances in Boundary Element Techniques V, Proceedings of BETEQ 2004 – International Conference on Boundary Element Techniques V*, EC Ltd, UK, pp. 1-7.

Krishnasamy G.; Rizzo F. J.; Rudolphi T. J. (1992): Continuity Requirements for Density Functions in the Boundary Integral Equation Method. In: *Computational Mechanics*, vol. 9: pp. 267–284

Kupradze, V. D. (1979): *Three-Dimensional Problems of the Mathematical Theory of Elasticity and Thermoelasticity*. North-Holland Publishing Company, Amsterdam.

Martin, P. A.; Rizzo, F. J. (1996): Hypersingular integrals; how smooth must the density be? In: *International Journal for Numerical Methods in Engineering*, vol. 39, n. 4, pp. 687–704.

Martin, P. A.; Rizzo, F. J.; Cruse, T. A. (1998): Smoothness relaxation strategies for singular and hypersingular integral equations. In: *International Journal for Numerical Methods in Engineering*, vol. 42, n. 5, pp. 885–906.

Mustoe, G. G.W.; Volait, F.; Zienkiewicz, O. C. (1982). A symmetric boundary integral equation method for 2 dimensional elastostatics. In: *Res Mechanica*, vol. 4, n. 1, pp. 57–82.

Richardson, J. D.; Cruse, T. A. (1999): Weakly Singular Stress-BEM for 2D Elastostatics. In: *International Journal for Numerical Methods in Engineering*, vol. 45, n. 1, pp. 13–35.

Richardson, J. D.; Cruse, T. A; Huang, Q. (1997): On the validity of conforming BEM algorithms for hypersingular boundary integral equations. In: *Computational Mechanics*, vol. 20, n. 3, pp. 213–220.

Sladek, V.; Sladek, J. (1998): Singular Integrals in Boundary Element Methods. In: *Advances in Boundary Elements Series*, Computational Mechanics Publications, Southampton, pp.1-31.