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Residue approach for evaluating the 3D anisotropic elastic Green's function: multiple roots

A.-V. Phan[a,*], L.J. Gray[b,c], T. Kaplan[b]

[a]*Department of Mechanical Engineering, University of South Alabama, Mobile, AL 36688-0002, USA*
[b]*Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6367, USA*
[c]*Grupo de Elasticidad y Resistencia de Materiales, Escuela Superior de Ingenieros, Universidad de Sevilla, 41092 Sevilla, Spain*

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Abstract

A numerical algorithm based upon the residue calculus for computing the three-dimensional anisotropic elastic Green's function and its derivatives has been presented by, among the others, Sales and Gray. Although this residue approach is in general faster than the standard Wilson–Cruse interpolation scheme, the convergence rate and accuracy can seriously degrade in the neighborhood of a non-simple pole. In this paper, explicit expressions, also based on the residue calculus, are obtained for computing the Green's function and its first-order derivatives in the presence of a multiple root. Further, the computation time for the residue algorithm proposed here has been significantly reduced by implementing the double-subscript-notation for the elastic constants that define the Christoffel tensor.
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Keywords: Green's function; Anisotropic elasticity; Residue calculus; Boundary element analysis

1. Introduction

A computational analysis using boundary integral equations requires numerous evaluations of both the Green's function (or fundamental solution) and its derivatives [1–3]. While these functions are relatively simple for many problems, e.g. potential theory or isotropic elasticity, they are far more complicated in case of materials of general anisotropy. An effective scheme for evaluating these complicated functions is therefore crucial for the success of an anisotropic boundary element analysis (BEA).

Approaches for computing the three-dimensional (3D) anisotropic elastic Green's function have been investigated by numerous research groups, including Nakamura and Tanuma [4], Ting and Lee [5], Wang [6], Sales and Gray [7], Pan and Yuan [8], Tonon et al. [9], and Phan et al. [10]. While most of the above studies focus on the Green's function for an homogeneous domain, the work by Pan and Yuan [8] was devoted to the bimaterial Green's function. Among the others, technique based upon the residue calculus has been pursued in [5–7,9,10]. The results are obtained in terms of the residue of poles whose positions are determined by the roots of a sixth degree polynomial. While the work of Ting and Lee, as well as Wang primarily focused on the derivation of explicit expressions for the Green's function, Sales and Gray devoted efforts to a practical algorithm for computing this function and its derivatives. Recently, numerical implementations for the calculation of the Green's displacements and stresses, as well as their derivatives have also been introduced by Tonon et al., and a comparison study of the two algorithms [7,9] is under investigation [9]. A limitation of both these studies is that all the roots of the sixth degree polynomial are assumed to be distinct which is not always the case. An explicit solution in terms of the Stroh eigenvalues for the 3D anisotropic elastic Green's function is presented in [5] where the solution remains valid for multiple roots. While this solution is general, it appears to be lengthier than the explicit expressions derived separately for the cases of simple, double and triple poles that are presented in this paper. Further, the development was limited to the Green's function only. In this work, analytical expressions for not only the Green's function but also its first-order derivatives,

* Corresponding author. Tel.: +1 251 460 7453; fax: +1 251 460 6549.
E-mail address: vphan@jaguar1.usouthal.edu (A.-V. Phan).

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in the presence of a multiple root, are discussed herein as they are required by a standard BEA.

Although the algorithm proposed by Sales and Gray is technically sound, it has been shown that numerical problems arise when the sixth degree polynomial has multiple roots. In this situation, or when the roots are nearly equal, the Newton algorithm employed to calculate the root can converge slowly. This issue has been partly addressed in a short publication [10] where the capability to evaluate the Green's function (but not derivatives) in case of a multiple pole was discussed. The evaluation of both the Green's function and its first-order derivatives, which is required in a standard boundary integral analysis, is the subject of this full-length paper. Explicit expressions based on the residue calculus are fully derived for the cases of double and triple roots. In addition, the present algorithm implements the double subscript notation for the fourth-rank elastic constant tensor C_{jlkm}, and consequently requires less memory storage and is more computationally efficient than that in [7]. Numerical results for the Green's function and its first-order derivatives in the presence of both double and triple roots are in excellent agreement with those obtained by means of direct integration using the symbolic computation package `Maple`.

2. Residue calculus approach to the Green's function

2.1. Green's function U_{jk}

Consider an unbounded anisotropic elastic body subjected to a point load. Let $U_{jk}(P,Q)$ be the Green's function corresponding to the displacement field in the x_k direction, at $\mathbf{x}$, produced by the load in the x_j direction at $\mathbf{x}_0$. The function $U_{jk}(\mathbf{x}_0,\mathbf{x})$ can be expressed as a line integral [11,12]

$$U_{jk}(\mathbf{x},\mathbf{x}_0) = \frac{1}{8\pi^2 r}\oint_{S^1} K_{jk}^{-1}(\xi)\mathrm{d}s(\xi) \equiv \frac{1}{8\pi^2 r}\bar{U}_{jk}, \tag{1}$$

where $\mathbf{x}_0$ is the *source point*, and $\mathbf{x}$ is the *observation* or *field point*. Here, $\xi \in \mathcal{R}^3$, K_{jk} is the Christoffel tensor defined in terms of the elastic constants C_{jlkm} of the material [13]

$$K_{jk} = C_{jlkm}\xi_l\xi_m, \tag{2}$$

and $r = \|\mathbf{x}-\mathbf{x}_0\|$. The integration path is the unit circle in the plane having normal $\mathbf{x}-\mathbf{x}_0$

$$S^1 = S^1(\mathbf{x},\mathbf{x}_0) = \{\xi \in \mathcal{R}^3 | \ \ \|\xi\| = 1, \xi\cdot(\mathbf{x}-\mathbf{x}_0) = 0\}. \tag{3}$$

2.2. General solution of the Green's function U_{jk}

In a spherical coordinate system located at the source point $\mathbf{x}_0$ (see Fig. 1), the contour integral in Eq. (1) may be written as

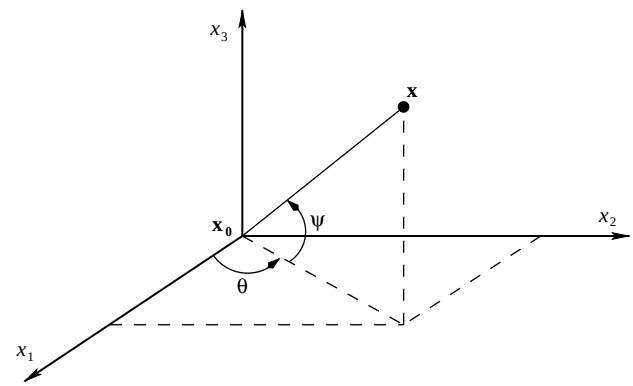

Fig. 1. A spherical coordinate system.

$$\bar{U}_{jk}(\theta,\psi) = \int_0^{2\pi} K_{jk}^{-1}(\xi(t,\theta,\psi))\mathrm{d}t, \tag{4}$$

where θ and ψ are spherical angles defining the unit direction vector $(\mathbf{x}-\mathbf{x}_0)/r$ ($0 \le \psi \le \pi$ denotes the polar angle measured from the equator, and $0 \le \psi \le 2\pi$ the azimuthal angle in the x_1x_2 plane from the x_1 axis). The parametric equation of the unit circle of the integration path is given by

$$\xi(t,\theta,\psi) = \begin{Bmatrix} \xi_1(t,\theta,\psi) \\ \xi_2(t,\theta,\psi) \\ \xi_3(t,\theta,\psi) \end{Bmatrix} = \begin{Bmatrix} \sin(\theta)\cos(t) + \cos(\theta)\cos(\psi)\sin(t) \\ -\cos(\theta)\cos(t) + \sin(\theta)\cos(\psi)\sin(t) \\ -\sin(\psi)\sin(t) \end{Bmatrix}. \tag{5}$$

The integral in Eq. (4) can be evaluated using residue calculus by transforming the integrand into a rational function, the range of integration becoming the real axis. One way to achieve this transformation is to use the change of variable [14]:

$$Z = \tan(t). \tag{6}$$

With this transformation, the components of K_{jk}^{-1} become rational functions of Z, and Eq. (4) can be written in the form [7]

$$\bar{U}_{jk}(\theta,\psi) = 2\int_{-\infty}^{\infty} \frac{P_{jk}(Z)}{Q(Z)}\mathrm{d}Z = 4\pi\mathrm{i}\sigma, \tag{7}$$

where $P_{jk}(Z)$ and $Q(Z)$ are the fourth degree and sixth degree polynomials of Z, respectively; and σ is the sum of the residues $\mathrm{Res}(\lambda_n)$ of $P_{jk}(Z)/Q(Z)$ at the poles λ_n of $Q(Z)$ which lie in the upper half plane. From now on, $P_{jk}(Z)$ and $Q(Z)$ should be understood as functions of not only Z, but also of θ and ψ, i.e. $P_{jk}(Z) \equiv P_{jk}(Z,\theta,\psi)$ and $Q(Z) \equiv Q(Z,\theta,\psi)$.

Note that [7] only considered $\mathrm{Res}(\lambda_n)$ for the case of a simple pole, i.e. distinct roots ($\lambda_j \neq \lambda_k$, $j \neq k$). In general, $\mathrm{Res}(\lambda_n)$ can be determined from the expression [15]:

$$\mathrm{Res}(\lambda_n) = \frac{1}{(m-1)!}\left[\frac{\mathrm{d}^{m-1}}{\mathrm{d}Z^{m-1}}\left\{(Z-\lambda_n)^m \frac{P_{jk}(Z)}{Q(Z)}\right\}\right]_{Z=\lambda_n}. \tag{8}$$

- In case of a *simple pole* ($m=1$)

$$\bar{U}_{jk}(\theta,\psi) = 4\pi\mathrm{i}\sum_{n=1}^{3}\mathrm{Res}(\lambda_n), \tag{9}$$

where

$$\mathrm{Res}(\lambda_n) = \left[(Z-\lambda_n)\frac{P_{jk}(Z)}{Q(Z)}\right]_{Z=\lambda_n} = \left[\frac{P_{jk}(Z)}{Q_{(n)}(Z)}\right]_{Z=\lambda_n} = \frac{P_{jk}(\lambda_n)}{Q_{(n)}(\lambda_n)}. \tag{10}$$

In Eq. (10), the polynomials $P_{jk}(\lambda_n)$ and $Q_{(n)}(\lambda_n)$ may be written in the following forms:

$$P_{jk}(\lambda_n) = \sum_{l=0}^{4} p_{jkl}\lambda_n^l, \tag{11}$$

$$Q_{(n)}(\lambda_n) = q_6(\lambda_n - \bar{\lambda}_n)\prod_{\substack{o=1\\ o\neq n}}^{3}(\lambda_n-\lambda_o)(\lambda_n-\bar{\lambda}_o), \tag{12}$$

where p_{jkl} is a coefficient associated with the lth-order term in Eq. (11), and q_6 is a coefficient associated with the sixth-order term in Eq. (12).

- In case of a *double pole* ($m=2$), for example, $\lambda_1=\lambda_2$, one gets

$$\bar{U}_{jk}(\theta,\psi) = 4\pi\mathrm{i}[\mathrm{Res}(\lambda_n)+\mathrm{Res}(\lambda_3)], \tag{13}$$

where n could either be 1 or 2, and (a subscript comma implies partial differentiation with respect to the variable following)

$$\begin{aligned}\mathrm{Res}(\lambda_n) &= \left[\frac{\mathrm{d}}{\mathrm{d}Z}\left\{(Z-\lambda_n)^2\frac{P_{jk}(Z)}{Q(Z)}\right\}\right]_{Z=\lambda_n}\\ &= \left[\frac{\mathrm{d}}{\mathrm{d}Z}\left\{\frac{P_{jk}(Z)}{Q_{(n^2)}(Z)}\right\}\right]_{Z=\lambda_n}\\ &= \frac{1}{Q_{(n^2)}(\lambda_n)}\left[P_{jk,Z}(\lambda_n)\right.\\ &\left.-\left(\frac{1}{\lambda_n-\lambda_3}+\frac{2}{\lambda_n-\bar{\lambda}_n}+\frac{1}{\lambda_n-\bar{\lambda}_3}\right)P_{jk}(\lambda_n)\right],\end{aligned} \tag{14}$$

$$P_{jk,Z}(\lambda_n) = \sum_{l=0}^{3}(l+1)p_{jk(l+1)}\lambda_n^l, \tag{15}$$

$$Q_{(n^2)}(\lambda_n) = q_6(\lambda_n-\lambda_3)(\lambda_n-\bar{\lambda}_n)^2(\lambda_n-\bar{\lambda}_3), \tag{16}$$

$$\mathrm{Res}(\lambda_3) = \frac{P_{jk}(\lambda_3)}{Q_{(3)}(\lambda_3)}. \tag{17}$$

- In case of a *triple pole* ($m=3$), we have $\lambda_1=\lambda_2=\lambda_3$, thus

$$\bar{U}_{jk}(\theta,\psi) = 4\pi\mathrm{i}\mathrm{Res}(\lambda_n), \tag{18}$$

where n could either be 1, 2 or 3, and

$$\begin{aligned}\mathrm{Res}(\lambda_n) &= \frac{1}{2}\left[\frac{\mathrm{d}^2}{\mathrm{d}Z^2}\left\{(Z-\lambda_n)^3\frac{P_{jk}(Z)}{Q(Z)}\right\}\right]_{Z=\lambda_n}\\ &= \frac{1}{2}\left[\frac{\mathrm{d}^2}{\mathrm{d}Z^2}\left\{\frac{P_{jk}(Z)}{Q_{(n^3)}(Z)}\right\}\right]_{Z=\lambda_n}\\ &= \frac{1}{Q_{(n^3)}(\lambda_n)}\left\{\frac{P_{jk,ZZ}(\lambda_n)}{2}-\frac{3P_{jk,Z}(\lambda_n)}{\lambda_n-\bar{\lambda}_n}\right.\\ &\left.+\frac{6P_{jk}(\lambda_n)}{(\lambda_n-\bar{\lambda}_n)^2}\right\},\end{aligned} \tag{19}$$

$$P_{jk,ZZ}(\lambda_n) = \sum_{l=0}^{2}(l+1)(l+2)p_{jk(l+2)}\lambda_n^l, \tag{20}$$

$$Q_{(n^3)}(\lambda_n) = q_6(\lambda_n-\bar{\lambda}_n)^3. \tag{21}$$

3. Residue calculus approach for the first-order derivatives of $U_{jk}(\mathbf{x},\mathbf{x}_0)$

According to Eqs. (1) and (4), the partial derivatives of $U_{jk}(\mathbf{x},\mathbf{x}_0)$ with respect to $\mathbf{x}$ or $\mathbf{x}_0$ can be expressed in terms of those of $\bar{U}_{jk}(\theta,\psi)$ with respect to angles θ or ψ. In the following, α represents either angle.

- In case of a *simple pole* ($m=1$) in $Q(Z)$

$$\begin{aligned}\bar{U}_{jk,\alpha}(\theta,\psi) &= 2\int_{-\infty}^{\infty}\frac{P_{jk,\alpha}(Z)Q(Z)-P_{jk}(Z)Q_{,\alpha}(Z)}{Q^2(Z)}\mathrm{d}Z\\ &= 4\pi\mathrm{i}\sum_{n=1}^{3}\mathrm{Res}(\lambda_n).\end{aligned} \tag{22}$$

As $Q^2(Z)$ has three double poles, use of Eq. (8) yields

$$\mathrm{Res}(\lambda_n) = \left[\frac{\mathrm{d}}{\mathrm{d}Z}\left\{\frac{P_{jk,\alpha}(Z)Q(Z)-P_{jk}(Z)Q_{,\alpha}(Z)}{Q^2_{(n)}(Z)}\right\}\right]_{Z=\lambda_n}, \tag{23}$$

where

$$Q_{(n)}(Z) = q_6(Z - \bar{\lambda}_n) \prod_{\substack{o=1 \\ o\neq n}}^{3} (Z - \lambda_o)(Z - \bar{\lambda}_o). \tag{24}$$

Noting that $Q(\lambda_n)=0$, the result is,

$$\begin{aligned}\mathrm{Res}(\lambda_n) &= \frac{P_{jk,\alpha}(\lambda_n)Q_{,Z}(\lambda_n) - P_{jk,Z}(\lambda_n)Q_{,\alpha}(\lambda_n) - P_{jk}(\lambda_n)Q_{,\alpha Z}(\lambda_n)}{Q^2_{(n)}(\lambda_n)} \\ &\quad + \frac{2P_{jk}(\lambda_n)Q_{,\alpha}(\lambda_n)Q_{(n),Z}(\lambda_n)}{Q^3_{(n)}(\lambda_n)}.\end{aligned} \tag{25}$$

- In case of a *double pole* ($m=2$) in $Q(Z)$, for example, $\lambda_1=\lambda_2$ (i.e. $n=1$ or 2), one gets

$$\bar{U}_{jk,\alpha}(\theta,\psi) = 4\pi\mathrm{i}[\mathrm{Res}(\lambda_n) + \mathrm{Res}(\lambda_3)], \tag{26}$$

where $\mathrm{Res}(\lambda_3)$ is determined by Eq. (23). As $Q^2(Z)$ has a quadruple pole, $\mathrm{Res}(\lambda_n)$ is given by Eq. (8) as follows:

$$\mathrm{Res}(\lambda_n) = \frac{1}{6}\left[\frac{\mathrm{d}^3}{\mathrm{d}Z^3}\left\{\frac{P_{jk,\alpha}(Z)Q(Z) - P_{jk}(Z)Q_{,\alpha}(Z)}{Q^2_{(n^2)}(Z)}\right\}\right]_{Z=\lambda_n}, \tag{27}$$

$$Q_{(n^2)}(Z) = q_6(Z - \lambda_3)(Z - \bar{\lambda}_n)^2(Z - \bar{\lambda}_3). \tag{28}$$

More specifically, Eq. (27) is represented as

$$\begin{aligned}\mathrm{Res}(\lambda_n) = &\frac{1}{6Q^2_{(n^2)}}(3P_{jk,\alpha ZZ}Q_{,Z} + 3P_{jk,\alpha Z}Q_{,ZZ} + P_{jk,\alpha}Q_{,ZZZ} \\ &- P_{jk,ZZZ}Q_{,\alpha} - 3P_{jk,ZZ}Q_{,\alpha Z} - 3P_{jk,Z}Q_{,\alpha ZZ} \\ &- P_{jk}Q_{,\alpha ZZZ}) - \frac{1}{Q^3_{(n^2)}}[Q_{(n^2),Z}(2P_{jk,\alpha Z}Q_{,Z} \\ &+ P_{jk,\alpha}Q_{,ZZ} - P_{jk,ZZ}Q_{,\alpha} - 2P_{jk,Z}Q_{,\alpha Z} \\ &- P_{jk}Q_{,\alpha ZZ}) + Q_{(n^2),ZZ}(P_{jk,\alpha}Q_{,Z} - P_{jk,Z}Q_{,\alpha} \\ &- P_{jk}Q_{,\alpha Z}) + Q_{(n^2),ZZZ}P_{jk}Q_{,\alpha}/3] \\ &+ \frac{3}{Q^4_{(n^2)}}[Q^2_{(n^2),Z}(P_{jk,\alpha}Q_{,Z} - P_{jk,Z}Q_{,\alpha} - P_{jk}Q_{,\alpha Z}) \\ &- Q_{(n^2),ZZ}Q_{(n^2),Z}P_{jk}Q_{,\alpha}] + \frac{4Q^3_{(n^2),Z}P_{jk}Q_{,\alpha}}{Q^5_{(n^2)}},\end{aligned} \tag{29}$$

where all the polynomials are evaluated at $Z=\lambda_n$, i.e. $P_{jk}=P_{jk}(\lambda_n)$ and so on.

- In case of a *triple pole* in $Q(Z)$ ($m=3$), we have

$$\bar{U}_{jk,\alpha}(\theta,\psi) = 4\pi\mathrm{i}\mathrm{Res}(\lambda_n), \tag{30}$$

where

$$\mathrm{Res}(\lambda_n) = \frac{1}{120}\left[\frac{\mathrm{d}^5}{\mathrm{d}Z^5}\left\{\frac{P_{jk,\alpha}(Z)Q(Z) - P_{jk}(Z)Q_{,\alpha}(Z)}{Q^2_{(n^3)}(Z)}\right\}\right]_{Z=\lambda_n}, \tag{31}$$

$$Q_{(n^3)}(Z) = q_6(Z - \bar{\lambda}_n)^3. \tag{32}$$

The result is

$$\begin{aligned}\mathrm{Res}(\lambda_n) = &\frac{1}{Q^2_{(n^3)}}(5P_{jk,\alpha ZZZZ}Q_{,Z} + 10P_{jk,\alpha ZZZ}Q_{,ZZ} \\ &+ 10P_{jk,\alpha ZZ}Q_{,ZZZ} + 5P_{jk,\alpha Z}Q_{,ZZZZ} \\ &+ P_{jk,\alpha}Q_{,ZZZZZ} - P_{jk,ZZZZZ}Q_{,\alpha} - 5P_{jk,ZZZZ}Q_{,\alpha Z} \\ &- 10P_{jk,ZZZ}Q_{,\alpha ZZ} - 10P_{jk,ZZ}Q_{,\alpha ZZZ} \\ &- 5P_{jk,Z}Q_{,\alpha ZZZZ} - P_{jk}Q_{,\alpha ZZZZZ}) \\ &- \frac{2}{Q^3_{(n^3)}}[5Q_{(n^3),Z}(4P_{jk,\alpha ZZZ}Q_{,Z} + 6P_{jk,\alpha ZZ}Q_{,ZZ} \\ &+ 4P_{jk,\alpha}Q_{,ZZZ} + P_{jk,\alpha}Q_{,ZZZ} - P_{jk,ZZZZ}Q_{,\alpha} \\ &- 4P_{jk,ZZZ}Q_{,\alpha Z} - 6P_{jk,ZZ}Q_{,\alpha ZZ} - 4P_{jk,Z}Q_{,\alpha ZZZ} \\ &- P_{jk}Q_{,\alpha ZZZZ}) \\ &+ 10Q_{(n^3),ZZ}(3P_{jk,\alpha ZZ}Q_{,Z} + 3P_{jk,\alpha Z}Q_{,ZZ} \\ &+ P_{jk,\alpha}Q_{,ZZZ} - P_{jk,ZZZ}Q_{,\alpha} - 3P_{jk,ZZ}Q_{,\alpha Z} \\ &- 3P_{,Z}Q_{,\alpha ZZ} - P_{jk}Q_{\alpha,ZZZ}) \\ &+ 10Q_{(n^3),ZZZ}(2P_{jk,\alpha Z}Q_{,Z} + P_{jk,\alpha}Q_{,ZZ} \\ &- P_{jk,ZZ}Q_{,\alpha} - 2P_{jk,Z}Q_{,\alpha Z} - P_{jk}Q_{\alpha ZZ}) \\ &+ 5Q_{(n^3),ZZZZ}(P_{jk,\alpha}Q_{,Z} - P_{jk,Z}Q_{,\alpha} - P_{jk}Q_{,\alpha Z}) \\ &- Q_{(n^3),ZZZZZ}P_{jk}Q_{,\alpha}] \\ &+ \frac{30}{Q^4_{(n^3)}}[2Q^2_{(n^3),Z}(3P_{jk,\alpha ZZ}Q_{,Z} + 3P_{jk,\alpha Z}Q_{,ZZ} \\ &+ P_{jk,\alpha}Q_{,ZZZ} - P_{jk,ZZZ}Q_{,\alpha} - 3P_{jk,ZZ}Q_{,\alpha Z} \\ &- 3P_{jk,Z}Q_{,\alpha ZZ} - P_{jk}Q_{,\alpha ZZZ}) \\ &+ 6Q_{(n^3),ZZ}Q_{(n^3),Z}(2P_{jk,\alpha Z}Q_{,Z} + P_{jk,\alpha}Q_{,ZZ} \\ &- P_{jk,ZZ}Q_{,\alpha} - 2P_{jk,Z}Q_{,\alpha Z} - P_{jk}Q_{,\alpha ZZ}) \\ &+ (3Q^2_{(n^3),ZZ} + 4Q_{(n^3),ZZZ}Q_{(n^3),Z})(P_{jk,\alpha}Q_{,Z} \\ &- P_{jk,Z}Q_{,\alpha} - P_{jk}Q_{,\alpha Z}) \\ &- P_{jk}Q_{,\alpha}(2Q_{(n^3),ZZZ}Q_{(n^3),ZZ} + Q_{(n^3),ZZZZ}Q_{(n^3),Z})] \\ &- \frac{120}{Q^5_{(n^3)}}[2Q^3_{(n^3),Z}(2P_{jk,\alpha Z}Q_{,Z} + P_{jk,\alpha}Q_{,ZZ} \\ &- P_{jk,ZZ}Q_{,\alpha} - 2P_{jk,Z}Q_{,\alpha Z} - P_{jk}Q_{,\alpha ZZ}) \\ &+ 6Q_{(n^3),ZZ}Q^2_{(n^3),Z}(P_{jk,\alpha}Q_{,Z} - P_{jk,Z}Q_{,\alpha} \\ &- P_{jk}Q_{,\alpha Z}) - (2Q_{(n^3),ZZZ}Q^2_{(n^3),Z} \\ &+ 3Q^2_{(n^3),ZZ}Q_{(n^3),Z})P_{jk}Q_{,\alpha}] \\ &+ \frac{600}{Q^6_{(n^3)}}[Q^4_{(n^3),Z}(P_{jk,\alpha}Q_{,Z} - P_{jk,Z}Q_{,\alpha} - P_{jk}Q_{,\alpha Z}) \\ &- 2Q_{(n^3),ZZ}Q^3_{(n^3),Z}P_{jk}Q_{,\alpha}] \\ &+ \frac{720Q^5_{(n^3),Z}P_{jk}Q_{,\alpha}}{Q^7_{(n^3)}}.\end{aligned} \tag{33}$$

4. Numerical implementation and computation time

As in Ref. [7], the three roots λ_n are found using Newton's method in conjunction with Horner's algorithm [16] for efficient polynomial evaluation.

Once the roots have been found, the quantities $|\lambda_1-\lambda_2|$, $|\lambda_2-\lambda_3|$ and $|\lambda_3-\lambda_1|$ are compared with $\varepsilon=10^{-4}$ to determine whether a multiple root occurs. Then depending on the order m of the roots, appropriate equations among (9), (13) and (18) need be selected to compute the tensor elements of $\bar{U}_{jk}$.

It is well known that the description of both elastic strain and stress tensors involve only six independent components, conveniently identified using a double subscript notation. As these quantities, as well as K_{jk} in Eq. (2), are symmetric with respect to an interchange of the subscripts, it will be convenient to abbreviate each double subscript notation uv in $K_{jk}=C_{(jl)(km)}\bar{\xi}_{lm}$ ($\bar{\xi}_{lm}=\xi_l\xi_m$) to a single subscript (Voight notation) running from 1 to 6; i.e. $uv=11$, 22, 33, 23/32, 31/13, 12/21. Due to these symmetries, the fourth-order elastic constant tensor C_{jlkm} can be replaced by 21 independent components c_{ij} of a (6×6) symmetric matrix as widely employed in the literature. As a result, the six independent components of the tensor K_{jk} are simply given by

$$\begin{Bmatrix} K_{11} \\ K_{22} \\ K_{33} \\ K_{23} \\ K_{31} \\ K_{12} \end{Bmatrix} = \begin{bmatrix} c_{11} & c_{66} & c_{55} & 2c_{56} & 2c_{15} & 2c_{16} \\ c_{66} & c_{22} & c_{44} & 2c_{24} & 2c_{46} & 2c_{26} \\ c_{55} & c_{44} & c_{33} & 2c_{34} & 2c_{35} & 2c_{45} \\ c_{56} & c_{24} & c_{34} & (c_{23}+c_{44}) & (c_{36}+c_{45}) & (c_{25}+c_{46}) \\ c_{15} & c_{46} & c_{35} & (c_{35}+c_{45}) & (c_{13}+c_{55}) & (c_{14}+c_{56}) \\ c_{16} & c_{26} & c_{45} & (c_{25}+c_{46}) & (c_{14}+c_{56}) & (c_{12}+c_{66}) \end{bmatrix} \times \begin{Bmatrix} \xi_1\xi_1 \\ \xi_2\xi_2 \\ \xi_3\xi_3 \\ \xi_2\xi_3 \\ \xi_3\xi_1 \\ \xi_1\xi_2 \end{Bmatrix}, \tag{34}$$

The use of single subscript notation eliminates the unnecessary storage for symmetric components in the elastic constant tensor C_{jlkm} and the Green's function U_{jk}: the handling of a $(3\times3\times3\times3)$ fourth-rank tensor C_{jlkm}, and (3×3) matrices K_{jk} and P_{jk} has been replaced by a (6×6) matrix and (6×1) vectors as shown in Eq. (34). However, the main consequence is computational efficiency. The computation times resulting from this numerical implementation are even be better than those reported in Ref. [7].

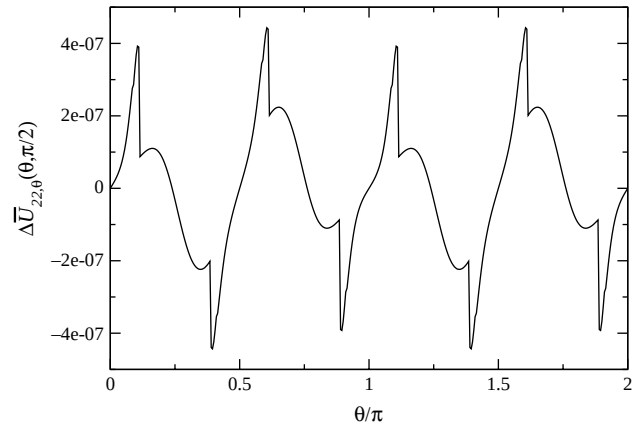

Fig. 2. Discrepancy of $\bar{U}_{22,\theta}(\theta,\pi/2)$ for germanium.

5. Numerical examples

5.1. Simple roots

To start, $\bar{U}_{jk}$ is evaluated in case of distinct roots (simple poles) in the polynomial $Q(Z)$ using the numerical implementation proposed above. The materials germanium (Ge) and tin (Sn), which, respectively, are cubic and tetragonal crystal systems, are employed. The elastic constants for germanium are (in units of 10^{10} Pa) [17] $c_{11}=12.85$, $c_{12}=4.83$ and $c_{44}=6.68$. Tin has a piezo-elasto-dielectric matrix type defined by the following six elastic constants (in the same units) [17]: $c_{11}=7.35$, $c_{33}=8.7$, $c_{44}=2.2$, $c_{66}=2.265$, $c_{12}=2.34$ and $c_{13}=2.8$.

Residue calculus results for $\bar{U}_{jk,\alpha}(\theta,\psi)$ are compared with those obtained via direct integration of Eq. (7) using the symbolic computation package `Maple`. The discrepancies of $\bar{U}_{22,\theta}(\theta,\pi/2)$ and $\bar{U}_{13,\psi}(\theta,\pi/2)$ for germanium, and $\bar{U}_{12,\theta}(\pi,\psi)$ and $\bar{U}_{33,\psi}(\pi,\psi)$ for tin are shown in Figs. 2–5, respectively. Excellent agreements can be observed considering that the elastic constants c_{ij} are typically only known to three significant digits.

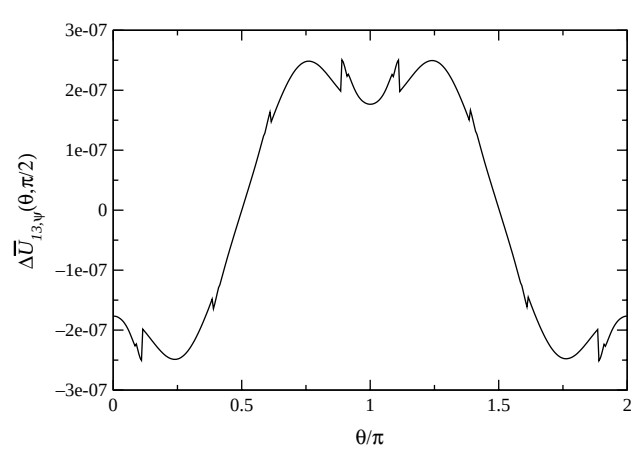

Fig. 3. Discrepancy of $\bar{U}_{13,\psi}(\theta,\pi/2)$ for germanium.

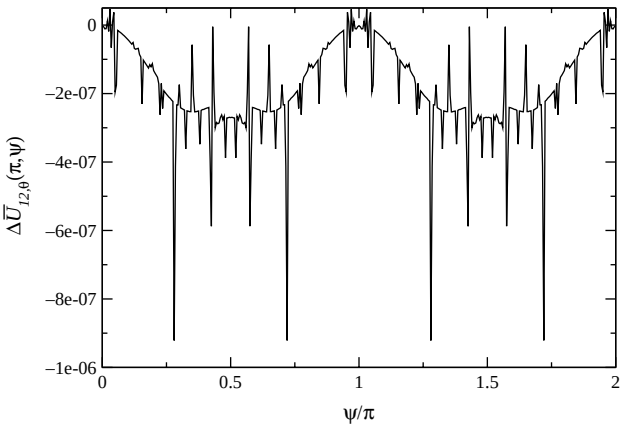

Fig. 4. Discrepancy of $\bar{U}_{12,\theta}(\pi,\psi)$ for tin.

5.2. Multiple roots

In this section, the evaluation of $\bar{U}_{jk,\alpha}(\theta,\psi)$ in case of multiple roots in the polynomial $Q(Z)$ is carried out to validate the numerical implementation of Eqs. (13) and (18). For these tests, it is convenient to prescribe $P_{jk}(Z)$ and $Q(Z)$ as functions of the angles θ and ψ, rather than use a particular material. The gradients $\bar{U}_{jk,\theta}(\pi/2,0)$ and $\bar{U}_{jk,\psi}(\pi/2,0)$ are evaluated using residue calculus and are compared with those obtained from the direct integration of the following equation using the package `Maple`:

$$\bar{U}_{kj,\alpha} = 2\int_{-\infty}^{\infty} \frac{\mathrm{d}}{\mathrm{d}\alpha}\left\{\frac{P_{jk}(Z)}{Q(Z)}\right\}\mathrm{d}Z. \tag{35}$$

- *Double pole:* Consider the following polynomials:

$$P_{jk}(Z) = [40-\cos(\theta)]Z^4 + 2\cos(\theta)Z^3 - [5+\sin(\psi)]Z^2 - 10\sin(\psi)Z + 25, \tag{36}$$

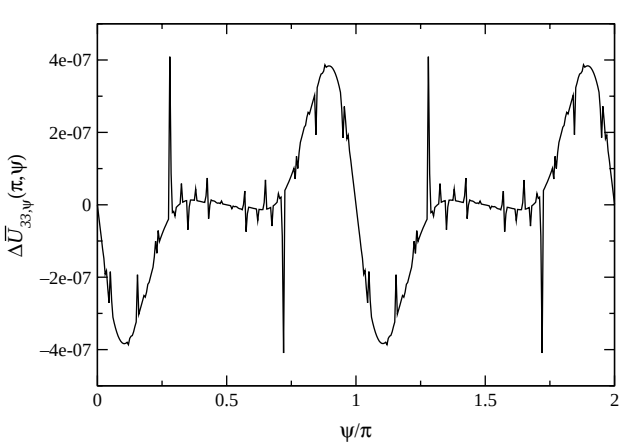

Fig. 5. Discrepancy of $\bar{U}_{33,\psi}(\pi,\psi)$ for tin.

Table 1
Evaluation of $\bar{U}_{jk,\alpha}(\pi/2,0)$ in case of a double pole

	Residue calculus	Maple solution	% Discrepancy
$\bar{U}_{jk,\theta}(\pi/2,0)$	−9.222024040	−9.222024152	1.214×10^{-6}
$\bar{U}_{jk,\psi}(\pi/2,0)$	−2.787466587	−2.787466638	1.830×10^{-6}

and

$$Q(Z) = 3\sin(\theta)\cos(\psi)Z^6 + 18Z^5 + 93[1-\cos(\theta)]Z^4 + 180Z^3 + 513[1+\sin(\psi)]Z^2 + 546Z + 2535\sin(\theta). \tag{37}$$

This is the case of a double pole since at $\theta=\pi/2$ and $\psi=0$

$$Q(Z) = 3Z^6 + 18Z^5 + 93Z^4 + 180Z^3 + 513Z^2 + 546Z + 2535 = 3(Z-\lambda_1)(Z-\lambda_2)^2(Z-\bar{\lambda}_1)(Z-\bar{\lambda}_2)^2, \tag{38}$$

where $\lambda_1 = 1+2\mathrm{i}$, and $\lambda_2=\lambda_3=-2+3\mathrm{i}$.The results obtained from residue calculus and from using the symbolic package `Maple` are shown in Table 1 along with the percentage discrepancies. The data suggest that the residue calculus implementation for double-pole cases is very accurate.

- *Triple pole:* Now, consider the following pair:

$$P_{jk}(Z) = \sin(\psi)Z^4 - \sin^2\left(\frac{\theta}{2}\right)Z^3 - [1-\cos(\theta)]Z^2 + \cos(\psi)Z + 1 \tag{39}$$

and

$$Q(Z) = 2\sin(\theta)\cos(\psi)Z^6 - 36\cos(2\theta)Z^5 + 276Z^4 + 1152Z^3 + 2760[1-\sin(2\theta)]Z^2 + 3600Z + 2000[1+\sin(\psi)]. \tag{40}$$

At $\theta=\pi/2$ and $\psi=0$, $Q(Z)$ has a triple pole since it can be written as

$$Q(Z) = 2Z^6 + 36Z^5 + 276Z^4 + 1152Z^3 + 2760Z^2 + 3600Z + 2000 = 2(Z-\lambda_1)^3(Z-\bar{\lambda}_1)^3, \tag{41}$$

where $\lambda_1=\lambda_2=\lambda_3=-3+\mathrm{i}$.

Table 2
Evaluation of $\bar{U}_{jk,\alpha}(\pi/2,0)$ in case of a triple pole

	Residue calculus	Maple solution	% Discrepancy
$\bar{U}_{jk,\theta}(\pi/2,0)$	−65972.66056	−65972.66046	1.516×10^{-7}
$\bar{U}_{jk,\psi}(\pi/2,0)$	−2115.666303	−2115.666308	2.363×10^{-7}

Again, the residue calculus results are compared with those obtained using the package `Maple` as shown in (Table 2), and it is seen that they can be considered as identical.

6. Conclusion

Explicit expressions based upon the residue calculus for the 3D anisotropic elastic Green's function and its first-order derivatives are obtained for the case of a multiple pole. A new numerical scheme is proposed which improves the computational effectiveness of the algorithm initially proposed by Sales and Gray [7] through the use of double subscript notation in expressing the fourth-order elastic constant tensor. Numerical results for the Green's function and its first-order derivatives in the presence of both single and multiple roots are in excellent agreement with those obtained using the symbolic computation package `Maple`. A numerical implementation of the residue calculus for the calculation of the second derivatives of the 3D anisotropic elastic Green's function in the presence of a multiple root is currently being pursued by the authors as these derivatives are required in a BEA based upon the hypersingular (traction/stress) boundary integral equation, such as a dual BEA [18] or a symmetric Galerkin BEA [19].

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