

COMPUTATIONAL MICROMECHANICS FOR COMPOSITES WITH FINITE BOUNDARIES

S. Nomura^{1*} and T. Pathapalli¹

¹Mechanical and Aerospace Engineering Department, The University of Texas at Arlington, Arlington, TX 76019-0023 USA

* Corresponding author (nomura@uta.edu)

Keywords: *Micromechanics, elliptic inclusions, computer algebra system*

Abstract

A semi-analytical approach is presented to solve general boundary value problems (BVPs) that arise in the analysis of composite materials. As an illustration, a rectangular shaped medium that contains elliptical inclusions will be considered. Permissible functions, which satisfy the homogeneous boundary conditions and the continuity conditions at the matrix-inclusion interface, are analytically derived. The eigenfunctions are subsequently derived from the permissible functions using the Galerkin method. The mechanical and physical fields (temperature or elastic deformation), with an arbitrarily given source term, can be expressed as a linear combination of the eigenfunctions. The method is favorably compared with numerical results obtained from the finite element method.

1 Introduction

The conventional micromechanics [1], pioneered by Eshelby [2], has been widely used to analyze the microstructure of elastic solids that contain inclusions. However, the major limitation of micromechanics is that the medium is assumed to be infinitely extended (no boundary) and the geometry of the microstructure is strictly limited, thus making it inconvenient to accurately represent actual composite materials. Although purely numerical methods such as the finite element method can be employed for the analysis of composites, analytical or semi-analytical solutions, if available, are needlessly valuable. This paper presents a new semi-analytical method for heterogeneous materials that makes use of both analytical and numerical techniques to obtain mechanical and physical fields associated with the given BVP. The method

primarily involves determining a set of continuous permissible functions that satisfy the boundary conditions and continuity conditions at the matrix-inclusion interface, expressing the BVP (governing equation) in terms of the Sturm-Liouville (S-L) system [3], subjecting the S-L problem (eigenvalue problem) to the Galerkin method to obtain an orthonormal set of eigenfunctions, and finally, representing the mechanical/physical field as a linear combination of the evaluated eigenfunctions. In order to facilitate the analytical derivation of the permissible functions in terms of the relevant material and geometrical parameters, a computer algebra system [4, 5] has been extensively used. As a demonstration example, a steady-state heat conduction problem for a rectangular shaped medium with elliptical inclusions is presented. The results are favorably compared with those obtained from the finite element method.

2 Formulations

The governing differential equations for both elasticity and steady-state heat conduction can be expressed as

$$L[u(x)] + b(x) = 0, \quad (1)$$

where L is a self-adjoint differential operator, $u(x)$ is the unknown physical field (temperature or displacement) and $b(x)$ is the source term (heat source or body force). For steady state heat conduction, L takes the following form:

$$L[u(x)] = \nabla \cdot (k(x) \nabla u(x)), \quad (2)$$

where $k(x)$ is the thermal conductivity and for the static elasticity case, L takes the form:

$$(L[u(x)])_i = (C_{ijkl} u_{k,l})_{,j}, \quad (3)$$

where C_{ijkl} is the elastic modulus. For isotropic materials, it can be expressed in terms of the shear modulus, G , and the bulk modulus, K , as:

$$C_{ijkl} = \left(K - \frac{2G}{3}\right) \delta_{ij} \delta_{kl} + G(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \quad (4)$$

where δ_{ij} is the Kronecker delta.

Based on the Sturm-Liouville theory, the solution to equation (1) can be obtained if the eigenfunction, $\phi_n(x)$, is available. The eigenfunction is defined as

$$L[\phi_n(x)] + \lambda_n \phi_n(x) = 0, \quad (5)$$

where λ_n and $\phi_n(x)$ are the n^{th} eigenvalue and eigenfunction, respectively. An intrinsic property of the Sturm-Liouville system is that its differential operator, L , is Hermitian, hence suggesting that all the eigenvalues are real and the eigenfunctions are mutually orthogonal as

$$\int_D \phi_m(x) \phi_n(x) dx = \delta_{mn}. \quad (6)$$

The solution to equation (5) can be obtained by expressing the eigenfunctions, $\phi_n(x)$, as a series of N permissible functions as

$$\phi_n(x) = \sum_{i=1}^N c_{ni} f_i(x), \quad (7)$$

where $f_i(x)$ is a permissible function chosen from elementary functions such as polynomials to satisfy the homogeneous boundary conditions and the continuity conditions across the matrix-inclusion interface. The quantity, c_{ni} , is the coefficient of $f_i(x)$ of the n^{th} eigenfunction and is determined using the Galerkin method. By substituting equation (7) into equation (5), multiplying $f_j(x)$ on both sides and integrating them over the entire domain, equation (5) can be converted to the following generalized eigenvalue problem:

$$A c + \lambda B c = 0, \quad (8)$$

where

$$A_{ij} = \int_D L[f_i(x)] f_j(x) dx, \quad (9)$$

$$B_{ij} = \int_D f_i(x) f_j(x) dx. \quad (10)$$

The components of A_{ij} and B_{ij} are obtained using equations (9) and (10). Therefore, equation (8) can be solved using a standard numerical techniques to obtain the eigenvalues, λ_n , and the corresponding set of unknown coefficients, c_{ni} .

In accordance with the Sturm-Liouville theory, the solution to equation (1) can be expressed as a linear combination of eigenfunctions as

$$u(x) = \sum_{n=1}^{\infty} \frac{b_n}{\lambda_n} \phi_n(x), \quad (11)$$

where b_n is the eigenfunction expansion coefficient of the source term, $b(x)$, and can be obtained as

$$b_n = \int_D b(x) \phi_n(x) dx. \quad (12)$$

The most demanding task is to obtain the permissible function, $f_i(x)$, that satisfies the boundary conditions and the required continuity conditions at the interface. For instance, a 2-D body that contains an elliptical inclusion, the permissible function needs to be defined separately for each phase. For the inclusion phase, $f_i(x, y)$ is assumed to be in the polynomial form as

$$f_i^{inc}(x, y) = \sum_{j=0}^M \sum_{k=0}^j a_{jk}^{inc} x^{j-k} y^k, \quad (13)$$

where M represents the order of the polynomial and the summation ensures that the permissible function, $f_i^{inc}(x, y)$, encompasses all the polynomials up to the M^{th} order. Similarly, for the matrix phase, $f_i^{mat}(x, y)$ is assumed to be of the form:

$$f_i^{mat}(x, y) = g(x, y) \sum_{j=0}^M \sum_{k=0}^j a_{jk}^{inc} x^{j-k} y^k, \quad (14)$$

where $g(x, y)$ is a function that vanishes at the boundary (for the boundary condition of the first kind). For example, if the boundary is rectangular

shaped with x_1, x_2, y_1, y_2 defining the corners of the rectangle, then, $g(x, y)$ takes the form:

$$g(x, y) = (x - x_1)(x - x_2)(y - y_1)(y - y_2), \quad (15)$$

The homogeneous boundary condition is categorically satisfied by equation (14).

Equations (13) and (14) also need to satisfy the continuity conditions at the matrix-inclusion interface. This is achieved by satisfying the following conditions:

$$f_i^{inc}|_{interface} = f_i^{mat}|_{interface}, \quad (16)$$

$$C_{inc} \frac{\partial f_i^{inc}}{\partial n}|_{interface} = C_{mat} \frac{\partial f_i^{mat}}{\partial n}|_{interface}, \quad (17)$$

where C_{inc} and C_{mat} are material constants associated with the inclusion and matrix, respectively. For steady state heat conduction, the material constant would be thermal conductivity, $k(x)$, and for the elastic equilibrium equation, it would be the shear modulus, G , and the bulk modulus, K . The term, $\frac{\partial}{\partial n}$, represents the directional derivative on the matrix-inclusion interface. The surface normal, \mathbf{n} , for an elliptical boundary is defined as

$$\mathbf{n} = \left(\frac{\frac{x/a^2}{\sqrt{x^2/a^4 + y^2/b^4}}}{\frac{y/b^2}{\sqrt{x^2/a^4 + y^2/b^4}}} \right), \quad (18)$$

where a and b are the semi-major and semi-minor axis of the ellipse respectively.

In the case of steady state heat conduction, equations (16) and (17) represent the continuity of temperature and heat flux respectively. The same equations, in the case of elastic equilibrium, represent the continuity of displacement and traction force across the matrix-inclusion interface.

3 Examples

The Poisson type equation is considered that governs the steady state heat conduction in a square shaped matrix medium consisting of two elliptical inclusions with the inclusions and matrix having

different thermal conductivities, k_1 and k_2 , as shown in Fig. 1. The governing equation is expressed as

$$\nabla \cdot (k(x, y) \nabla T(x, y)) = c, \quad (19)$$

where $T(x, y)$ is the unknown temperature field and c represents the heat source. The boundaries of the square shaped region are subjected to the boundary condition of the first kind ($T(x, y) = 0$). The associated continuity conditions are

$$T_1(x, y)|_{interface} = T_2(x, y)|_{interface}, \quad (20)$$

$$k_1 \frac{\partial T_1(x, y)}{\partial n}|_{interface} = k_2 \frac{\partial T_2(x, y)}{\partial n}|_{interface}, \quad (21)$$

where the indices, 1 and 2, represent the inclusion phase and matrix phase, respectively.

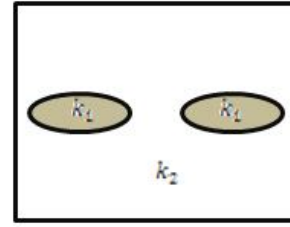


Figure 1. Elliptical Inclusions.

A set of continuous permissible functions are analytically derived that satisfy the homogeneous boundary condition and the continuity conditions indicated above. Despite the simplicity of the BVP, the procedure involved in obtaining the permissible functions is a cumbersome one. This is facilitated with the aid of a computer algebra system, *Mathematica* [6]. For illustration purposes, one of the computer generated permissible functions is shown below:

$$f(x, y) = -\frac{a^2 b^6 k_2}{3k_1} + \frac{a^2 b^4 d^2 k_2}{k_1} + \frac{b^6 d^2 k_2}{k_1} - \frac{2b^4 d^4 k_2}{k_1} - \frac{2b^6 d^2 x^2 k_2}{a^2 k_1} + \frac{2b^4 d^4 x^2 k_2}{a^2 k_1} + \frac{b^6 x^4 k_2}{a^2 k_1} - \frac{b^4 d^2 x^4 k_2}{a^2 k_1} + \frac{b^6 d^2 x^4 k_2}{a^4 k_1} - \frac{2b^6 x^6 k_2}{3a^4 k_1} - \frac{2a^2 b^2 d^2 y^2 k_2}{k_1} + \frac{2b^2 d^4 y^2 k_2}{k_1} + \frac{a^2 b^2 y^4 k_2}{k_1} + \frac{a^2 d^2 y^4 k_2}{k_1} - \frac{b^2 d^2 y^4 k_2}{k_1} - \frac{2a^2 y^6 k_2}{3k_1}, \quad (22)$$

where d is half the length of the square shaped matrix, a and b represent the semi-major and semi-minor axes of the elliptical inclusion, k_1 and k_2 are the thermal conductivities of the inclusion and matrix, respectively. From the above equation, it can be observed that $f(x,y)$ is a function of both the geometrical and material parameters.

From the permissible functions, the matrix elements of equations (9) and (10) are computed, following which an orthonormal set of eigenfunctions are obtained using equation (7). Figures 2, 3, and 4 show three arbitrary eigenfunctions for aspect ratios of 1 (circular inclusion), 2, and 5, respectively. A noticeable feature in all of the representations below is the shape of the inclusions being clearly reflected in each of the eigenfunctions. A closer examination also reveals that the eigenfunctions in each of the aspect ratios are mutually orthogonal (independent) to each other as indicated by equation (6).

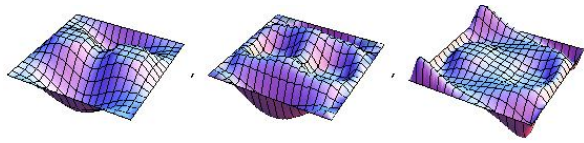


Figure 2. Eigenfunctions for an aspect ratio = 1.

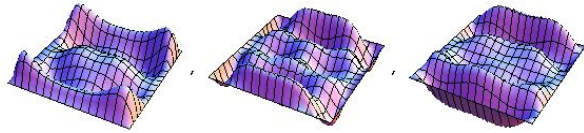


Figure 3. Eigenfunctions for an aspect ratio = 2.

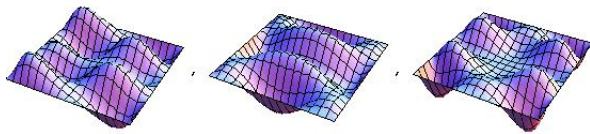


Figure 4. Eigenfunctions for an aspect ratio = 5.

The unknown physical field (temperature), can now be obtained in terms of the eigenfunctions by expressing them as a linear combination as described in equation (11).

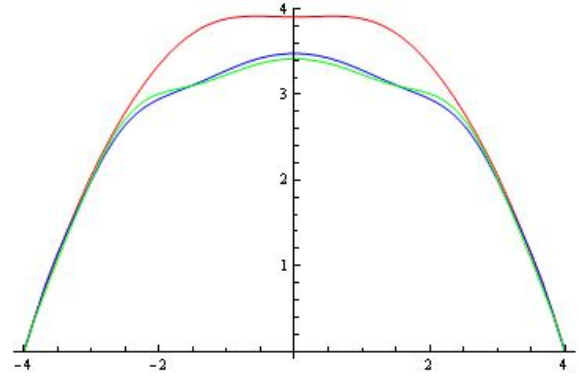


Figure 5. Cross-sectional profile of $T(x,y)$.

Figure 5 depicts the cross sectional views of temperature ($T(x,y)$) at $x = 0$ for each of the aspect ratios, 1, 2, and 5. The profile in red represents the temperature distribution for an aspect ratio = 1 (two circular inclusions). The profiles in blue and green represent the temperature distribution for two elliptical inclusions with aspect ratios of 2 and 5, respectively. For aspect ratios greater than 5, it was seen that there is but negligible difference in the temperature profile. The results depicted in Figure 5 are in good agreement with those obtained from the finite element method for the same geometrical configuration and material properties.

As a precursor to the boundary value problems associated with the elastic equilibrium equation, the permissible functions were analytically derived. Shown below is a computer generated sample output of one such function:

$$\begin{aligned}
 f(x,y) = & -\frac{a^2 b^6 k_2}{3k_1} + \frac{a^2 b^4 d^2 k_2}{k_1} \\
 & + \frac{b^6 d^2 k_2}{k_1} - \frac{2b^4 d^4 k_2}{k_1} \\
 & - \frac{2b^6 d^2 x^2 k_2}{a^2 k_1} \\
 & + \frac{2b^4 d^4 x^2 k_2}{a^2 k_1} + \frac{b^6 x^4 k_2}{a^2 k_1} \\
 & - \frac{b^4 d^2 x^4 k_2}{a^2 k_1} + \frac{b^6 d^2 x^4 k_2}{a^4 k_1} \\
 & - \frac{2b^6 x^6 k_2}{3a^4 k_1} \\
 & - \frac{2a^2 b^2 d^2 y^2 k_2}{k_1} \\
 & + \frac{2b^2 d^4 y^2 k_2}{k_1} \\
 & + \frac{a^2 b^2 y^4 k_2}{k_1} + \frac{a^2 d^2 y^4 k_2}{k_1} \\
 & - \frac{b^2 d^2 y^4 k_2}{k_1} - \frac{2a^2 y^6 k_2}{3k_1},
 \end{aligned} \tag{23}$$

where G and K represent the shear and bulk moduli, respectively, and the indices, 1 and 2, represent the inclusion phase and matrix phase, respectively.

4 Conclusions

An analytical procedure was introduced to systematically derive the permissible functions that satisfy the boundary condition and continuity conditions for a body having elliptical shaped inclusions that arise in heat conduction and elasticity. A computer algebra system was extensively used to carry out tedious algebra. Temperature fields were obtained by the Galerkin method with the derived permissible functions. This approach gives a unified methodology to solve general boundary value problems.

References

- [1] T. Mura, "Micromechanics of defects in solids," Martinus Nijhoff, 1987.
- [2] J. D. Eshelby "The determination of elastic fields of an ellipsoidal inclusion, and related problems," *Proc. Roy. Soc.*, A241. pp 376-11, 1967.

- [3] R. Courant and D. Hilbert, "Methods of Mathematical Physics," vol.1, Wiley, 1989.
- [4] D. Choi and S. Nomura, "Application of symbolic computations to two-dimensional elasticity," *Computers and Structures*, vol.42, pp.645-649, 1992.
- [5] S. Nomura, "A new analytical method for particulate composites," *Composites Science and Technology*, vol.69, pp.2282-2284, 2009.
- [6] S. Wolfram, "Mathematica Book," Wolfram Media, 2003.