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ELASTIC FIELDS DUE TO EIGENSTRAINS PART I: INCLUSION IN INFINITE SPACE

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Abstract: A fast algorithm to predict elastic fields due to arbitrarily shaped eigenstrains in an elastic, isotropic infinite space is advanced in this paper. The inclusion domain is partitioned in a set of cuboids of uniform eigenstrains, and solutions for each individual cuboid, derived by Chiu in closed form expressions, are superimposed. Computation is accelerated by implementing three-dimensional spectral methods, in a hybrid convolution-correlation algorithm. The newly proposed algorithm can be used as a partial solution when assessing elastic fields due to eigenstrains in an isotropic half-space.

1. INTRODUCTION

Eigenstrains such as plastic strains, misfits strains, thermal expansion or phase transformation, generate a linear elastic stress field in an isotropic half-space. Usually, assessment of this field, also referred to as the inclusion problem, is performed using a problem decomposition method originally suggested by Chiu [3]. His formulation requires the solution to the inclusion problem in infinite isotropic space. Although this problem has received a great deal of attention in the last four decades, [9-12], closed form solutions exist only in a few cases of simple, regular shapes, such as spherical or cuboidal eigenstrains. In most real-life designing situations, these limiting assumptions are not met, thus imposing the use of numerical approach.

It has become standard practice to divide the inclusion domain into a collection of non-intersecting cuboids of uniform eigenstrains, by means of a rectangular three-dimensional mesh, and to approximate the effect of the arbitrarily shaped inclusion by superimposing the individual contributions of each cuboidal inclusion. Assuming a continuous distribution as piece-wise constant may induce an important discretization error if the step of the imposed grid is not small enough. However, this approach remains the most efficient to date, as integration over arbitrarily shaped domains is substituted by summation over all grid elements, which can be performed numerically in an efficient manner.

2. PROBLEM DISCRETIZATION

The choice for the grid must consider two requirements. Firstly, union of all elementary domains should cover the inclusion domain, and secondly, the contribution of each individual grid element, also referred to as the influence coefficient (IC), should be known from existing analytical solutions. These requirements are both met if a rectangular grid is imposed. A supplementary condition is needed if spectral methods, which speed up the computation dramatically, are used. If the grid is uniformly spaced, the number of different influence coefficients to be computed is reduced to the number of different distances between cell control points. This allows reformulation of multi-summation operation as a discrete convolution, which can be evaluated efficiently in the frequency domain, according to convolution and/or correlation theorems.

A uniformly-spaced rectangular grid is thus established in a cuboidal domain including the arbitrarily shaped eigenstrains. According to superposition principle, problem solution is obtained by superimposing the solution of each cuboidal inclusion. Eigenstrains are assumed constant in the elementary cell, but otherwise can vary along computational

domain. Therefore, the solution for a cuboidal inclusion of constant eigenstrains in an infinite space, namely the IC, is needed.
The first closed form solution for the IC was advanced by Chiu, [2]. A Cartesian coordinate system (x_1', x_2', x_3') is attached to the center of the cuboid. In the presence of plastic strains ε_{ij}^p, displacements u_i are related to strains by the strain-displacement equations:

$$\varepsilon_{ij}^e + \varepsilon_{ij}^p = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right), \tag{1}$$

where $\boldsymbol{\varepsilon}^e$ is the elastic component of strains, and a single comma in the subscript denotes the derivative with respect to the corresponding direction: $u_{i,j} = \partial u_i / \partial x_j'$. By substituting ε_{ij}^e into the constitutive equation (Hooke's law), one can find the stresses induced by the eigenstrains ε_{ij}^p. The gradients of displacements needed in eq. (1) were obtained by Chiu, [2], using the Galerkin vector:

$$2\mu u_{i,q}(x_1', x_2', x_3') = \frac{1}{8\pi^3}\sum_{m=1}^{8}(-1)^m \left[\begin{array}{l} \dfrac{1-2\nu}{1-\nu}\lambda\varepsilon_{kk}^p D_{,iqnn}(\mathbf{c}_m) + 4\mu\varepsilon_{ij}^p D_{,jqnn}(\mathbf{c}_m) - \\ -\dfrac{2\mu}{1-\nu}\varepsilon_{nj}^p D_{,iqnj}(\mathbf{c}_m) \end{array}\right], \tag{2}$$

where μ and λ are Lame's constants, $\mathbf{c}_m$, $m = \overline{1,8}$ are the eight vectors linking the corners of the cuboid to the observation point, and $D(\mathbf{c}_m)$ is a function whose fourth derivates with respect to coordinates x_j' are obtained by circular permutation in one of four categories, $D_{,1111}$, $D_{,1112}$, $D_{,1122}$ and $D_{,1123}$, given in [2]. Einstein summation convention is employed throughout this paper.
The elastic fields σ_{ij} induced in the observation point (x_1', x_2', x_3') by a cuboidal inclusion of uniform eigenstrains $\varepsilon_{k\ell}^p$, centered in origin, can then be expressed in terms of influence coefficients $A_{ijk\ell}$, computed with the aid of Eqs. (1) and (2):

$$\sigma_{ij}(x_1', x_2', x_3') = A_{ijk\ell}(x_1', x_2', x_3')\varepsilon_{k\ell}^p(0,0,0). \tag{3}$$

Chiu's decomposition method [3] for the inclusion problem in isotropic half-space requires superposition of elastic fields induced by the mirror image of the original inclusion with respect to half-space boundary:

$$\boldsymbol{\varepsilon}^{pm} = \begin{bmatrix} \varepsilon_{11}^p & \varepsilon_{12}^p & -\varepsilon_{13}^p \\ \varepsilon_{12}^p & \varepsilon_{22}^p & -\varepsilon_{23}^p \\ -\varepsilon_{13}^p & -\varepsilon_{23}^p & \varepsilon_{33}^p \end{bmatrix}, \tag{4}$$

Summation of elastic fields induced by $\boldsymbol{\varepsilon}^p$ and $\boldsymbol{\varepsilon}^{pm}$ in a coordinate system with the origin on the half-space boundary yields the following equation:

$$\sigma_{ij}(x_1,x_2,x_3)=A_{ijk\ell}(x_1-x_1',x_2-x_2',x_3-x_3')\varepsilon^{p}_{k\ell}(x_1',x_2',x_3')+ \\ +A_{ijk\ell}(x_1-x_1',x_2-x_2',x_3+x_3')\varepsilon^{pm}_{k\ell}(x_1',x_2',-x_3'). \tag{5}$$

where (x_1,x_2,x_3) is the observation point and (x_1',x_2',x_3') the source point (the control point of the elementary cuboid with uniform eigenstrains).
It has become standard practice to break up an arbitrarily shaped inclusion into multiple cuboids of uniform eigenstrains and to apply the superposition principle in order to evaluate the resulting stress state. As all distributions are assumed piece-wise constant, it is convenient to index the collection of cuboids by a sequence of three integers ranging from 1 to N_1,N_2 and N_3 respectively, with $N=N_1N_2N_3$, and to express all distributions as functions of these integers instead of coordinates. After superimposing the individual contributions of all cuboids, Eq. (5) becomes:

$$\sigma^{r(space)}_{\xi\zeta}(i,j,k)=\sum_{\ell=1}^{N_1}\sum_{m=1}^{N_2}\sum_{n=1}^{N_3}A_{\xi\zeta\varsigma\gamma}(i-\ell,j-m,k-n)\varepsilon^{p}_{\varsigma\gamma}(\ell,m,n)+ \\ +\sum_{\ell=1}^{N_1}\sum_{m=1}^{N_2}\sum_{n=1}^{N_3}A_{\xi\zeta\varsigma\gamma}(i-\ell,j-m,k+n)\varepsilon^{p}_{\varsigma\gamma}(\ell,m,n), \tag{6}$$

which expresses the stress field induced in infinite space at cell (i,j,k) by all cuboids of uniform eigenstrains (ℓ,m,n) and their mirror images.

3. ACCELERATION OF COMPUTATION

Convolution product is used to derive the answer of a linear elastic system subjected to an input, when the unit impulse response, also referred to as the Green function, is known. For contact problems, the response of an elastic isotropic half-space to a unit concentrated force applied on the boundary is known from the Boussinesq [1] and/or Cerruti fundamental solutions. The product of this solution (or Green function) with a shape function, as defined in [6], yields the influence coefficient, which expresses the effect of an element of the grid into another. Superposition principle is then applied, implying summation of individual contributions over all grid elements. This multi-summation process, which is in fact a convolution product, is very time-consuming, being of order $O(N^2)$ for a grid with N elements. The solution currently applied is to compute the convolution in the frequency domain, according to convolution theorem, thus reducing the computational effort to $O(N\log N)$. An important issue when using discrete cyclic convolution to assess continuous linear convolution is the periodization of the problem, which induce the so called periodicity error [6]. If the Green function is known in the time-space domain, the Discrete Convolution Fast Fourier Transform (DCFFT) technique proposed by Liu, Wang and Liu, [6], eliminates completely the periodicity error, as discrete cyclic convolution approaches the linear continuous convolution the way quadrature estimates continuous integral.
The two terms in Eq. (6) imply multi-summation over three dimensions, as both source and observation domains are three-dimensional. Computation of these distributions by direct multiplication method (DMM) is very time-consuming, therefore a non-conventional approach is required. When analyzing the products to be computed, one can see that the first term in Eq. (6) is a three-dimensional convolution, while the second term is a

convolution with respect to directions of $\vec{x}_1$ and $\vec{x}_2$ and a correlation with respect to direction of $\vec{x}_3$. Liu and Wang [7] suggested that correlation theorem, together with convolution theorem, could be used together in a hybrid convolution-correlation multidimensional algorithm.

Beginning with Ju and Farris, [5], spectral methods are intensively used in contact mechanics to rapidly evaluate convolution-type products. Jacq et al. [4] applied a two-dimensional fast Fourier transform algorithm to speed up the computation of convolution products arising in Eq. (6). His approach reduces the computational requirements from $O(N_1^2 N_2^2 N_3^2)$ to $O(N_3^2 N_1 N_2 \log N_1 N_2)$. However, using a two-dimensional algorithm to solve a problem which is essentially three-dimensional is not likely to produce optimum results. Therefore, in this paper, a three dimensional spectral algorithm is proposed, capable of evaluating both convolution and hybrid convolution-correlation type products in $O(N_1 N_2 N_3 \log N_1 N_2 N_3)$ operations.

The newly advanced algorithm is based on the notorious DCFFT technique by Liu, Wang and Liu [6]. If the ICs are known in the time/space domain, this algorithm can evaluate the linear convolution by means of a cyclic convolution with no periodicity error. The concepts of "zero-padding" and "wrap-around order", presented in [6], can be extended naturally to the three-dimensional case, and applied to compute the first term in the right side of Eq. (6). However, for the second term, due to positioning of the mirror-image element relative to global coordinate system (linked to half-space boundary), convolution turns to correlation with respect to direction of $\vec{x}_3$. In order to use three-dimensional FFT and convolution theorem to evaluate the convolution-correlation product, the following algorithm is proposed:

1. The influence coefficients $\mathbf{A}$ are computed as a three dimensional array of $N_1 \times N_2 \times 2N_3$ elements, using the formulas derived from Eqs. (1) and (2).
2. $\mathbf{A}$ is extended into a $2N_1 \times 2N_2 \times 2N_3$ array by applying zero-padding and wrap around order with respect to directions of $\vec{x}_1$ and $\vec{x}_2$, as requested by the classic DCFFT algorithm.
3. Eigenstrains $\boldsymbol{\varepsilon}^p$ are inputted as a three-dimensional array of $N_1 \times N_2 \times N_3$ elements.
4. $\boldsymbol{\varepsilon}^p$ is extended to a $2N_1 \times 2N_2 \times 2N_3$ array by zero-padding.
5. Elements of $\boldsymbol{\varepsilon}^p$ are rearranged in reversed order with respect to direction of $\vec{x}_3$.
6. The Fourier transforms of $\mathbf{A}$ and $\boldsymbol{\varepsilon}^p$ are computed by means of a three dimensional FFT algorithm, thus obtaining the complex arrays $\hat{\mathbf{A}}$ and $\hat{\boldsymbol{\varepsilon}}^p$, where $(\hat{g})$ is used to denote the discrete Fourier transform of any time/space array g.
7. The spectral array of residual stresses is computed as element-by-element product between convolution terms: $\hat{\sigma}^{r(space)} = \hat{A} \cdot \hat{\varepsilon}^p$.
8. The time/space array of residual stresses is finally obtained by means of an inverse discrete Fourier transform: $\sigma^{r(space)} = IFFT(\hat{\sigma}^{r(space)})$.
9. The terms in the extended domain are discarded, thus keeping the terms $N_1 \times N_2 \times N_3$ of $\sigma^{r(space)}$ as output.

Domain extension with respect to directions of $\vec{x}_1$ and $\vec{x}_2$ in step 2 is required by the DCFFT technique, and no additional treatment is needed to evaluate the corresponding discrete cyclic convolutions. On the other hand, according to discrete correlation theorem, [13], a correlation product can be evaluated as a convolution between one member of the

correlation and the complex conjugate of the other. Therefore, DCFFT can be applied with respect to direction of $\bar{x}_3$ too, if the second term, namely the eigeinstrains array, is substituted by its complex conjugates in the frequency domain. The fastest way to achieve this is to rearrange the terms of $\boldsymbol{\varepsilon}^p$, as indicated in step 4. Indeed, when FFT is applied on a series of real terms g, thus obtaining $\hat{g}$, one can obtain its complex conjugate, $\hat{g}^*$, simply by reading g in reversed order. This remarkable property allows for combining convolutions and correlations products with respect to different directions in a hybrid algorithm. By applying three-dimensional FFT, the computational effort for computing the inclusion problem in infinite, elastic and isotropic space is reduced considerably from $O(N_3^2 N_1 N_2 \log N_1 N_2)$, in Jacq's approach, [4], to $O(N_1 N_2 N_3 \log N_1 N_2 N_3)$ operations for the newly proposed algorithm.

4. PROGRAM VALIDATION

In order to verify the formulas for the ICs, a cuboid of sides Δ_1, Δ_2 and Δ_3 is considered in an infinite elastic isotropic space with Poisson's ratio ν and Young's modulus E. A Cartesian coordinate system is attached to the center of the cuboid. The orientation of the axes is depicted on each of the following figures. The cuboidal domain is assumed to have vanishing eigenstrains, except for ε_{11}^p, uniformly distributed. Dimensionless coordinates $\bar{x}_i$ are defined as ratios to corresponding cuboid sides, $\bar{x}_i = x_i / \Delta_i$. Normal stresses $\bar{\sigma}_{ii11}$ induced by strains ε_{11}^p are normalized by $E\varepsilon_{11}^p$. Results for different Δ_1/Δ_3 ratios are depicted in Figs. 1 - 4, revealing a good match with existing solutions.

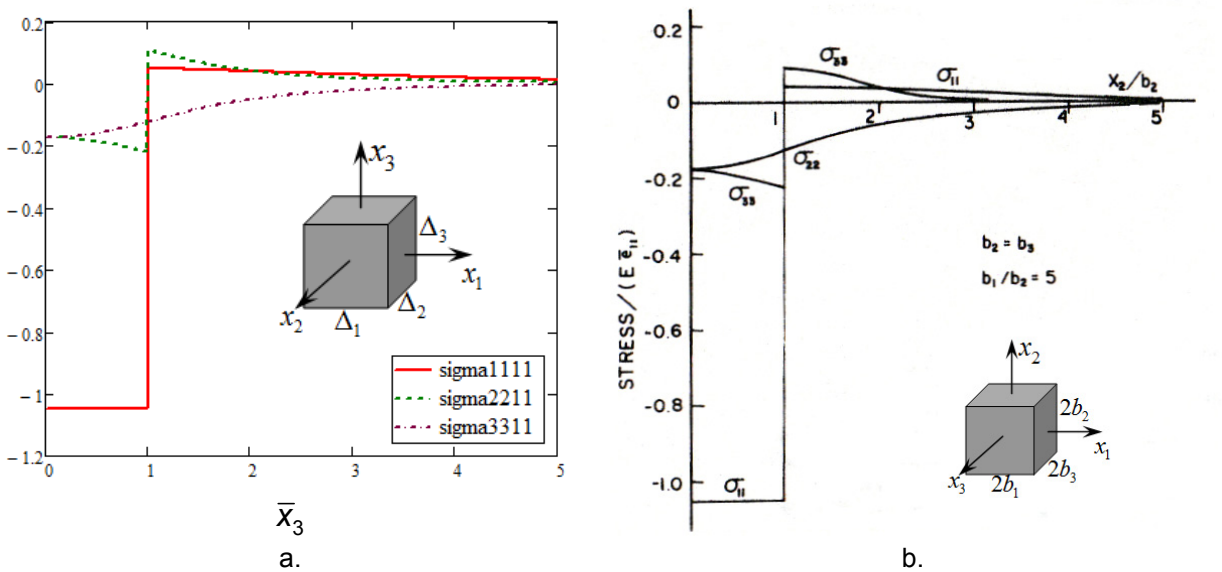
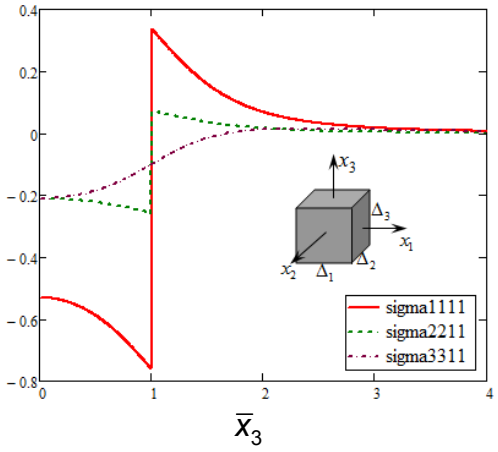
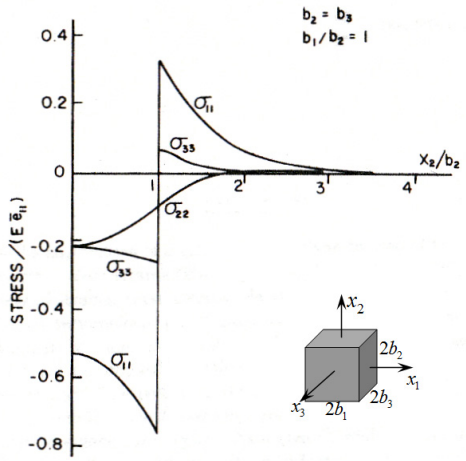


Figure 1. Normal stresses due to a cuboidal inclusion of uniformly distributed plastic strains ε_{11}^p, $\Delta_1/\Delta_3 = 5$ ***: a. this code, b. Chiu's results [2]***

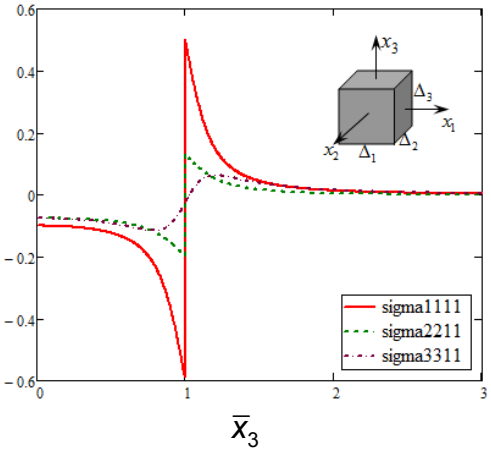


a.

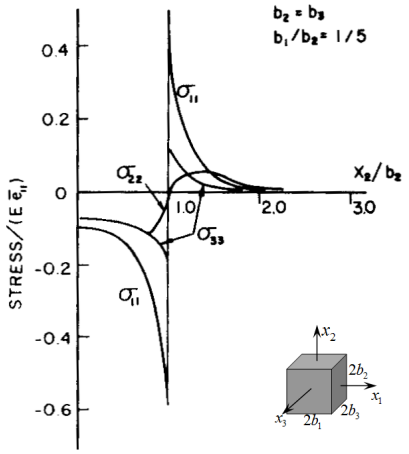


b.

Figure 2. Normal stresses due to a cuboidal inclusion of uniformly distributed plastic strains ε_{11}^{p}, $\Delta_1/\Delta_3 = 1$***: a. this code, b. Chiu's results [2]***

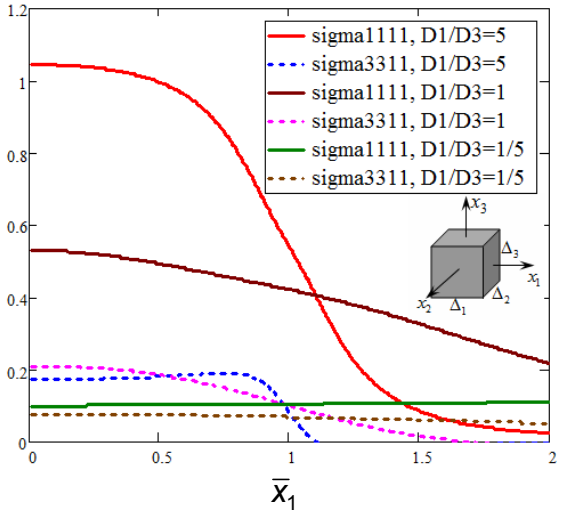


a.

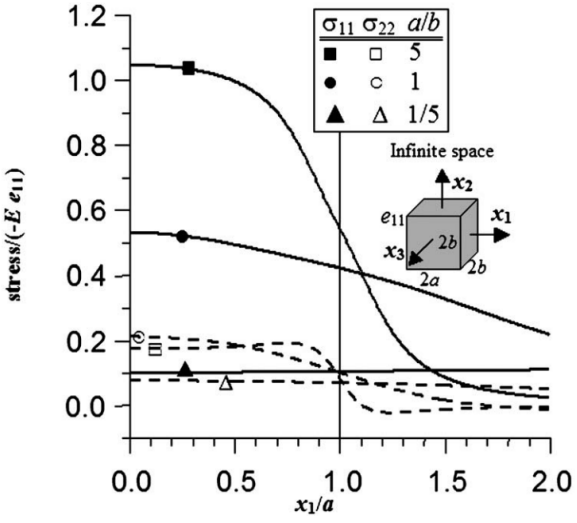


b.

Figure 3. Normal stresses due to a cuboidal inclusion of uniformly distributed plastic strains ε_{11}^{p}, $\Delta_3/\Delta_1 = 5$***: a. this code, b. Chiu's results [2]***



a.



b.

Figure 4. Normal stresses due to a cuboidal inclusion of uniformly distributed plastic strains ε_{11}^{p}, ***various*** Δ_1/Δ_3 ***: a. this code, b. Liu and Wang's results [7]***

5. CONCLUSIONS

A new algorithm to compute numerically elastic fields due to arbitrarily shaped eigenstrains in an infinite, elastic and isotropic space is proposed in this paper. The numerical formulation is based on breaking up the inclusion domain in a set of cuboids of uniform eigenstrains, and on superimposing the solutions for each individual cuboidal inclusion, also known as the influence coefficients.

Three-dimensional spectral methods are implemented for acceleration of computation. A new convolution-correlation hybrid algorithm is advanced, based on the DCFFT technique by Liu, Wand and Liu, [6]. This algorithm reduces the computational effort from the existing $O(N_3^2 N_1 N_2 \log N_1 N_2)$ to $O(N_1 N_2 N_3 \log N_1 N_2 N_3)$ operations.

The newly proposed algorithm can be used as a partial solution to the problem of elastic fields due to eigenstrains in an isotropic half-space, if Chiu's decomposition method, [3], is used.

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