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Fundamental solutions for general anisotropic multi-field materials based on spherical harmonics expansions

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ABSTRACT

A unified method to evaluate the fundamental solutions for generally anisotropic multi-field materials is presented. Based on the relation between the Rayleigh expansion and the three-dimensional Fourier representation of a homogenous partial differential operator, the proposed technique allows to obtain the fundamental solutions and their derivatives up to the desired order as convergent series of spherical harmonics. For a given material, the coefficients of the series are computed only once, and the derivatives of the fundamental solutions are obtained without any term-by-term differentiation, making the proposed approach attractive for boundary integral formulations and efficient for numerical implementation. Useful general relationships for the computation of derivatives of various order of the fundamental solutions are presented. Furthermore, no particular treatment is needed for mathematically degenerate cases. The fundamental solutions of the Laplace equation and isotropic elastic solids are exactly retrieved as special cases. Numerical results are presented to demonstrate the accuracy of the approach for isotropic elastic, generally anisotropic elastic, transversely isotropic and generally anisotropic piezo-electric and magneto-electro-elastic materials.

1. Introduction

Fundamental solutions, or Green's functions, are essential to the solution of many boundary value problems in engineering (Mura, 2013) and represent the key ingredient in boundary integral formulations (Aliabadi, 2002; Banerjee and Butterfield, 1981; Wrobel, 2002). Simple and closed form expressions are available only for simple cases, such as potential problems or isotropic elasticity. Therefore, the development of efficient schemes for computing the fundamental solutions of generic linear systems of partial differential equations (PDEs) still represents a challenge of great scientific interest.

In the field of materials engineering, several works have been devoted to finding the displacements field (Fredholm, 1900; Lifshitz and Rozentsveig, 1947) and its derivatives (Barnett, 1972) due to a point force in a three-dimensional anisotropic elastic medium. The formal expression of the fundamental solutions of a second order partial differential operator has been classically obtained using either Fourier or Radon transforms, which lead to expressions in terms of a contour integral on a unit circle (Synge, 1957). By using suitable variable transformations, several researchers replaced the contour integral by an infinite line integral (Wang, 1997), whose solution has been obtained by means of the Cauchy's residue theorem in terms of the Stroh eigenvalues (Lee, 2003; Sales and Gray, 1998; Wu, 1998) or eigenvectors (Malen, 1971; Nakamura and Tanuma, 1997). However, when the Stroh's eigenvalues or eigenvectors approach is used, the issue of *degeneracy* needs to be robustly addressed, in particular when such an approach is used in a numerical code, e.g. in boundary element implementations. Non-degenerate cases were first studied by Dederichs and Leibfried (Dederichs and Leibfried, 1969) for cubic crystals. Phan et al. (2004; 2005) presented a technique to compute the fundamental solutions of a 3D anisotropic elastic solid and their first derivatives in presence of multiple roots and using the residue approach. Shiah et al. (2008) used the spherical coordinates differentiation to obtain the explicit expressions of the derivatives of the fundamental solutions for an anisotropic elastic solid up to the second order. Although being exact, the main disadvantage of these approaches is the necessity of using different expressions for each different case of different roots, two coincident roots, and three coincident roots. A unified formulation, valid for degenerate as well as non-degenerate cases, has been first presented by Ting and Lee (1997). Their approach has been further investigated by the recent work of Xie et al. (2016b), in which the authors developed

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a unified approach to compute the fundamental solutions of 3D anisotropic solids valid for partially degenerate, fully degenerate and non-degenerate materials. Although not suffering from material's degeneracy, the expressions presented in the work of Xie et al. (2016b) are valid only for anisotropic elastic materials, are given up to second order differentiation and are rather long and complex, in particular when the derivatives are considered. A 2D Radon transform approach has been also used in the literature as an alternative approach to the problem (Buroni and Denda, 2014; Xie et al., 2016a).

The aforementioned works have been mainly devoted to the derivation of the fundamental solution or Green's functions of elastic anisotropic materials. Recently, multi-field materials have received increasing interest for their application in composite multi-functional devices (Nan et al., 2008; Peng et al., 2014). Closed form expressions can be found for transversely isotropic materials showing piezo-electric (Dunn, 1994; Dunn and Wienecke, 1996) and magneto-electro-elastic (Ding et al., 2005; Hou et al., 2005; Soh et al., 2003; Wang and Shen, 2002) coupling. Pan and Tonon (2000) used the Cauchy's residue theorem to derive the fundamental solutions of non-degenerate anisotropic piezo-electric solids, and a finite difference scheme to obtain their derivatives. Buroni and Sáez (2010) used the Cauchy's residue theorem and the Stroh's formalism to obtain the fundamental solutions of degenerate or non-degenerate anisotropic magneto-electro-elastic materials. Their scheme was recently employed in a boundary element code for fracture analysis (Muñoz-Reja et al., 2016).

From a numerical perspective, the fundamental solutions represent the essential ingredient in boundary integral formulations, such as the Boundary Element Method (BEM) (Aliabadi, 2002; Banerjee and Butterfield, 1981; Wrobel, 2002). In practical BEM analyses of engineering interest, the fundamental solutions and their derivatives are computed in the order of million times and the availability of efficient schemes for their evaluation is thus of great interest, especially for large 3D problems. To accelerate the computations for anisotropic elastic materials, Wilson and Cruse (1978) proposed pre-computing the values of the fundamental solutions at regularly spaced points of a spatial grid and using an interpolation scheme with cubic splines to approximate their values in general points during the subsequent BEM analysis. Such an approach and similar interpolation techniques (Schclar, 1994) have been widely employed in the BEM literature (Benedetti and Aliabadi, 2013a; 2013b; Benedetti et al., 2016; 2009; Gulizzi et al., 2015; Milazzo et al., 2012). Mura and Kinoshita (1971) represented the fundamental solutions of a general anisotropic elastic medium in terms of spherical harmonics expansions and used a term-by-term differentiation to obtain the first derivative. Aubry and Arsenlis (2013) used the spherical harmonics expansions for dislocation dynamics in anisotropic elastic media and pointed out that line integrals and double line integrals could be obtained analytically once the series coefficients were computed. Recently, Shiah et al. (2012) proposed an alternative scheme to compute the fundamental solutions of 3D anisotropic elastic solids based on a double Fourier series representation. The authors expressed the fundamental solutions as given by Ting and Lee (1997) in the spherical reference system and then built their Fourier series representation relying on their periodic nature. The authors underlined that the coefficients of the series were computed only once for a given material and employed their method in a BEM code (Tan et al., 2013). They also obtained the first and the second derivatives of the fundamental solutions whose complexity increases with the order of differentiation, despite the use of the spherical coordinates to obtain the derivatives. The interested reader is referred to the book by Pan and Chen (2015) and to the recent paper by Xie et al. (2016a) for a comprehensive overview of the available methods to obtain the fundamental solutions.

In the present work, given a generic linear system of PDEs defined by a homogeneous partial differential operator, the fundamental solutions and their derivatives are computed in a unified fashion in terms of spherical harmonics expansions. It is here demonstrated that the formula found by Mura and Kinoshita (1971) is in fact a particular case of a more general representation of the fundamental solutions and their derivatives, which are not obtained by a term-by-term differentiation and can be computed up to the desired order. The coefficients of the series depend on the material constants and need to be computed only once, thus making the present scheme attractive for efficient boundary integral formulations. Eventually, mathematically degenerate media do not require any specific treatment and the present scheme can be generally employed to cases ranging from simply isotropic to more complex general anisotropic differential operators. To the best of the authors' knowledge, it is the first time that the fundamental solutions for generally anisotropic multi-field materials and their derivatives up to any order are represented in such compact unified fashion.

The paper is organised as follows: Section 2 introduces the class of systems of partial differential equations and the corresponding fundamental solutions that will be addressed in the present study; Section 3 illustrates the mathematical steps needed to obtain the expressions of the fundamental solutions and their derivatives in terms of spherical harmonics; Section 4 presents a few results from the proposed scheme: first it is shown that, in the case of isotropic operators, the proposed representation leads to exact expressions of the fundamental solutions; then a few numerical tests covering generally anisotropic elastic, transversely isotropic and generally anisotropic piezo-electric and magneto-electro-elastic media are presented and discussed. Section 5 draws the final considerations.

2. Problem statement

The linear behaviour of different classes of *multi-field* materials, such as Piezo-Electric (PE), Magneto-Electric (ME), or Magneto-Electro-Elastic (MEE) materials, can be represented through a system of generally coupled partial differential equations (PDEs)

$$\mathscr{L}_{ij}(\partial_x)\phi_j(\boldsymbol{x}) + f_i(\boldsymbol{x}) = 0 \tag{1}$$

where $\boldsymbol{x} = \{x_k\} \in \mathbb{R}^3,\ k = 1, 2, 3,$ is the spatial independent variable, $\phi_j(\boldsymbol{x})$ represent the *unknown* functions of $\boldsymbol{x}$, $f_i(\boldsymbol{x})$ represent the known *generalized* volume forces, and $i, j = 1, \dots, N$ where N is the number of equations as well as the number of unknown functions. $\mathscr{L}_{ij}(\partial_x)$ is supposed to be a general *homogeneous* partial differential operator involving a linear combination of second order derivatives of $\boldsymbol{x}$, i.e. $\mathscr{L}_{ij}(\partial_x) = c_{ijkl}\partial^2(\cdot)/\partial x_k \partial x_l$, where c_{ijkl} are the material constants. The system of PDEs (1) may be specialised to several specific problems ranging from the classical Laplace equation up to the governing equations for general anisotropic magneto-electro-elastic materials, as shown in Section 4.

The system of PDEs in Eq. (1) is defined $\forall \boldsymbol{x} \in V \subseteq \mathbb{R}^3$, being V the material domain, and it is mathematically closed by enforcing a suitable set of boundary conditions over the frontier $S = \partial V$ of V. A well-established technique for numerically solving Eq. (1) is the Boundary Element Method (BEM) (Aliabadi, 2002; Banerjee and Butterfield, 1981; Wrobel, 2002), which is based on the integral representation of the unknown field components $\phi_i(\boldsymbol{x})$. In particular, using the Green's identities, it is possible to express the values of the functions $\phi_i(\boldsymbol{y})$ at any interior point $\boldsymbol{y} \in V$ in terms of the values of $\phi_i(\boldsymbol{x})$ and their derivatives on the boundary S as

$$\phi_p(\boldsymbol{y}) = \int_S \left[\Phi_{pi}(\boldsymbol{x},\boldsymbol{y})\tau_i(\boldsymbol{x}) - T_{pi}(\boldsymbol{x},\boldsymbol{y})\phi_i(\boldsymbol{x})\right]\mathrm{d}S(\boldsymbol{x}) + \int_V \Phi_{pi}(\boldsymbol{x},\boldsymbol{y}) f_i(\boldsymbol{x})\mathrm{d}V(\boldsymbol{x}), \tag{2}$$