COMMUNICATIONS IN NUMERICAL METHODS IN ENGINEERING
Commun. Numer. Meth. Engng 2004; **20**:335–341 (DOI: 10.1002/cnm.675)

On the residue calculus evaluation of the 3-D anisotropic elastic Green's function

A.-V. Phan[1,*,†], L. J. Gray[2] and T. Kaplan[2]

[1]*Department of Mechanical Engineering, University of South Alabama, Mobile, AL 36688-0002, U.S.A.*
[2]*Oak Ridge National Laboratory, Computer Science and Mathematics Division, Oak Ridge, TN 37831-6367, U.S.A.*

SUMMARY

An algorithm based upon the residue calculus for computing three-dimensional anisotropic elastic Green's function and its derivatives has been presented in Sales and Gray (*Comput. Structures* 1998; **69**:247–254). It has been shown that the algorithm runs three to four times faster than the standard Wilson–Cruse interpolation scheme. However, the main concern of the Sales–Gray algorithm is its numerical instability that could lead to significant errors due to the existence of multiple poles of the residue. This paper proposes a remedy for the problem by adding the capability to evaluate the Green's function in case of multiple poles of the residue. Further, an improved numerical implementation based on the use of double-subscript-notation elastic constants in determining the Christoffel tensor is also at issue. Copyright © 2004 John Wiley & Sons, Ltd.

KEY WORDS: Green's function; anisotropic elasticity; residue calculus; boundary element analysis

1. INTRODUCTION

Boundary element analysis requires numerous evaluations of a Green's function (fundamental solutions) and its derivatives. While these functions are relatively simple for isotropic elasticity, they are far more complicated in case of materials of general anisotropy. Thus, an effective scheme for evaluating these complicated functions is very crucial for the success of a boundary element anisotropic analysis.

An approach based upon the residue calculus to computing the three-dimensional (3-D) anisotropic elastic Green's function has been investigated by Wang [1], and Sales and Gray [2]. The results are obtained in terms of the residue of poles whose positions are determined by the roots of a sixth degree polynomial equation. While the work of Wang primarily focused

*Correspondence to: A.-V. Phan, Department of Mechanical Engineering, University of South Alabama, Mobile, AL 36688-0002, U.S.A.
†E-mail: vphan@jaguar1.usouthal.edu

Contract/grant sponsor: University of South Alabama Research Council
Contract/grant sponsor: U.S. Department of Energy; contract/grant number: DE-AC05-00OR22725

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Received 23 May 2003
Accepted 22 October 2003

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. Although the proposed algorithm is technically sound, potential problems in terms of numerical instability could arise when the residue is not a single pole. The objective of this paper is to address the above concern by adding the capability to evaluate the Green's function in case of multiple poles, whereas a full-length paper on the development of the derivatives in this case will be the subject of a subsequent publication. Further, by using double subscript notation in expressing the fourth-rank elastic constant tensor C_{jklm}, an improved numerical implementation versus that proposed in Reference [2] is also discussed herein.

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 uniformly distributed load. Let U_{jk} be the Green's function corresponding to the displacement field in the x_k direction produced by the load in the x_j direction. U_{jk} can be expressed as a line integral [3, 4]

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

where $\mathbf{x}_0$ is the *pole* or *source point*, $\mathbf{x}$ is the *observation* or *field point*, $\boldsymbol{\xi}\in\mathscr{R}^3$, K_{jk} is the Christoffel tensor defined in terms of the elastic constants C_{jklm} of the material

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

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

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

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

The contour integral in Equation (1) can be written as

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

where $\boldsymbol{\xi}$ is written parametrically as

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

The integral in Equation (4) can be evaluated using residue calculus by transforming the integrand into a rational function and expanding the range of the integral to include all real numbers. One way to achieve this transformation is using the following change of variable [5]:

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

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By using this transformation, the components of K_{jk}^{-1} become rational functions of Z. Finally, the integral in Equation (4) can be written in the form [2]

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

where $P_{jk}(Z)$ and $Q(Z)$ are polynomials of Z, 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 plan.

Note that only $\mathrm{Res}(\lambda_n)$ for the case of simple poles (or distinct roots $\lambda_1 \neq \lambda_2 \neq \lambda_3$) was reported in Reference [2]. In general, $\mathrm{Res}(\lambda_n)$ can be determined using the following expression (e.g. Reference [6]):

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

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

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

where

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

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

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

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

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

where n can either be 1 or 2, and

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

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

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

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

$$\bar{U}_{jk}=4\pi \mathrm{i}\,\mathrm{Res}(\lambda_n) \tag{17}$$

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

$$\begin{aligned}\mathrm{Res}(\lambda_n)&=\frac{1}{2}\left[\frac{\mathrm{d}^2}{\mathrm{d}Z^2}\left\{(Z-\lambda_n)^3\,\frac{P_{jk}(Z)}{Q(Z)}\right\}\right]_{Z=\lambda_n}\\&=\frac{1}{Q_{\mathrm{t}}(\lambda_n)}\left\{\frac{P_{jk,ZZ}(\lambda_n)}{2}-\frac{3\,P_{jk,Z}(\lambda_n)}{\lambda_n-\bar{\lambda}_n}+\frac{6P_{jk}(\lambda_n)}{(\lambda_n-\bar{\lambda}_n)^2}\right\}\end{aligned} \tag{18}$$

$$P_{jk,ZZ}(\lambda_n)=\sum_{l=0}^{2}(l+1)(l+2)\,p_{jk(l+2)}\,\lambda_n^l \tag{19}$$

$$Q_{\mathrm{t}}(\lambda_n)=q_6(\lambda_n-\bar{\lambda}_n)^3 \tag{20}$$

2.3. Numerical implementation and computation time

As in Reference [2], the three roots λ_n are found using Newton's approach in conjunction with Horner's method [7] 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 (17) need to 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 identifiable by a double subscript notation. Since both these quantities as well as K_{jk} in Equation (2) are symmetric with respect to an interchange of the subscripts, it will be convenient to abbreviate the double subscript notation ($K_{jk}=C_{jklm}\,\xi_l\,\xi_m$) to a single subscript ($k_u=c_{uv}e_v$) with u/v running from 1 to 6 for $jk/lm=11,22,33,23/32,31/13,12/21$, respectively.

The use of single subscript notation will eliminate the unnecessary storage for symmetric components in the elastic constant tensor C_{jklm} and Green's function U_{jk} since the handling of a fourth-rank tensor C_{jklm} and a (3×3) matrix U_{jk} can be reduced to that of a (3×3) matrix c_{ij} and a (6×1) vector k_j, respectively. Thus, the computation time resulted from this numerical implementation will even be better than that reported in Reference [2].

3. NUMERICAL EXAMPLES

3.1. Simple roots

First, we evaluate $\bar{U}_{jk}$ 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^{11} dynes/cm^2) [8] $c_{11}=12.85$, $c_{12}=4.83$ and $c_{44}=6.68$. Tin

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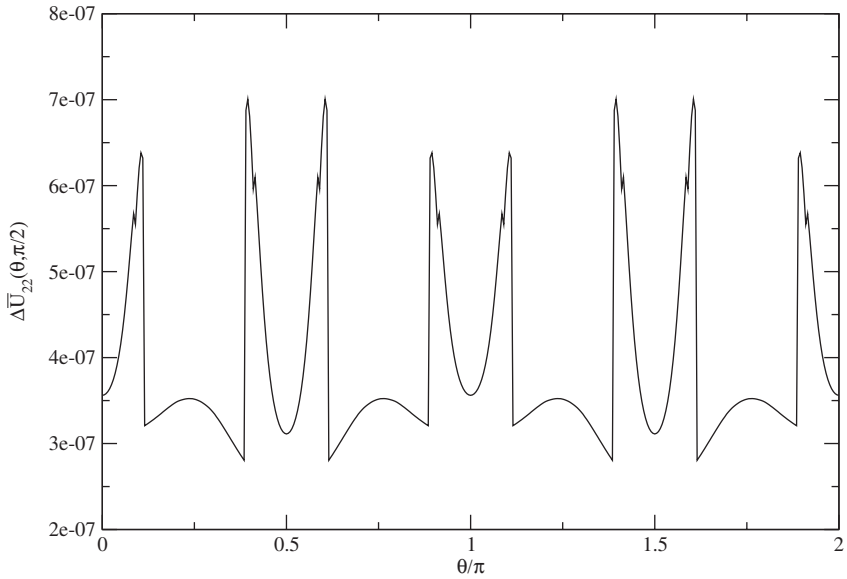

Figure 1. Error of $\bar{U}_{22}(\theta, \pi/2)$ for germanium.

has a piezo-elasto-dielectric matrix type defined by the following six elastic constants (in the same units) [8]: $c_{11} = 7.35$, $c_{33} = 8.7$, $c_{44} = 2.2$, $c_{66} = 2.265$, $c_{12} = 2.34$ and $c_{13} = 2.8$.

Residue calculus results for $\bar{U}_{jk}(\theta, \psi)$ are compared with those obtained from a direct numerical quadrature. The absolute errors of $\bar{U}_{22}(\theta, \pi/2)$ for germanium and $\bar{U}_{13}(\pi, \psi)$ for tin are, respectively, shown in Figures 1 and 2. Excellent agreements can be concluded considering that the elastic constants c_{ij} are typically only known to three significant digits.

3.2. Multiple roots

In this section, the evaluation of $\bar{U}_{jk}$ in case of multiple roots in the polynomial $Q(Z)$ is carried out to validate the numerical implementation of Equations (13) and (17).

Assume that the contour integral term $\bar{U}_{11}$ is given by

$$\bar{U}_{11} = 2 \int_{-\infty}^{\infty} \frac{P_{11}(Z)}{Q(Z)} \, \mathrm{d}Z \tag{21}$$

where

$$P_{11}(Z) = 3Z^4 + 2Z^3 - 5Z^2 - 10Z + 25 \tag{22}$$

and

$$Q(Z) = 3Z^6 + 18Z^5 + 93Z^4 + 180Z^3 + 513Z^2 + 546Z + 2535 \tag{23}$$

or

$$Q(Z) = 2Z^6 + 36Z^5 + 276Z^4 + 1152Z^3 + 2760Z^2 + 3600Z + 2000 \tag{24}$$

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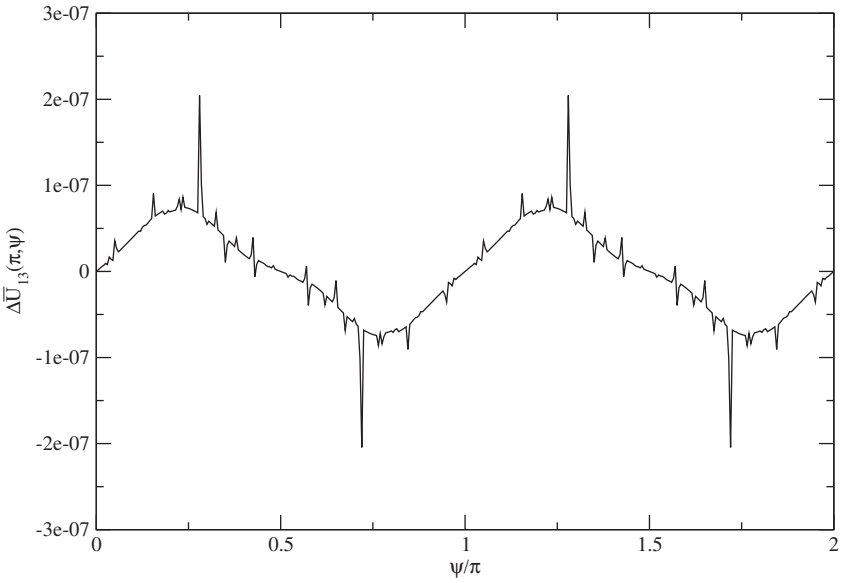

Figure 2. Error of $\bar{U}_{13}(\pi,\psi)$ for tin.

Table I. Evaluation of $\bar{U}_{11}$ in case of a double pole.

Maple solution	Residue calculus	Error (%)
1.063000129	1.0630001286	0.211×10^{-8}

- *Double pole*: This is the case of Equation (23) in which $Q(Z)$ can be written as

$$\begin{aligned} Q(Z) &= 3Z^6 + 18Z^5 + 93Z^4 + 180Z^3 + 513Z^2 + 546Z + 2535 \\ &= 3(Z-\lambda_1)(Z-\lambda_2)^2(Z-\bar{\lambda}_1)(Z-\bar{\lambda}_2)^2 \end{aligned} \tag{25}$$

where $\lambda_1 = 1 + 2\mathrm{i}$, and $\lambda_2 = \lambda_3 = -2 + 3\mathrm{i}$.

- *Triple pole*: This is the case where $Q(Z)$ is given by Equation (24) since we have

$$\begin{aligned} Q(Z) &= 2Z^6 + 36Z^5 + 276Z^4 + 1152Z^3 + 2760Z^2 + 3600Z + 2000 \\ &= 2(Z-\lambda_1)^3(Z-\bar{\lambda}_1)^3 \end{aligned} \tag{26}$$

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

The residue calculus results are compared with those obtained using the symbolic package `Maple`. These results are shown in Tables I and II where they can actually be considered as identical.

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Table II. Evaluation of $\bar{U}_{11}$ in case of a triple pole.

Maple solution	Residue calculus	Error (%)
292.5608159	292.5608158655	-0.194×10^{-5}

4. CONCLUSION

An improved numerical scheme based upon the residue calculus for evaluating the 3-D anisotropic elastic Green's function is presented. The scheme is not only able to determine the Green's function in case of multiple poles of the residue which was not addressed in Reference [2], but also enhances the computational effectiveness of the algorithm initially proposed by that work through the use of double subscript notation in expressing the fourth-order elastic constant tensor. Evaluation of the derivatives of the Green's function will be the subject of a subsequent full-length publication which is currently pursued by the authors.

ACKNOWLEDGEMENTS

This research was supported in part by the University of South Alabama Research Council and the Applied Mathematical Sciences Research Program of the Office of Mathematical, Information, and Computational Sciences, U.S. Department of Energy under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

REFERENCES

1. Wang C-Y. Elastic fields produced by a point source in solids of general anisotropy. *Journal of Engineering Mathematics* 1997; **32**:41–52.
2. Sales MA, Gray LJ. Evaluation of the anisotropic Green's function and its derivatives. *Computers and Structures* 1998; **69**:247–254.
3. Lifschitz IM, Rozentsweig LN. *Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki* 1947; **17**:783.
4. Barnett DM. The precise evaluation of derivatives of the anisotropic elastic Green's functions. *Physica Status Solidi B* 1972; **49**:741–748.
5. Dederichs PH, Liebfried G. Elastic Green's function for anisotropic cubic crystals. *Physical Review* 1969; **188**:1175–1183.
6. Hildebrand FB. *Advanced Calculus for Applications.* Prentice-Hall: New Jersey, 1976.
7. Burden RL, Faires JD. *Numerical Analysis.* PWS-Kent Publishing: Boston, 1989.
8. Seitz F, Turnbull D (eds). *Solid State Physics*, Vol. 7. Academic Press: New York, 1958.

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