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ALTERNATIVE FORMS OF FUNDAMENTAL SOLUTIONS FOR 3-D ANISOTROPIC HEAT TRANSFER

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Abstract. This work presents two new methods to derive the fundamental solution for threedimensional heat transfer problems in the general anisotropic media. Initially, the basic integral equations used in the definition of the general anisotropic fundamental solution are revisited. We show the relationship between three, two and one-dimensional integral definitions, either by purely algebraic manipulation as well as through Fourier and Radon transforms. Two of these forms are used to derive the fundamental solutions for the general anisotropic media. The first method gives the solution analytically for which the solution for the orthotropic case agrees with the well known result obtained by the domain mapping, while the fundamental solution for the general anisotropic media is new. The second method expresses the solution by a line integral over a semi-circle. The advantages and disadvantages of the two methods are discussed with numerical examples.

1 INTRODUCTION

The steadily increasing use of new and non-conventional materials by the modern industry has created a demand for reliable simulation methods in the design and analysis of mechanical components. Many of these new materials exhibit non-isotropic properties, making the differential operator of the governing equations somewhat more complicated than the well known isotropic case.

The Poisson's equation can be used to solve a wide range of engineering problems such as heat transfer, electro-magnetism, torsion etc., commonly referred to as potential problems. Among the numerical methods traditionally used to solve the potential problems is the boundary element method (BEM), due to its high accuracy, applicability to infinite domains, and ability to capture singularities with less discretization effort than other methods (Brebbia et al. 1984; Kane, 1994; Mera et al. 2001a). Additionally, only boundary discretization is required in most linear problems. On the other hand, the BEM needs the particular solution of the differential equation, or the fundamental solution of the problem. In spite of a good number of references dealing with the application of the BEM for the isotropic potential problems, the number of anisotropic counterparts is much smaller and, notably, solved in the principal diffusivity coordinate system, only.

The numerical or analytical treatment of orthotropic potential problems is generally accomplished by coordinate transformations which map the original problem into an equivalent isotropic one (Mulholland and Gupta, 1977; Chang and Tsou, 1977; Poon et al. 1979). This method has the clear advantage of allowing the use of analytical solutions and/or computer codes developed for the isotropic media. However, the flux boundary conditions must also be transformed before their imposition on the new domain. While this is not a problem in domains composed of a single material, the application of the compatibility conditions along the interfaces of multi-material problems (Atalay et al. 2004] can be cumbersome because the transformation for each subregion is different and therefore boundary interfaces in the original domain may no longer be aligned after the transformation. This is an important issue in problems that require the knowledge of the fluxes during the solution phase, like in the iterative solution methods or the inverse problems (Mera et al. 2001b) where the flux boundary conditions is measured from the actual components.

Most of the published works on non-isotropic potential problems are based on the transformation of the coordinate axes into the principal ones. In this situation, the thermal diffusion tensor (K) is diagonal, but the aforementioned drawbacks persist. In particular, the current trend for design, analysis and development of porous materials (Feng et al. 2004), composite materials containing different types of inclusions (Ram and Singh, 2004), and cellular materials for optimal thermal performance requires behavior prediction based on numerical models containing thousands of inhomogeneities. This is necessary in cases when the distribution of cavities/inclusions is non-periodic, precluding analytical solutions, particularly for high volume fractions. Furthermore, special cases such as the functionally graded materials cannot be handled because there are no guarantees that the mapping will be invertible. In the BEM context, Shiah and Tan (1997) applied the coordinate transformation technique and the BEM to solve two-dimensional problems. Hsieh and Ma (2002) introduced a linear coordinate transformation method to solve the heat conduction on a thin layer of anisotropic medium subjected to arbitrary thermal loadings applied inside the domain or on the boundary surfaces. Ma and Chang (2004) studied the two-dimensional steady-state thermal conduction problems in the anisotropic multi-layered media. They have used the linear coordinate transformation to simplify the governing equation without complicating the boundary and interface conditions. Shiah and Tan (2004) extended their earlier work and showed how to solve a three-dimensional anisotropic field problems by applying the two-dimensional coordinate transformations on the three coordinate planes.

It is interesting to derive the fundamental solution for the heat transfer referring to the generic, non-principal set of coordinate axes. To the best of authors' knowledge, no closed form fundamental solution for the fully anisotropic potential problems has been derived yet without the use of coordinate transformation. This is intrinsically due to the higher complexity of the differential equation when the thermal diffusion tensor is fully populated, making the separation of variables only conditionally possible. Wang (1994) showed how to derive the two-dimensional fundamental solution for the isotropic Poisson's equation using the integral definitions. Similar ideas will be used here for the three-dimensional, anisotropic case.

We first review the integral representations for the fundamental solutions as generally used to derive solutions for the vector-field problems. These representations have seldom been used for the isotropic or orthotropic scalar problems since the direct derivation of solutions for these cases can be accomplished with little analytical effort. In the anisotropic case, however, the non-diagonal form of the constitutive tensor makes the use of such integral representations a more straightforward way to derive the fundamental solution. One of these definitions are applied to the general anisotropic heat transfer case, and then particularized to the orthotropic one. The agreement of the later with the well known orthotropic fundamental solution for Poisson's problems validates the applicability of the procedure. Furthermore, both cases can be reduced to the isotropic case, something not always possible in crystal physics.

This one-step analytical approach, however, can be applied with relative ease only in cases of point source fundamental solutions. Other types of fundamental solutions will require more intense analytical effort, and although the explicit evaluation of the line integrals is all that is required, the calculation of the derivatives of the fundamental solution will become tedious, or even impossible. In such cases, the explicit use of Radon transform (Deans, 1983) to derive the fundamental solutions has proven to be a very interesting alternative, because other line integral forms can be employed (Wang and Achenbach, 1994; Wang and Denda, 2007). This approach has been previously applied for crystal elasto dynamics such as time-transient wave scattering (Wang and Achenbach, 1994) and eigenvalue problems (Denda et al. 2004), and not only allowed the analytical evaluation of the surface integrals over the boundary elements, but also reduced the computational effort drastically. More important, the fundamental solutions remain expressed by line integrals over a semi-circle for potential and flux as well. This is a significant advantage over the conventional analytical procedure which, as already mentioned, may fail to deliver fully analytical, closed form expressions for the later. We derive and test fundamental solutions for three-dimensional anisotropic heat transfer problems using both approaches.

2 GENERAL EXPRESSIONS FOR SCALAR FUNDAMENTAL SOLUTIONS

The steady-state heat conduction equation in three-dimensions, defined in the coordinate system \mathbf{x} , can be written as

$$L(\partial_{\mathbf{x}})u(\mathbf{x}) = b(\mathbf{x}) \qquad \mathbf{x} \in \mathbb{R}^3 \quad , \tag{1}$$

where u and b are the temperature and heat source fields, respectively. The differential operator,

$$L(\partial_{\mathbf{x}}) = k_{ij} \partial_i \partial_j , \qquad (2)$$

is the Laplace's operator defined in terms of the thermal diffusion tensor k_{ij} . As a companion of this differential operator, define a scalar-valued quadric,

$$L(\mathbf{x}) = k_{ij} x_i x_j , \qquad (3)$$

in terms of k_{ij} which is called Green-Christoffel tensor or acoustic tensor (Mura and Kinoshita, 1971; Nye, 1957). The fundamental solution for the scalar differential operator $L(\partial_x)$ is defined by the unit source applied at y and is given by the solution of the equation (Stakgold 1979),

$$L(\partial_{\mathbf{x}})u^*(\mathbf{x},\mathbf{y}) = -\delta(\mathbf{x} - \mathbf{y}) \qquad \mathbf{x}, \mathbf{y} \in \mathbb{R}^3,$$
(4)

in an infinite space, where δ is the Dirac's delta operator. It is generically called the potential fundamental solution. The dual fundamental solution, which is the heat flux in the unit normal direction **n**, can be determined by the Fourier law,

$$q^*(\mathbf{x}, \mathbf{y}) = n_i(\mathbf{x}) k_{ij} u^*_{,i}(\mathbf{x}, \mathbf{y}).$$
⁽⁵⁾

The solution of eq.(4) can be obtained, using the Fourier transform (Synge, 1957), to give the fundamental solution,

$$u^{*}(\mathbf{x},\mathbf{y}) = \frac{1}{8\pi^{3}} \int \int \int_{S^{3}} L^{-1}(\boldsymbol{\xi}) e^{-i\boldsymbol{\xi}\cdot(\mathbf{x}-\mathbf{y})} dS^{3}(\boldsymbol{\xi}), \qquad (6)$$

where the integral is carried out over the unit sphere, in the transformed space, with the center located at the origin as shown in Fig.1. Notice that $L^{-1}(\xi)$ is the inverse of the scalar valued quadric defined by (3).

We observe from eq.(6) that the fundamental solution is constructed by the superposition of the wave functions. Applying the theory of harmonic functions, it can be further reduced to an integral over an arbitrary closed surface containing \mathbf{y} (Mura and Kinoshita, 1971),

$$u^{*}(\mathbf{x},\mathbf{y}) = \frac{1}{16\pi^{2}} \Delta_{\mathbf{y}} \iint_{S^{2}} L^{-1}(\boldsymbol{\xi}) \left| \boldsymbol{\xi} \cdot (\mathbf{x} - \mathbf{y}) \right| dS^{2}(\boldsymbol{\xi}), \tag{7}$$

where Δ_y is the Laplacian operator. The final result of (7) does not depend on the size and shape of S^2 , so a unity sphere $S^2 = \{ \boldsymbol{\xi} | \boldsymbol{\xi} \in \mathbb{R}^3, \|\boldsymbol{\xi}\| = 1 \}$ is generally used (fig.1). According to eq.(7), the fundamental solution u^* is constructed in terms of the surface wave functions of the form $|\boldsymbol{\xi} \cdot \mathbf{r}|$. This equation can further be transformed to give the line integral representation (Kröner, 1953; Synge, 1957),

$$u^{*}(\mathbf{x}, \mathbf{y}) = \frac{1}{8\pi^{2}r} \oint_{S^{1}} L^{-1}(\boldsymbol{\xi}) \, dS^{1}(\boldsymbol{\xi}), \qquad (8)$$

where the integration is performed on a circumference S^1 formed by the intersection of the plane perpendicular to **x**-**y** and the unit sphere S^2 , i.e., $S^1 = \{ \boldsymbol{\xi} | \boldsymbol{\xi} \in \mathbb{R}^3, \| \boldsymbol{\xi} \| = 1, \ \boldsymbol{\xi} \cdot (\mathbf{x} - \mathbf{y}) = 0 \}$ (Fig.1). This equation can be more conveniently written in the spherical coordinates as Li and Wang 2007)

$$u^{*}(\mathbf{x},\mathbf{y}) = \frac{1}{8\pi^{2}r} \int_{0}^{2\pi} L^{-1}(\boldsymbol{\xi}^{0}) d\varphi(\boldsymbol{\xi}^{0}) , \qquad (9)$$

where ξ^0 is a parametric coordinate.



Figure 1: Relationship between the various integral forms for Green.s functions and their domain of integration.

Equation (8) is often recognized as a direct consequence of the application of Radon transform (Deans, 1983; Gelfand et al. 1966), although by no means that is the only way to derive it. Its two most remarkable features are the relative simplicity of the integration needed compared with other equivalent expressions, and the preservation of the distribution properties necessary for continuous differentiation, as in eq.(5). It is worth mentioning that this form of line integral representation is seldom used in the scalar potential problems.

The operational forms of eqs.(6), (7) and (8) may vary depending on the analytical procedures adopted in their derivation, but the equivalence between them has been proved (Synge, 1957; Gelfand et al. 1966). The development of the fundamental solutions for the potential problems given by (1) can use either eq.(6), (7) or (8), as they are all continuously differentiable. We consider (7) to be the best starting point for the general methodology for three reasons. First, it is easier to integrate since it incorporates a reduction, by one dimension, in the original integration order of (6). Secondly, although a number of one-dimensional forms

like (8) can be obtained from (7), the apparent simplicity of line integral does not remain so when evaluating its derivatives as in eq.(5). Finally, eq.(7) is directly related to Radon transform whose inversion process is simpler than the corresponding inversion of the Fourier transform. As shown in Appendix, the fundamental solution obtained by Radon transform is given in the form,

$$u^{*}(\mathbf{x},\mathbf{y}) = \frac{1}{8\pi^{2}} \iint_{S^{2}} L^{-1}(\boldsymbol{\xi}) \,\delta(\boldsymbol{\xi} \cdot (\mathbf{x}-\mathbf{y})) \, dS^{2}(\boldsymbol{\xi}). \tag{10}$$



Figure 2: Local coordinate system centered on a unit circle over the field point.

Transformations among eqs.(8), (9) and (10) can be performed in a number of ways. For example, eq. (8) can be reduced to an infinite integral along a line belonging to the plane perpendicular to $\mathbf{x} - \mathbf{y}$ (Ting and Lee, 1997; Tonon et al. 2001) using the symmetry property of L^{-1} and the fact the integration is independent on the shape of S^2 . This is accomplished by decomposing $\boldsymbol{\xi}$ in terms of an arbitrary parameter $\boldsymbol{\psi}$ (Fig.2),

$$\boldsymbol{\xi} = \mathbf{n}\cos\boldsymbol{\psi} + \mathbf{m}\sin\boldsymbol{\psi},\tag{11}$$

and writing eq.(8) as

$$u^{*}(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi^{2}r} \int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} L^{-1}(\psi) d\psi, \qquad (12)$$

where **n** and **m** form a triad of mutually orthogonal vectors along with **x-y**. Further introduction of the variable change, $p = \tan \psi$, will give

$$u^{*}(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi^{2}r} \int_{-\infty}^{+\infty} L^{-1}(p) \, dp.$$
(13)

One should note that the simplicity of the Laplacian operator allows the direct integration of any of eqs.(6), (7) and (8) or the alternative expressions given by either eqs.(10), (12) or (13). The choice of one particular form depends on the complexity of the integrand in each case. For example, eq.(10) can be integrated only if a suitable expression for the Dirac's delta is used (Wang et al. 2006; Wang and Denda, 2007), while eqs.(8), (12) and (13) relies on

simpler one dimensional integration. Most of them have been extensively used in the past to obtain tensorial fundamental solutions in crystal physics, in which L is a matrix that requires the matrix inversion. In comparison, the present case of potential fundamental solution is much simpler as shown below.

3 FUNDAMENTAL SOLUTION FOR 3D ANISOTROPIC LAPLACIAN OPERATOR

3.1 Analytical form

In this section, eq.(12) will be used to derive the fundamental solution of an anisotropic diffusive medium. The general anisotropic thermal diffusion tensor is given by

$$\mathbf{K} = \begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{22} & k_{23} \\ \text{sym.} & k_{33} \end{bmatrix}.$$

The quadric is given by

$$L(\boldsymbol{\xi}) = \boldsymbol{\xi}^{T} \mathbf{K} \boldsymbol{\xi} = \xi_{1}^{2} k_{11} + \xi_{2}^{2} k_{22} + \xi_{3}^{2} k_{33} + 2 \xi_{1} \xi_{2} k_{12} + 2 \xi_{1} \xi_{3} k_{13} + 2 \xi_{3} \xi_{2} k_{23}.$$

If we substitute eq.(11) into the above quadric we get

$$L(\psi) = n_i n_j k_{ij} \cos^2 \psi + (n_j m_i k_{ij} + n_i m_j k_{ij}) \sin \psi \cos \psi + m_i m_j k_{ij} \sin^2 \psi$$
$$= Q \cos^2 \psi + R \sin \psi \cos \psi + T \sin^2 \psi.$$

The parameters Q, R and T are the scalar counterparts of the similar (tensorial) terms found in crystal physics (Ting, 1997). Use this result in eq.(12) to get

$$u^*(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi^2 r} \int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \left(\frac{1}{Q\cos^2 \psi + R\sin\psi\cos\psi + T\sin^2\psi} \right) d\psi$$
$$= \frac{1}{4\pi r} \frac{1}{\sqrt{\Delta}}.$$

where

$$\Delta = QT - R^2 / 4 = n_i n_j m_k m_l k_{ij} k_{kl} - \frac{1}{4} \left(n_j \left(m_i k_{ij} \right) + m_j \left(n_i k_{ij} \right) \right)^2.$$

This can be factored as

$$\Delta = d_{12}^2 k_{11} k_{22} + d_{13}^2 k_{11} k_{33} + d_{23}^2 k_{22} k_{33} + 2d_{12} d_{13} k_{11} k_{23} - 2d_{12} d_{23} k_{13} k_{22} + + 2d_{13} d_{23} k_{12} k_{33} - 2d_{12} d_{13} k_{12} k_{13} + 2d_{12} d_{23} k_{12} k_{23} - 2d_{13} d_{23} k_{13} k_{23} + - d_{12}^2 k_{12}^2 - d_{23}^2 k_{23}^2 - d_{13}^2 k_{13}^2 ,$$

where $d_{ij} = (n_i m_j - n_j m_i)$. Recalling that **m** and **n** are the unit vectors perpendicular to $\mathbf{r} = \mathbf{x} \cdot \mathbf{y}$, one can rewrite Δ in terms of the components of **r** as follows:

$$r^{2}\Delta = r_{3}^{2}k_{11}k_{22} + r_{2}^{2}k_{11}k_{33} + r_{1}^{2}k_{22}k_{33} + 2r_{3}r_{2}(k_{11}k_{23} - k_{12}k_{13}) + +2r_{3}r_{1}(k_{12}k_{23} - k_{13}k_{22}) + 2r_{2}r_{1}(k_{12}k_{33} - k_{13}k_{23}) + -r_{3}^{2}k_{12}^{2} - r_{1}^{2}k_{23}^{2} - r_{2}^{2}k_{13}^{2}.$$

If we define

$$\overline{r}^{2} = \frac{r^{2}\Delta}{k_{11}k_{22}k_{33}} = \frac{r_{1}^{2}}{k_{11}} + \frac{r_{2}^{2}}{k_{22}} + \frac{r_{3}^{2}}{k_{33}} + 2r_{3}r_{2}\frac{\left(k_{11}k_{23} - k_{12}k_{13}\right)}{k_{11}k_{22}k_{33}} + 2r_{3}r_{1}\frac{\left(k_{12}k_{23} - k_{13}k_{22}\right)}{k_{11}k_{22}k_{33}} + 2r_{2}r_{1}\frac{\left(k_{12}k_{33} - k_{13}k_{23}\right)}{k_{11}k_{22}k_{33}} + \frac{r_{3}^{2}k_{12}^{2} + r_{1}^{2}k_{23}^{2} + r_{2}^{2}k_{13}^{2}}{k_{11}k_{22}k_{33}}$$

then we can write u^* as

$$u^* = \frac{1}{4\pi \bar{k}\bar{r}} \tag{14}$$

where $\overline{k} = \sqrt{k_{11}k_{22}k_{33}}$. Equation (14) represents the fundamental solution for a Laplacian operator when the coordinate axes are scaled so that the quadric in eq.(3) becomes a sphere. The coordinate system, however, are not aligned with the principal axes of **K**. The use of arbitrary coordinate systems is then possible, exempting the need for coordinate transformations. When **K** is diagonal (ortotropic case), eq.(14) reduces to the classical solution obtained by applying the coordinate transformation $z_i = y_i / \sqrt{k_i}$ (Brebbia et al. 1984; Rucker and Richter, 1988):

$$u_{\text{ORT}}^* = \frac{1}{4\pi k} \frac{1}{\sqrt{\frac{n^2}{k_{11}} + \frac{n^2}{k_{22}} + \frac{n^2}{k_{33}}}}$$
(15)

Evidently eq.(15) must be used with a coordinate system aligned with the principal directions. As for the heat flux, eq.(5) can be rewritten from eq.(14) using the chain rule:

$$q^* = \frac{-1}{4\pi \overline{k}\overline{r}^2} n_i k_{ij} \frac{\partial \overline{r}}{\partial r_k} \delta_{kj} = \frac{-1}{4\pi \overline{k}\overline{r}^2} n_i k_{ij} \frac{\partial \overline{r}}{\partial r_j}$$

which results in:

$$q^{*} = \frac{-1}{2\pi \bar{k}^{3} \bar{r}^{2}} \left(\bar{q}_{1} n_{1} + \bar{q}_{2} n_{2} + \bar{q}_{3} n_{3} \right)$$
(16)

where the terms \overline{q}_i are given by:

$$\begin{split} \overline{q}_{1} &= \left(c_{2233}k_{11} + c_{1233}k_{12} + c_{1223}k_{13}\right)r_{1} + \left(c_{1233}k_{11} + c_{1133}k_{12} + c_{1123}k_{13}\right)r_{2} + \\ &\left(c_{1223}k_{11} + c_{1123}k_{12} + c_{1122}k_{13}\right)r_{3}, \\ \overline{q}_{2} &= \left(c_{2233}k_{12} + c_{1233}k_{22} + c_{1223}k_{23}\right)r_{1} + \left(c_{1233}k_{12} + c_{1133}k_{22} + c_{1123}k_{23}\right)r_{2} + \\ &\left(c_{1223}k_{12} + c_{1123}k_{22} + c_{1122}k_{23}\right)r_{3}, \\ \overline{q}_{3} &= \left(c_{2233}k_{13} + c_{1233}k_{23} + c_{1223}k_{33}\right)r_{1} + \left(c_{1233}k_{13} + c_{1133}k_{23} + c_{1123}k_{33}\right)r_{2} + \\ &\left(c_{1223}k_{13} + c_{1123}k_{23} + c_{1122}k_{33}\right)r_{3}, \end{split}$$

and the symbol $c_{ijkl} = k_{ij}k_{kl} - k_{il}k_{jk}$ is used for compactness.

3.2 Line integral form

Let $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ be a set of unit orthogonal base vectors in the global coordinate system. If we express the unit sphere S^2 by

$$\boldsymbol{\xi} = \sin\varphi\cos\theta\,\boldsymbol{e}_1 + \sin\varphi\sin\theta\,\boldsymbol{e}_2 + \cos\varphi\,\boldsymbol{e}_3, \tag{17}$$

then the integral (10) can be written as

$$u^{*}(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi^{2}} \int_{0}^{\pi} \int_{0}^{\pi} \mathcal{L}^{-1}(\boldsymbol{\xi}) \,\delta[\boldsymbol{\xi} \cdot (\mathbf{x} - \mathbf{y})] \sin \varphi \, d\varphi \, d\theta.$$
(18)

In deriving equation (18), symmetry with respect to θ has been used. This equation can further be modified if we introduce

$$\mathbf{s} = \frac{\boldsymbol{\xi}}{\sin \varphi} = \cos \theta \mathbf{e}_1 + \sin \theta \mathbf{e}_2 + \operatorname{ctan} \varphi \mathbf{e}_3$$

and the change of variable $\lambda = \operatorname{ctan} \varphi$. Then (18) can be written as

$$u^{*}(\mathbf{x},\mathbf{y}) = \frac{1}{4\pi^{2}} \int_{0}^{\pi} \int_{-\infty}^{\infty} L^{-1}(\mathbf{s}) \delta[\mathbf{s} \cdot (\mathbf{x} - \mathbf{y})] d\mathbf{\lambda} d\theta.$$
(19)

The infinite integral in (19) can be reduced to the Cauchy integral along the λ -axis, which can be evaluated by the Residue theorem to give

$$u^{*}(\mathbf{x}, \mathbf{y}) = -\Re \int_{0}^{\pi} \overline{u}^{*}(\theta) \frac{\operatorname{sign}(x_{3} - y_{3})}{(\mathbf{x} - \mathbf{y}) \cdot \mathbf{s}^{*}(\theta)} d\theta,$$
(20)

where

$$\mathbf{s}^*(\boldsymbol{\theta}) = \cos \boldsymbol{\theta} \, \mathbf{e}_1 + \sin \boldsymbol{\theta} \, \mathbf{e}_2 + \boldsymbol{\lambda}^* \, \mathbf{e}_3, \tag{21}$$

$$\overline{u}^*(\theta) = \frac{1}{2\pi^2} \frac{1}{\partial_\lambda L(\mathbf{s}^*(\theta))},\tag{22}$$

and λ^* is one of the two characteristic roots of L(s) with positive imaginary part. The corresponding flux across the plane with the unit normal **n** is given by

$$q^*(\mathbf{x}, \mathbf{y}) = \Re \int_0^{\pi} \overline{q}^*(\theta) \frac{\operatorname{sign}(x_3 - y_3)}{\left[(\mathbf{x} - \mathbf{y}) \cdot \mathbf{s}^*(\theta) \right]^2} d\theta,$$
(23)

where

$$\overline{q}^*(\theta) = n_i s_i k_{ij} \overline{u}^*(\theta) = n_i \overline{q}_i^*(\theta) .$$
⁽²⁴⁾

The integrands of the line integrals (20) and (23) are given by the product of a function of the material properties only (i.e., independent of location vectors \mathbf{x} and \mathbf{y}) and a simple algebraic function. Notice that the partial differentiation of the integral can be performed by changing the order of the integration and differentiation.

There is no question on the advantage of the analytical form (14) of the fundamental solution. However the advantage stops here. If we want to use the analytical solution for the continuous distribution of the heat sources, then it is not straightforward to integrate the distribution analytically. Derivation of the fundamental flux solution in such cases, if not impossible, is tedious. In contrast to this, the line integral form (20) of the fundamental solution is much simpler than the analytical solution and is flexible. Any associated fundamental solutions that can be obtained from this either by differentiation or integration can be obtained by simply applying the operation to the integrand of (20). Since the integrand is a simple plane wave function its derivative and integration can be performed readily. The only disadvantage is the need for numerical integration, which can be performed by the standard Gauss quadrature. On the other hand, the integrand functions in eqs.(20) and (23) are very well behaved. Figure 3 shows the integrand of (20), while the integrands of (23) associated to $\mathbf{n} = (1,0,0)$, $\mathbf{n} = (0,1,0)$, and $\mathbf{n} = (0,0,1)$ are illustrated in fig.4. In the numerical evaluation of these fundamental solutions, the typical number of divisions of the integration interval $[0, \pi]$ is 10, and the number of the Gauss quadrature points for each division is 3. This combination gives a very accurate solution without the need of higher order quadrature rules. For accuracy assessment purposes, eqs.(20) and (23) were evaluated for the integration interval divided in n_{D} parts, and applying n_{C} Gauss points for each division. The results were compared with their analytical counterparts given by eqs.(14) and (16), respectively. The percentage errors to the analytical solutions are presented in Table 1 for temperatures and Table 2 for fluxes.

4 NUMERICAL EXAMPLES

In order to assert the validity of the fundamental solutions developed for the anisotropic case, eq.(14) was implemented for three types of materials with hexagonal and trigonal symmetries. They are Graphite (hexagonal), Quartz (trigonal), and Calcite (trigonal), respectively with the following thermal diffusivity written in their principal axes (Nye, 1957):

$$\mathbf{K}_{G} = \begin{bmatrix} 355 & 0 & 0 \\ & 355 & 0 \\ & & 89 \end{bmatrix} [W/m^{\circ}C],$$
$$\mathbf{K}_{Q} = \begin{bmatrix} 6.5 & 0 & 0 \\ & 6.5 & 0 \\ & & 11.3 \end{bmatrix} [W/m^{\circ}C],$$

$$\mathbf{K}_{C} = \begin{bmatrix} 4.18 & 0 & 0 \\ 4.18 & 0 \\ 4.98 \end{bmatrix} \quad [W/m^{\circ}C].$$



Figure 3: Behavior of the integrand of eq.(20) as a function of the polar angle θ .



Figure 4: Behavior of the integrands of eq.(23) as functions of the polar angle θ in three canonic directions.

	n _G								
n _D	1	2	3	4	6	8			
1	-0.203E+01	0.182E+01	-0.109E+01	0.251E+00	-0.784E-02	-0.712E-03			
2	0.207E+01	-0.512E+00	0.573E-01	-0.499E-02	-0.476E-04	-0.439E-06			
3	-0.216E-03	0.191E-03	-0.114E-03	0.271E-04	0.306E-06	0.803E-09			
4	-0.210E-01	0.271E-04	-0.471E-03	0.222E-04	0.942E-08	-0.630E-11			
6	0.216E-03	-0.519E-04	0.484E-05	-0.230E-06	-0.129E-09	-0.148E-12			
8	-0.221E-05	0.532E-06	-0.496E-07	0.236E-08	0.130E-11	-0.104E-12			
10	0.227E-07	-0.545E-08	0.509E-09	-0.242E-10	-0.148E-13	-0.889E-13			
16	-0.148E-13	0.148E-13	-0.148E-13	-0.148E-13	-0.148E-13	-0.104E-12			
24	-0.148E-13	-0.148E-13	-0.444E-13	-0.444E-13	-0.148E-13	-0.119E-12			
32	-0.148E-13	-0.148E-13	-0.148E-13	-0.148E-13	0.000E+00	0.133E-12			
36	-0.296E-13	-0.148E-13	0.000E+00	-0.296E-13	-0.296E-13	-0.119E-12			

Table 1: Percentage difference between the temperature fields evaluated by eqs.(14) and (20). n_D is the number of divisions used in the integration interval $[0,\pi]$ and n_D is the number of Gauss points used in each division.

	n _G								
n _D	1	2	3	4	6	8			
1	0.778E+01	-0.714E+01	0.424E+01	-0.938E+00	0.833E-01	0.552E-02			
2	-0.815E+01	2 0.208E+01	-0.279E+00	0.339E-01	0.497E-03	0.613E-05			
3	0.294E-02	-0.260E-02	0.156E-02	-0.370E-03	-0.418E-05	-0.108E-07			
4	0.184E+00	-0.443E-01	0.412E-02	-0.192E-03	-0.522E-07	0.130E-09			
6	-0.294E-02	0.708E-03	-0.661E-04	0.314E-05	0.177E-08	0.171E-12			
8	0.409E-04	-0.985E-05	0.919E-06	-0.437E-07	-0.245E-10	-0.107E-12			
10	-0.530E-06	0.128E-06	-0.119E-07	0.566E-09	0.299E-12	-0.107E-12			
16	0.938E-12	-0.213E-12	0.000E+00	-0.213E-13	-0.213E-13	-0.107E-12			
24	-0.213E-13	0.000E+00	-0.213E-13	-0.427E-13	-0.427E-13	-0.128E-12			
32	0.000E+00	0.000E+00	0.000E+00	-0.213E-13	-0.213E-13	-0.107E-12			
36	-0.213E-13	-0.427E-13	-0.213E-13	-0.213E-13	-0.427E-13	-0.853E-13			

Table 2: Percentage difference between the temperature fields evaluated by eqs.(16) and (23). n_D is the number of divisions used in the integration interval $[0,\pi]$ and n_D is the number of Gauss points used in each division.

The application of eq.(15) referenced to a coordinate system coincident with the principal axes is straighforward. The numerical test performed here was therefore limited to verifying if the fundamental solution obtained in a arbitrary coordinate system, as given by eq.(14), reproduces the same results obtained in the orthotropic case. Initially, a coordinate system (x, y, z) was used to evaluate u_{ORT}^* for all three materials as a function of a load point placed along the line (a, a, 0). These fundamental solutions are plotted as solid lines in fig. A new coordinate system (x', y', z') was generated by rotating the original one by 30°, 60°, and 90° along the axes x, y, and z, respectively. In the (x', y', z') system, the thermal diffusivity tensors become obviously non-diagonal, allowing the direct application of eq.(14), which are plotted as symbols in fig.5. Excellent agreement was found in all cases analyzed.

As a second example, a fundamental solution for Graphite was derived for its principal coordinate axes as in eq.(15), again considering the load point acting along the line (a, a, 0). The expression for u^* in this case is:

$$u^* = \frac{3.16567 \times 10^{-4}}{a}.$$
 (25)

The (x, y, z) system was then rotated along the direction $(0, \sqrt{2}/2, \sqrt{2}/2)$ by an angle of $\pi/6$, resulting the following diffusivity tensor:

$$\mathbf{K}'_{G} = \begin{bmatrix} 321.75 & 6.30 & 87.74 \\ 353.81 & -16.62 \\ 123.44 \end{bmatrix} \quad [W/m^{\circ}C]$$

These properties were used in eq.(14) and produced exactly the same function given by eq.(25).



Figure 5: Comparison of the Green.s functions obtained by eq.(15) in the principal (x,y,z) system (solid lines) and by eq.(14) in an abritrary (x',y',z') system (symbols) for three different materials.

5 CONCLUSIONS

In this paper we have initially presented a review of several integral identities used to derive fundamental solutions for the Laplace operator, aiming its application in integral equation methods. The relationship between the one, two and three-dimensional forms, as well as their relation to Fourier and Radon transforms have been shown. Although the tensorial form of these equations has been long known in elastodynamics, their use in potential problems has never been fully explored. In particular, the application of either eq.(7) and (8) or eq.(20) in analytical and semi-analytical derivations, respectively, to other types of scalar problems seems to be very attractive. By replacing the operator L it is possible to use the procedure outlined here to derive different types of fundamental solutions, such as time-dependent problems, problems with spatially variable constitutive parameters, and problems with heat sources distributed along lines and arcs, to name a few.

The methodology was applied to the fully anisotropic heat transfer equation, generating a less known solution for the problem, which exempts the need for coordinate transformations. A numerical version of the fundamental solution was also derived using the line integral method. Numerical examples show that both fundamental solutions agree.

The fundamental solutions derived can be interesting to solve problems composed by more than one non-isotropic material using the subregion technique, can be easily implemented in a standard BEM code, and avoids the overhead of handling mapped domains and flux boundary conditions. Composite materials modeled with representative volume elements containing large number of inclusions embedded in can be solved more efficiently using these new functions. However, analytical forms like eq.(14) or (16) may be impossible to obtain in cases subjected to excitations other than a unit source. In such cases, particular forms of the line integral (18) will provide a much easier solution for both potential and flux.

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APPENDIX

It may be instructive to derive another useful form of eq.(4) by applying Radon transform (Deans, 1983) to it :

$$L(\boldsymbol{\xi}) \frac{\partial^2 u^* \left(\boldsymbol{\xi}, p - \boldsymbol{\xi} \cdot \boldsymbol{r} \right)}{\partial p^2} = - \,\widehat{\delta} \left(\boldsymbol{\xi} \cdot \boldsymbol{r} \right) \quad , \tag{26}$$

where $\boldsymbol{\xi}$ and p are the variables in the transformed space, the symbol $\hat{f}(\boldsymbol{\xi}, p - \boldsymbol{\xi} \cdot \mathbf{r})$ denotes the Radon transform of $f(\boldsymbol{x}, \mathbf{y})$:

$$\widehat{f}\left(\boldsymbol{\xi}, p - \boldsymbol{\xi} \cdot \mathbf{y}\right) = \iint_{\mathbb{R}^{2}} f\left(\mathbf{x}, \mathbf{y}\right) \delta\left(p - \boldsymbol{\xi} \cdot \mathbf{r}\right) dS^{2}\left(\mathbf{x}\right) = \iint_{\mathbb{R}^{2} \mid \boldsymbol{\xi} \mathbf{r} = p} f\left(\mathbf{x}, \mathbf{y}\right) dS^{2}\left(\mathbf{x}\right)$$

and the integration is performed over the infinite plane $\boldsymbol{\xi} \cdot \mathbf{r} = p$. It follows that the inverse of Radon transform for the three-dimensional case is given by (Deans, 1983):

$$f(\mathbf{x}, \mathbf{y}) = \frac{-1}{8\pi^2} \iint_{S^2} \left[\frac{\partial^2 \widehat{f}(\boldsymbol{\xi}, p - \boldsymbol{\xi} \cdot \mathbf{r})}{\partial p^2} \right]_{\boldsymbol{\xi} \cdot \mathbf{r} = p} dS^2(\boldsymbol{\xi})$$
(27)

and one of the interesting properties of the Radon transform becomes apparent, namely, its inverse is obtained by integration over the unit sphere S^2 , and it is independent on its size. Another fundamental result is obtained by replacing $f(\mathbf{x}, \mathbf{y})$ by $\delta(\mathbf{r})$ (Gelfand et al. 1966):

$$\delta(\mathbf{r}) = \frac{-1}{8\pi^2} \Delta_{\mathbf{y}} \iint_{S^2} \delta(\boldsymbol{\xi} \cdot \mathbf{r}) \, dS^2(\boldsymbol{\xi}) = \widehat{\delta}(\boldsymbol{\xi} \cdot \mathbf{r}) \tag{28}$$

that is, the Radon transform of a Dirac's delta function is also a delta function. Using eq.(28) in (26):

$$\frac{\partial^2 \widehat{u^*}(\boldsymbol{\xi}, p - \boldsymbol{\xi} \cdot \mathbf{r})}{\partial p^2} = L^{-1}(\boldsymbol{\xi}) \,\delta(\mathbf{r}) \quad ,$$

and the application of the inverse transform leads to:

$$u^{*}(\mathbf{x},\mathbf{y}) = \frac{1}{8\pi^{2}} \iint_{S^{2}} L^{-1}(\boldsymbol{\xi}) \,\delta(\boldsymbol{\xi}\cdot\mathbf{r}) \,dS^{2}(\boldsymbol{\xi})$$
(29)

which happens to be an alternative form to eq.(7). In principle, a counterpart of eq.(29) could be found for a generic source excitation b replacing the unit source on the left hand side of (26), but certainly the Radon transform of such a function will lack the simplicity in eq.(29).