

## Development of 3D Trefftz Voronoi Cells with Ellipsoidal Voids &/or Elastic/Rigid Inclusions for Micromechanical Modeling of Heterogeneous Materials

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**Abstract:** In this paper, as an extension to the authors's work in [Dong and Atluri (2011a,b, 2012a,b,c)], three-dimensional Trefftz Voronoi Cells (TVCs) with ellipsoidal voids/inclusions are developed for micromechanical modeling of heterogeneous materials. Several types of TVCs are developed, depending on the types of heterogeneity in each Voronoi Cell (VC). Each TVC can include alternatively an ellipsoidal void, an ellipsoidal elastic inclusion, or an ellipsoidal rigid inclusion. In all of these cases, an inter-VC compatible displacement field is assumed at each surface of the polyhedral VC, with Barycentric coordinates as nodal shape functions. The Trefftz trial displacement fields in each VC are expressed in terms of the Papkovitch-Neuber solution. Ellipsoidal harmonics are used as the Papkovitch-Neuber potentials to derive the Trefftz trial displacement fields. Characteristic lengths are used for each VC to scale the Trefftz trial functions, in order to avoid solving systems of ill-conditioned equations. Two approaches for developing VC stiffness matrices are used. The differences between these two approaches are that, the compatibility between the independently assumed fields in the interior of the VC with those at the outer- as well as the inner-boundary, are enforced alternatively, by Lagrange multipliers in multi-field boundary variational principles, or by collocation at a finite number of preselected points. These VCs are named as TVC-BVP and TVC-C respectively. Several three-dimensional computational micromechanics problems are solved using these TVCs. Computational results demonstrate that both TVC-BVP and TVC-C can efficiently predict the overall properties of composite/porous materials. They can also accurately capture the stress concentration around ellipsoidal voids/inclusions, which can be used in future to study the damage of materials, in combination of tools of modeling micro-crack initiation and propagation. Therefore, we consider that the 3D TVCs developed in this study are very suitable for ground-breaking micromechanical study of heterogeneous materials.

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## 1 Introduction

In recent decades, increasing advancement of science, technology, and the wide application of heterogeneous materials, have been experienced in mechanical, aerospace and military industries. For example, metal/alloys with precipitates/pores, and metal/polymer/ceramic composite materials with fiber/whisker/particulate reinforcements are of particular interest. Development of efficient and accurate tools to model the micromechanical and macromechanical behavior of heterogeneous materials is of fundamental importance.

There are several widely-used analytical tools to predict the overall properties of heterogeneous materials. For example, [Hashin and Shtrikman (1963)] developed variational principles to estimate the upper and lower bounds of the elasticity or compliance tensor. [Hill (1965)] developed a self-consistent approach to estimate the homogenized material properties. For a useful reference, one can refer to the book [Nemat-Nasser and Hori (1999)]. Analytical methods have their unique values in the study of micromechanics. However, because most of these methods follow the work of [Eshelby (1957)], namely the elastic field of an ellipsoidal inclusion in an infinite media, it is expected that these methods can only accurately model heterogeneous materials with simple geometries and low volume fractions of inclusions.

The need for predicting the overall properties of a material with complex geometry, distribution, and arbitrary volume fraction of inclusions, promoted the development of computational tools for micromechanics. A popular way of doing this is to use finite elements to model a Representative Volume Element (RVE). By concept, a RVE is a microscopic material volume, which is statistically representative of the infinitesimal material neighborhood of the macroscopic material point of interest. By modeling simple loading cases of the RVE, the microscopic stress field and strain field in the RVE can be computed by the finite element method. And the homogenized material properties are calculated by relating the macroscopic (average) stress tensor to the macroscopic (average) strain tensor. Some useful references can be found in [Christman, Needleman and Suresh (1989), Bao, Hutchinson, McMeeking(1991)]. Finite element method and asymptotic homogenization theory were also combined to perform multi-scale modeling of structures composed of heterogeneous materials in [Guedes and Kikuchi (1990)].

However, it is well known that, primal finite elements, which involve displacement-

type of nodal shape functions, are highly inefficient for modeling stress concentration problems. Accurate computation of the fields around a single inclusion or void may need thousands of elements. Moreover, meshing of a RVE which contains a large number of inclusions/voids, can be human-labor intensive. For the expensive burden of computation as well as meshing, the above-mentioned computational models mostly use a Unit Cell as the RVE, assuming the microstructure of material is strictly periodic. This obviously cannot account for the complex shape and distribution of materials of different phases.

In order to reduce the burden of computation and meshing, [Ghosh and Mallett (1994); Ghosh, Lee and Moorthy (1995)] proposed the idea of Voronoi Cell Finite elements (VCFEMs). The RVE is meshed using Voronoi Diagram according to the locations of inclusions/voids, and each Voronoi Cell with/without an inclusion/void can be modeled using one single finite element. Ghosh's VCFEMs are all developed based on the hybrid stress model of [Pian (1964)], using the modified principle of complementary energy, and assuming inter-element compatible displacement fields and a priori equilibrated stress fields. The a priori equilibrated stress fields are generated by using Airy's stress functions in 2D or Maxwell's stress functions in 3D. However, the hybrid stress approach involves Lagrange multipliers, and involves both domain and boundary integration for each and every element. This makes the VCFEMs developed by Ghosh and his coworkers computationally inefficient, and also plagued by LBB conditions. The completeness of the stress fields generated by polynomial Airy's stress functions or Maxwell's stress functions is also of obvious questionability. Incomplete stress field assumptions lead to very poor results of computed stress/strain fields. Attempts were made to improve the accuracy by introducing additional stress fields. For example, in the 3D VCFEMs developed by [Ghosh and Moorthy (2004)], the analytical stress field around an ellipsoidal inclusion embedded in an infinite media subjected to remote loads was added to the stress field generated by the polynomial Maxwell's stress functions. However, the stress field is still not necessarily complete, even though some improvement was made by introducing this additional stress field. For detailed discussion of completeness, see [Muskhelishvili (1954)] for 2D problems, and [Lurie (2005)] for 3D problems.

In order to overcome the several aforementioned disadvantages, a different method was developed recently by the authors—Trefftz Voronoi Cells (TVCs)<sup>1</sup>, which are efficient and accurate for micromechanical modeling of heterogeneous materials. 2D cases of TVCs with/without circular inclusions/voids were presented in [Dong and Atluri(2011b); Dong and Atluri(2012a)]. 3D cases of TVCs with/without

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<sup>1</sup> Trefftz Voronoi Cells were original named T-Trefftz Voronoi Finite Elements by the authors in [Dong and Atluri (2011b, 2012a,b)].

spherical inclusions/voids were presented in [Dong and Atluri(2012b)]. The main difference of TVCs developed by the authors and the VCFEMs developed by Ghosh and his coworkers is that: a complete Trefftz trial displacement field which satisfies both equilibrium and compatibility is assumed in TVCs, instead of only the “a priori equilibrated” stress field used in [Ghosh, Lee and Moorthy (1995)]. For example, the well-known 2D general solution of [Muskhelishvili (1954)] by the techniques of complex variables and conformal mapping is used as the Trefftz trial displacement field for 2D TVCs with circular/elliptical inclusions/voids. And the Papkovitch-Neuber general solution with spherical harmonics is used as the Trefftz trial displacement field for 3D TVCs with spherical inclusions/voids. Because both the Trefftz trial displacement fields satisfy the governing Naviers equations a priori, only boundary integrals are needed in TVCs, instead of both the volume and surface integrals needed in the hybrid-stress VCFEMs developed by Ghosh et al. Therefore, TVCs developed by the authors are computationally more efficient. TVCs can also model the stress concentration around voids/inclusions much more accurately, because of the completeness of the Trefftz trial displacement fields, see [Dong and Atluri (2012c)].

In this study, we extend 3D TVCs to solve 3D problems with ellipsoidal inclusions/voids. 3D TVCs with an ellipsoidal void, with an ellipsoidal elastic inclusion, or with an ellipsoidal rigid inclusion are developed respectively. The inter-VC displacement field is assumed by using Barycentric coordinates as nodal shape functions. The Trefftz trial displacement fields are assumed in the form of Papkovitch-Neuber solutions. Ellipsoidal harmonics are used as Papkovitch-Neuber potentials. Two approaches for developing stiffness matrices are used. The compatibility between the independently assumed fields at the outer- as well as the inner-boundary, are enforced alternatively, by Lagrange multipliers in multi-field boundary variational principles, or by collocation at a finite number of preselected points. These VCs are named as TVC-BVP and TVC-C respectively. Numerical experiments show high-performance of the developed TVCs with ellipsoidal inclusions/voids.

The rest of this paper is organized as follows: in section 2, we use Barycentric coordinates to develop the inter-VC compatible displacement field; in section 3, we introduce the Trefftz trial displacement fields in the form of Papkovitch-Neuber solution; in section 4, we briefly discuss ellipsoidal harmonics as Papkovitch-Neuber potentials; in section 5, we develop 3D TVCs with ellipsoidal voids/inclusions; in section 6, we demonstrate the accuracy and efficiency of the developed TVCs by some numerical examples; in section 7, we complete this paper with some concluding remarks.

## 2 Boundary Displacement Fields with Barycentric Coordinates as Nodal Shape Functions

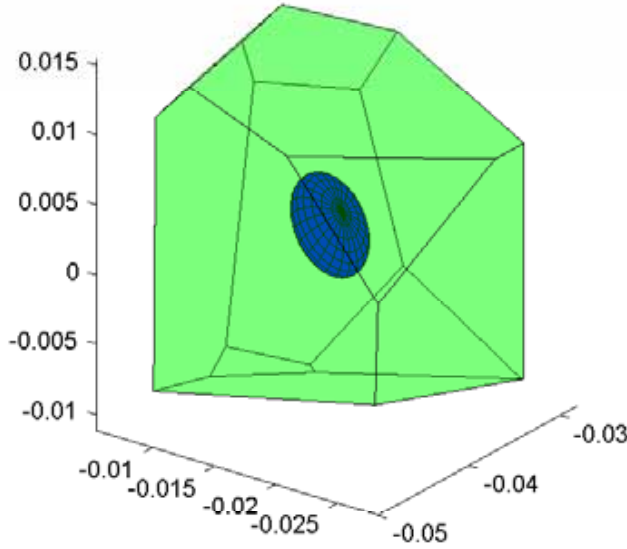


Figure 1: A 3D Trefftz Voronoi Cell with an ellipsoidal inclusion/void

For an arbitrary TVC in the 3D space, each surface is a polygon, see Fig. 1 for example. Constructing an inter-VC compatible displacement on the boundary of the polyhedral VC is not as simple as that for 2D TVCs. One way of doing this is to use Barycentric coordinates as nodal shape functions on each polygonal face of the 3D TVC. There are other ways, such as discretizing the VC boundary with 2D triangles, quadrangles, etc. But using Barycentric coordinates seems to be the simplest way, because no additional nodes are needed to be introduced to the polyhedron.

Consider a polygon face  $V_n$  with  $n$  nodes  $\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^n$ , the Barycentric coordinates, denoted as  $\lambda_i (i = 1, 2, \dots, n)$ .  $\lambda_i$  is a function of the position vector  $\mathbf{x}$ . To obtain a good performance of TVC, we only consider Barycentric coordinates which satisfy the following properties:

Non-negative:  $\lambda_i \geq 0$  in the polygon  $V_n$

Smooth:  $\lambda_i$  is at least  $C^1$  continuous in the polygon  $V_n$

Linear along each edge that composes the polygon  $V_n$

Linear completeness: For any linear function  $f(\mathbf{x})$ , the following equality holds:  
 $f(\mathbf{x}) = \sum_{i=1}^n f(\mathbf{x}^i) \lambda_i$

Partition of unity:  $\sum_{i=1}^n \lambda_i \equiv 1$ .

Dirac delta property:  $\lambda_i(\mathbf{x}^j) = \delta_{ij}$ .

Among the many Barycentric coordinates that satisfy these conditions, Wachspress coordinates [Wachspress (1975)] is among the most simple and efficient.

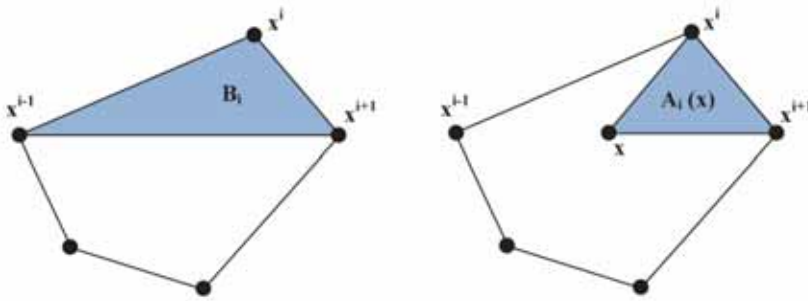


Figure 2: Definition of triangles  $B_i$  and  $A_i(\mathbf{x})$

Let  $\mathbf{x} \in V_n$ , and define the areas:  $B_i$  as the area of the triangle with  $\mathbf{x}^{i-1}$ ,  $\mathbf{x}^i$  and  $\mathbf{x}^{i+1}$  as its three vertices, and  $A_i(\mathbf{x})$  as the area of the triangle having  $\mathbf{x}$ ,  $\mathbf{x}^i$  and  $\mathbf{x}^{i+1}$  as its three vertices. This is illustrated in Fig. 2.

Define the Wachspress weight function as:

$$w_i(\mathbf{x}) = B_i \prod_{j \neq i, i-1} A_j(\mathbf{x}) \quad (1)$$

Then, the Wachspress coordinates are given by the rational functions:

$$\lambda_i(\mathbf{x}) = \frac{w_i(\mathbf{x})}{\sum_{j=1}^n w_j(\mathbf{x})} \quad (2)$$

Fig. 3 shows the Wachspress coordinate for one node of a regular pentagon. It can be seen that the Wachspress coordinate as shown in Fig. 3 have all the properties described previously in this section.

Similar to the well-known triangular Barycentric coordinates used in the 2D primal triangular elements, the nodal shape functions associated with the vertices of this polygonal surface displacement field are their corresponding Barycentric coordinates. An inter-VC compatible displacement field is therefore expressed in the

following form:

$$\tilde{u}_i(\mathbf{x}) = \sum_{k=1}^n \lambda_k(\mathbf{x}) u_i(\mathbf{x}^k) \quad \mathbf{x} \in V_n, V_n \subset \partial\Omega^e \quad (3)$$

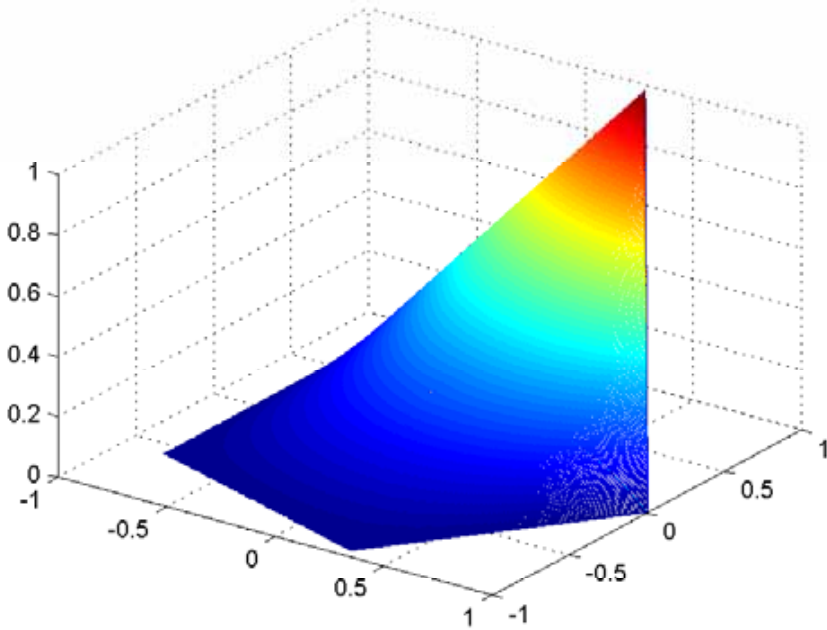


Figure 3: Barycentric coordinates as nodal shape functions

### 3 Trefftz Trial Displacement field: the Papkovitch-Neuber Solution

Consider a linear elastic solid undergoing infinitesimal elasto-static deformation. Cartesian coordinates  $x_i$  identify material particles in the solid.  $\sigma_{ij}, \varepsilon_{ij}, u_i$  are Cartesian components of the stress tensor, strain tensor and displacement vector respectively.  $\bar{f}_i, \bar{u}_i, \bar{t}_i$  are Cartesian components of the prescribed body force, boundary displacement and boundary traction vector.  $S_u, S_t$  are displacement boundary and traction boundary of the domain  $\Omega$ . We use  $(\cdot)_{,i}$  to denote differentiation with respect to  $x_i$ . The equations of linear and angular momentum balance, constitutive

equations, compatibility equations, and boundary conditions can be written as:

$$\sigma_{ij,j} + \bar{f}_i = 0 \text{ in } \Omega \quad (4)$$

$$\sigma_{ij} = \sigma_{ji} \text{ in } \Omega \quad (5)$$

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} \text{ (or } \varepsilon_{ij} = S_{ijkl} \sigma_{kl} \text{) in } \Omega \text{ for a linear elastic solid} \quad (6)$$

$$\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \equiv u_{(i,j)} \text{ in } \Omega \quad (7)$$

$$u_i = \bar{u}_i \text{ at } S_u \quad (8)$$

$$n_j \sigma_{ij} = \bar{t}_i \text{ at } S_t \quad (9)$$

For 3D isotropic media where body force is negligible, equation (4)-(6) can be rewritten in terms of displacements, which is the Navier's equation:

$$(\lambda + \mu) \theta_{,i} + \mu \Delta u_i = 0 \quad (10)$$

where

$$\begin{aligned} \theta &= u_{k,k} \\ \lambda &= \frac{Ev}{(1+\nu)(1-2\nu)} \\ \mu &= G = \frac{E}{2(1+\nu)} \end{aligned} \quad (11)$$

The Trefftz methods start by selecting a set of trial functions which satisfy (10) a priori. For 3D isotropic elasticity, this can be done by using the Papkovitch-Neuber solution, see [Lurie (2005)]:

$$\begin{aligned} \mathbf{u} &= [4(1-\nu)\mathbf{B} - \nabla(\mathbf{R} \cdot \mathbf{B} + \mathbf{B}_0)] / 2G \\ &= [(3-4\nu)\mathbf{B} - \mathbf{R} \cdot (\nabla \mathbf{B})^T - \nabla \mathbf{B}_0] / 2G \end{aligned} \quad (12)$$

$B_0, \mathbf{B}$  are scalar and vector harmonic functions, which are sometimes called Papkovitch-Neuber potentials

The second equation in (12) can be written in the following index form:

$$u_i = [(3-4\nu)B_i - x_k B_{k,i} - B_{0,i}] / 2G \quad (13)$$

An interesting fact of 3D Papkovitch-Neuber solution is that, the 3D displacements as in (13) have a very similar form to the displacements in 2D expressed in terms of complex potentials, as shown in [Muskhelishvili (1954)]. However, unlike the

approach of complex potentials, for a specific displacement field  $u_i$  in 3D, the harmonic potentials have large degrees of freedom. That is to say, there may exist many different sets of  $B_0, B_1, B_2, B_3$ , which are harmonic potentials of the same specific displacement field  $u_i$ . This prompts people to think about whether it is possible to drop the scalar harmonic function, to express the solution as:

$$\mathbf{u} = [4(1 - \nu)\mathbf{B} - \nabla\mathbf{R} \cdot \mathbf{B}] / 2G \quad (14)$$

It was proved by M.G. Slobodyansky that (14) is complete for the infinite region which is external to a closed surface for any  $\nu$ . However, for a simply-connected domain, (14) is complete only when  $\nu \neq 0.25$ .

By expressing  $B_0$  to be a specific function of  $\mathbf{B}$ , M.G. Slobodyansky has shown that a specific case of the Papkovitch Neuber solution is :

$$\mathbf{u} = [4(1 - \nu)\mathbf{B} + \mathbf{R} \cdot \nabla\mathbf{B} - \mathbf{R}\nabla \cdot \mathbf{B}] / 2G \quad (15)$$

which is complete for a simply connected domain, for any  $\nu$ .

For detailed discussion of the completeness of the Papkovitch-Neuber solution, see [Lurie (2005)].

#### 4 On Ellipsoidal Harmonics as Papkovitch-Neuber General Potentials

In this section, we make a brief introduction to ellipsoidal harmonics. One can refer to [Hobson (1931); Romain and Jean-Pierre (2001); Hu(2012)] for detailed discussion.

##### 4.1 Laplace Equation and Lamé Equation in an Ellipsoidal Coordinate System

Ellipsoidal coordinate systems are developed and used for solving specific problems of ellipsoid-shaped objects, for example, computation of the gravitational field of a celestial body, the electrical field of a molecule, and in this study, the stresses/strains around an ellipsoidal inclusion/void. Consider a background ellipsoid with semi-axes  $a > b > c$ , for any point with Cartesian coordinates  $x_1, x_2, x_3$ , the ellipsoidal coordinates  $\lambda_1, \lambda_2, \lambda_3$  are roots of the following equation:

$$\begin{aligned} \frac{x_1^2}{\lambda_1^2} + \frac{x_2^2}{\lambda_2^2 - h^2} + \frac{x_3^2}{\lambda_3^2 - k^2} &= 1 \\ \lambda_1^2 &\geq k \geq \lambda_2^2 \geq h \geq \lambda_3^2 \geq 0 \\ k &= \sqrt{a^2 - c^2}, h = \sqrt{a^2 - b^2} \end{aligned} \quad (16)$$

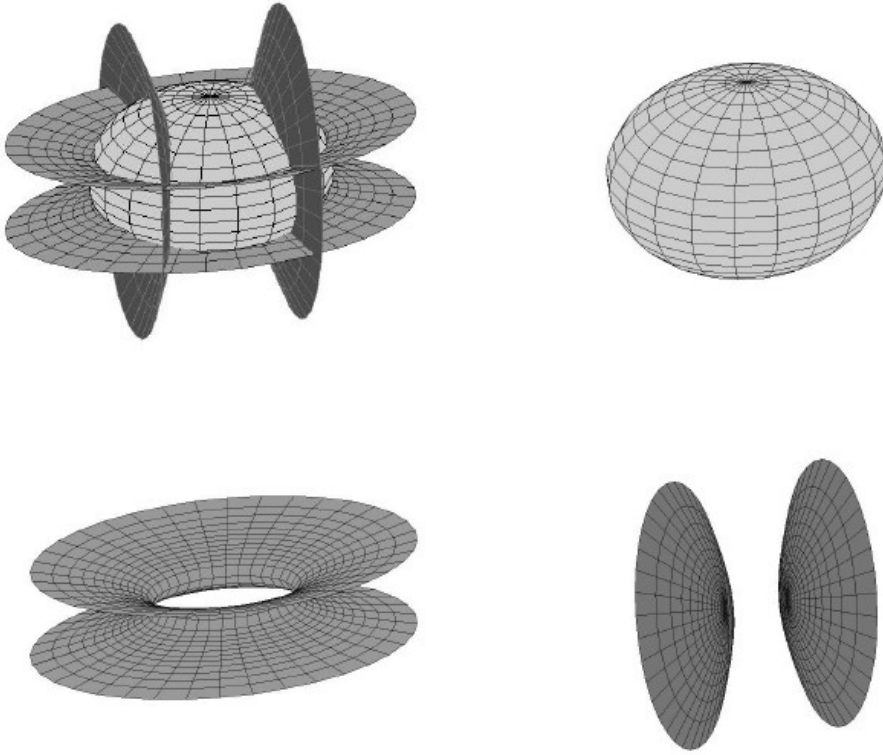


Figure 4: Coordinate surfaces of ellipsoidal coordinates  $\lambda_1, \lambda_2, \lambda_3$  are respectively an ellipsoid, a one-sheet hyperboloid, and a two-sheet hyperboloid

From (16), we find that the coordinate surfaces of ellipsoidal coordinates  $\lambda_1, \lambda_2, \lambda_3$  are respectively an ellipsoid, a one-sheet hyperboloid, and a two-sheet hyperboloid, as shown in Fig. 4.

The mapping from ellipsoidal to Cartesian coordinates is:

$$\begin{aligned}
 x_1^2 &= \frac{\lambda_1^2 \lambda_2^2 \lambda_3^2}{h^2 k^2} \\
 x_2^2 &= \frac{(\lambda_1^2 - h^2)(\lambda_2^2 - h^2)(h^2 - \lambda_3^2)}{h^2(k^2 - h^2)} \\
 x_3^2 &= \frac{(\lambda_1^2 - k^2)(k^2 - \lambda_2^2)(k^2 - \lambda_3^2)}{k^2(k^2 - h^2)}
 \end{aligned} \tag{17}$$

As seen in (16)(17), the signs of  $\lambda_1, \lambda_2, \lambda_3$  play no rule in defining  $x_1, x_2, x_3$ , and the signs of  $x_1, x_2, x_3$  cannot be uniquely defined by  $\lambda_1, \lambda_2, \lambda_3$ . Therefore, in this study,

$\lambda_1, \lambda_2, \lambda_3$  are prescribed to be non-negative. And the signs of  $x_1, x_2, x_3$  are always stored together with  $\lambda_1, \lambda_2, \lambda_3$  for a unique definition of the inverse mapping.

The Laplace operator of a scalar  $V$  has the following form in ellipsoidal coordinates:

$$\begin{aligned} \nabla^2 V &= (\lambda_2^2 - \lambda_3^2) \frac{\partial^2 V}{d\xi_1^2} + (\lambda_3^2 - \lambda_1^2) \frac{\partial^2 V}{d\xi_2^2} + (\lambda_1^2 - \lambda_2^2) \frac{\partial^2 V}{d\xi_3^2} = 0 \\ \xi_1(\lambda_1) &= \int_k^{\lambda_1} \frac{ds}{\sqrt{s^2 - h^2} \sqrt{s^2 - k^2}} \\ \xi_2(\lambda_2) &= \int_h^{\lambda_2} \frac{ds}{\sqrt{s^2 - h^2} \sqrt{k^2 - s^2}} \\ \xi_3(\lambda_3) &= \int_0^{\lambda_3} \frac{ds}{\sqrt{h^2 - s^2} \sqrt{k^2 - s^2}} \end{aligned} \quad (18)$$

By assuming  $V = E_1(\lambda_1) E_2(\lambda_2) E_3(\lambda_3)$ , the Laplace equation is changed to:

$$\begin{aligned} &(\lambda_2^2 - \lambda_3^2) \frac{1}{E_1(\lambda_1)} \frac{\partial^2 E_1(\lambda_1)}{d\xi_1^2} + (\lambda_3^2 - \lambda_1^2) \frac{1}{E_2(\lambda_2)} \frac{\partial^2 E_2(\lambda_2)}{d\xi_2^2} \\ &+ (\lambda_1^2 - \lambda_2^2) \frac{1}{E_3(\lambda_3)} \frac{\partial^2 E_3(\lambda_3)}{d\xi_3^2} = 0 \end{aligned} \quad (19)$$

From (19) one can readily see that functions  $E_1(\lambda_1), E_2(\lambda_2), E_3(\lambda_3)$  should have exactly the same form  $E(\lambda_i)$ , and they should all satisfy the following equation:

$$\frac{1}{E(\lambda_i)} \frac{d^2 E(\lambda_i)}{d\xi_i^2} = n(n+1) \lambda_i^2 - p \quad (20)$$

where  $n(n+1), p$  are separation constants.

Equation (20) is identical to:

$$\begin{aligned} &(\lambda_i^2 - h^2) (\lambda_i^2 - k^2) \frac{d^2 E_i(\lambda_i)}{d\lambda_i^2} + \lambda_i (2\lambda_i^2 - h^2 - k^2) \frac{dE_i(\lambda_i)}{d\lambda_i} \\ &+ (p - n(n+1) \lambda_i^2) E_i(\lambda_i) = 0 \end{aligned} \quad (21)$$

Equation (21) is called Lamé equation, the solution of which are called Lamé functions.

#### 4.2 Lamé Functions of the First Kind and Ellipsoidal Harmonics for Internal Problems

Solutions of the Lamé equation (21) are recorded in the monograph of [Hobson (1931)] in detail, where constants  $p$  for each natural number  $n$  are determined by

solving four eigenvalue problems. However, as shown in many recent works, this method is computationally unstable. Instead, the approach as shown in [Romain and Jean-Pierre (2001)] is used here because of its stability, accuracy and efficiency.

For each natural number  $n$ ,  $2n + 1$  different values of  $p$  can be found by solving four different eigenvalue problems. And the corresponding functions  $E_n^p(\lambda_i)$ , which satisfy (21) and are non-singular for any finite  $\lambda_i$ , are called Lamé functions of the first kind:

$$\begin{aligned} E_n^p(\lambda_i) &= \phi_n^p(\lambda_i) P_n^p(\lambda_i) \\ P_n^p(\lambda_i) &= \sum_{j=0}^m b_j \left(1 - \frac{\lambda_i^2}{h^2}\right)^j \end{aligned} \quad (22)$$

$m + 1$  is the size of matrices in these four different eigenvalue problems, and  $b_j$  are entries of the corresponding eigenvector of each  $p$ .

According to their expressions,  $\phi_n^p(\lambda_i)$  are categorized to four classes:

$$\begin{aligned} K_n^p(\lambda_i) &= \lambda_i^{n-2r}, \quad m = r \\ L_n^p(\lambda_i) &= \lambda_i^{1-n+2r} \sqrt{|\lambda_i^2 - h^2|}, \quad m = n - r - 1 \\ M_n^p(\lambda_i) &= \lambda_i^{1-n+2r} \sqrt{|\lambda_i^2 - k^2|}, \quad m = n - r - 1 \\ N_n^p(\lambda_i) &= \lambda_i^{n-2r} \sqrt{|\lambda_i^2 - h^2| (\lambda_i^2 - k^2)}, \quad m = r - 1 \end{aligned} \quad (23)$$

where  $r = \lceil \frac{n-1}{2} \rceil$ .

Each class of  $\phi_n^p(\lambda_i)$  corresponds to a specific one of the four different eigenvalue problems, from which eigenvalue  $p$  and eigenvector  $b_j$  are found, and thereafter  $P_n^p(\lambda_i)$  is defined.

The eigenvalue problem can be expressed in the following form:

$$\begin{bmatrix} d_0 & g_0 & 0 & \cdots & \cdots & 0 \\ f_1 & d_1 & g_1 & \ddots & \ddots & \vdots \\ 0 & f_2 & d_2 & g_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & f_{m-1} & d_{m-1} & g_{m-1} \\ 0 & \cdots & \cdots & 0 & f_m & d_m \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_{m-1} \\ b_m \end{Bmatrix} = p \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_{m-1} \\ b_m \end{Bmatrix} \quad (24)$$

For  $K_n^p$  with even  $n$ ,

$$\begin{cases} f_i = -(2r - 2i + 2)(2r + 2i - 1)\alpha \\ d_i = 2r(2r + 1)\alpha - 4i^2\gamma \\ g_i = -(2i + 2)(2i + 1)\beta \end{cases} \quad (25)$$

where

$$\alpha = h^2, \quad \beta = k^2 - h^2, \quad \gamma = \alpha - \beta \quad (26)$$

For  $K_n^p$  with odd  $n$ ,

$$\begin{cases} f_i = -(2r - 2i + 2)(2r + 2i + 1)\alpha \\ d_i = ((2r + 1)(2r + 2) - 4i^2)\alpha + (2i + 1)^2\beta \\ g_i = -(2i + 2)(2i + 1)\beta \end{cases} \quad (27)$$

For  $L_n^p$  with even  $n$ ,

$$\begin{cases} f_i = -(2r - 2i)(2r + 2i + 1)\alpha \\ d_i = (2r(2r + 1) - (2i + 1)^2)\alpha + (2i + 2)^2\beta \\ g_i = -(2i + 2)(2i + 3)\beta \end{cases} \quad (28)$$

For  $L_n^p$  with odd  $n$ ,

$$\begin{cases} f_i = -(2r - 2i + 2)(2r + 2i + 1)\alpha \\ d_i = (2r + 1)(2r + 2)\alpha - (2i + 1)^2\gamma \\ g_i = -(2i + 2)(2i + 3)\beta \end{cases} \quad (29)$$

For  $M_n^p$  with even  $n$ ,

$$\begin{cases} f_i = -(2r - 2i)(2r + 2i + 1)\alpha \\ d_i = 2r(2r + 1)\alpha - (2i + 1)^2\gamma \\ g_i = -(2i + 2)(2i + 1)\beta \end{cases} \quad (30)$$

For  $M_n^p$  with odd  $n$ ,

$$\begin{cases} f_i = -(2r - 2i + 2)(2r + 2i + 1)\alpha \\ d_i = ((2r + 1)(2r + 2) - (2i + 1)^2)\alpha + 4i^2\beta \\ g_i = -(2i + 2)(2i + 1)\beta \end{cases} \quad (31)$$

For  $N_n^p$  with even  $n$ ,

$$\begin{cases} f_i = -(2r-2i)(2r+2i+1)\alpha \\ d_i = 2r(2r+1)\alpha - (2i+2)^2\alpha + (2i+1)^2\beta \\ g_i = -(2i+2)(2i+3)\beta \end{cases} \quad (32)$$

For  $N_n^p$  with odd  $n$ ,

$$\begin{cases} f_i = -(2r-2i)(2r+2i+3)\alpha \\ d_i = (2r+1)(2r+2)\alpha - (2i+2)^2\gamma \\ g_i = -(2i+2)(2i+3)\beta \end{cases} \quad (33)$$

Solutions of these four eigenvalue problems are computationally stable, because of the well-posedness of these coefficient matrices, as compared to those ill-posed ones in the monograph of [Hobson (1931)].

Now that Lamé functions of the first kind are completely defined, and are non-singular for any finite  $\lambda_i$ , their products can be used to solve Laplace equation in a finite ellipsoidal domain. These ellipsoidal harmonics for internal problems exhibit several similar characteristics to spherical harmonics as shown in [Dong and Atluri (2012b)]. For example,  $E_n^p(\lambda_2)E_n^p(\lambda_3)$  are called ellipsoidal surface harmonics, which have the property of orthogonally with respect to the integral over the background ellipsoidal surface  $S$ :

$$\int_S E_n^p(\lambda_2)E_n^p(\lambda_3)E_l^q(\lambda_2)E_l^q(\lambda_3)dS = \delta_n^l\delta_p^q(\gamma_n^p)^2 \quad (34)$$

And they can be normalized as:

$$Y_n^p(\lambda_2, \lambda_3) = \frac{1}{\gamma_n^p} E_n^p(\lambda_2)E_n^p(\lambda_3) \quad (35)$$

Details of how to compute the  $\gamma_n^p$  is shown in [Romain and Jean-Pierre (2001)].

The first function  $E_n^p(\lambda_1)$  is similar to the function  $R^n$  in spherical harmonics, which increases drastically with respect to  $n$ . Therefore, a characteristic length  $\lambda_{1p}$  is introduced, which should be the largest  $\lambda_1$  at locations where boundary conditions are specified. Therefore,  $E_n^p(\lambda_1)$  is scaled to  $E_n^p(\lambda_1)/E_n^p(\lambda_{1p})$ , which is between 0 and 1 for any point at the boundary. Scaling of harmonic functions with characteristic lengths were firstly presented by [Liu (2007a,b)]. This method was used by authors of this paper to scale the Trefftz trial function of TVCs in a series of

paper [Dong and Atluri (2011b,2012a,b,c)], in order to avoid solving a system of ill-posed equations.

The ellipsoidal harmonics of internal problems are thereafter expressed as:

$$V_n^p(\lambda_1, \lambda_2, \lambda_3) = \frac{E_n^p(\lambda_1)}{E_n^p(\lambda_{1p})} \frac{E_n^p(\lambda_2) E_n^p(\lambda_3)}{\gamma_n^p} \quad (36)$$

### 4.3 Lamé Functions of the Second Kind and Ellipsoidal Harmonics for External Problems

Ellipsoidal harmonics as shown in (36) obviously cannot be used to solve external problems, because  $E_n^p(\lambda_1)$  becomes infinity when  $\lambda_1 \rightarrow \infty$ .

Using the usual technique of Wronskian, one can find a second solution of the Lamé equation:

$$\begin{aligned} F_n^p(\lambda_1) &= E_n^p(\lambda_1) I_n^p(\lambda_1) \\ I_n^p(\lambda_1) &= \int_{\lambda_1}^{\infty} \frac{ds}{[E_n^p(s)]^2 \sqrt{(s^2 - h^2)(s^2 - k^2)}} \\ &= \int_0^{1/\lambda_1} \frac{dt}{[E_n^p(1/t)]^2 \sqrt{(1 - h^2 t^2)(1 - k^2 t^2)}} \end{aligned} \quad (37)$$

$F_n^p(\lambda_1)$  is called Lamé function of the second kind.

As opposed to  $E_n^p(\lambda_1)$ , the function  $F_n^p(\lambda_1)$  is singular at  $\lambda_1 = 0$  only, and decreases drastically with respect to  $n$ . Therefore, a characteristic length  $\lambda_{1k}$  is introduced, which should be the smallest  $\lambda_1$  at locations where boundary conditions are specified. Therefore, Lamé functions of the second kind is scaled to  $F_n^p(\lambda_1)/F_n^p(\lambda_{1k})$ , which is between 0 and 1 for any point at the boundary.

And the ellipsoidal harmonics of external problems are thereafter expressed as:

$$V_n^p(\lambda_1, \lambda_2, \lambda_3) = \frac{F_n^p(\lambda_1)}{F_n^p(\lambda_{1k})} \frac{E_n^p(\lambda_2) E_n^p(\lambda_3)}{\gamma_n^p} \quad (38)$$

### 4.4 Spatial Differentiation of Ellipsoidal Harmonics

From the explicit formulas of  $E_n^p(\lambda_1)$ ,  $F_n^p(\lambda_1)$ ,  $E_n^p(\lambda_2)$ ,  $E_n^p(\lambda_3)$ , one can easily derive  $\frac{\partial V_n^p}{\partial \lambda_i}$ ,  $\frac{\partial^2 V_n^p}{\partial \lambda_i \partial \lambda_j}$ . And the spatial differentiation of ellipsoidal harmonics with re-

spect to  $x_1, x_2, x_3$  can be written as:

$$\begin{aligned}\frac{\partial V}{\partial x_i} &= \frac{\partial V}{\partial \lambda_m} \frac{\partial \lambda_m}{\partial x_i} \\ \frac{\partial^2 V}{\partial x_i \partial x_j} &= \frac{\partial}{\partial x_j} \left( \frac{\partial V}{\partial \lambda_m} \frac{\partial \lambda_m}{\partial x_i} \right) \\ &= \frac{\partial^2 V}{\partial \lambda_m \partial \lambda_n} \frac{\partial \lambda_m}{\partial x_i} \frac{\partial \lambda_n}{\partial x_j} + \frac{\partial V}{\partial \lambda_m} \frac{\partial^2 \lambda_m}{\partial x_i \partial \lambda_n} \frac{\partial \lambda_n}{\partial x_j}\end{aligned}\quad (39)$$

The formulas of  $P_{ij} = \frac{\partial \lambda_j}{\partial x_i}$  can be derived from (17):

$$\begin{aligned}P_{11} &= \frac{x_1 (\lambda_1^2 - k^2) (\lambda_1^2 - h^2)}{\lambda_1 (\lambda_1^2 - \lambda_2^2) (\lambda_1^2 - \lambda_3^2)}, P_{12} = \frac{x_1 (\lambda_2^2 - k^2) (\lambda_2^2 - h^2)}{\lambda_2 (\lambda_2^2 - \lambda_1^2) (\lambda_2^2 - \lambda_3^2)} \\ P_{13} &= \frac{x_1 (\lambda_3^2 - k^2) (\lambda_3^2 - h^2)}{\lambda_3 (\lambda_3^2 - \lambda_1^2) (\lambda_3^2 - \lambda_2^2)}, P_{21} = \frac{x_2 \lambda_1 (\lambda_1^2 - k^2)}{(\lambda_1^2 - \lambda_2^2) (\lambda_1^2 - \lambda_3^2)} \\ P_{22} &= \frac{x_2 \lambda_2 (\lambda_2^2 - k^2)}{(\lambda_2^2 - \lambda_1^2) (\lambda_2^2 - \lambda_3^2)}, P_{23} = \frac{x_2 \lambda_3 (\lambda_3^2 - k^2)}{(\lambda_3^2 - \lambda_1^2) (\lambda_3^2 - \lambda_2^2)} \\ P_{31} &= \frac{x_3 \lambda_1 (\lambda_1^2 - h^2)}{(\lambda_1^2 - \lambda_2^2) (\lambda_1^2 - \lambda_3^2)}, P_{32} = \frac{x_3 \lambda_2 (\lambda_2^2 - h^2)}{(\lambda_2^2 - \lambda_1^2) (\lambda_2^2 - \lambda_3^2)} \\ P_{33} &= \frac{x_3 \lambda_3 (\lambda_3^2 - h^2)}{(\lambda_3^2 - \lambda_1^2) (\lambda_3^2 - \lambda_2^2)}\end{aligned}\quad (40)$$

And the formulas of  $\frac{\partial P_{ij}}{\partial \lambda_1}$  are derived by differentiating (40):

$$\begin{aligned}\frac{\partial P_{11}}{\partial \lambda_1} &= 2x_1 \left( \frac{(2\lambda_1^2 - h^2 - k^2)}{(\lambda_1^2 - \lambda_2^2) (\lambda_1^2 - \lambda_3^2)} - \frac{(2\lambda_1^2 - \lambda_2^2 - \lambda_3^2)(\lambda_1^2 - h^2)(\lambda_1^2 - k^2)}{(\lambda_1^2 - \lambda_2^2)^2 (\lambda_1^2 - \lambda_3^2)^2} \right) \\ \frac{\partial P_{21}}{\partial \lambda_1} &= x_2 \left( \frac{4\lambda_1^4 - (3h^2 + 2k^2)\lambda_1^2 + h^2k^2}{(\lambda_1^2 - \lambda_2^2) (\lambda_1^2 - \lambda_3^2) (\lambda_1^2 - h^2)} - \frac{2\lambda_1^2(\lambda_1^2 - k^2)(2\lambda_1^2 - \lambda_2^2 - \lambda_3^2)}{(\lambda_1^2 - \lambda_2^2)^2 (\lambda_1^2 - \lambda_3^2)^2} \right) \\ \frac{\partial P_{31}}{\partial \lambda_1} &= x_3 \left( \frac{4\lambda_1^4 - (2h^2 + 3k^2)\lambda_1^2 + h^2k^2}{(\lambda_1^2 - \lambda_2^2) (\lambda_1^2 - \lambda_3^2) (\lambda_1^2 - k^2)} - \frac{2\lambda_1^2(\lambda_1^2 - h^2)(2\lambda_1^2 - \lambda_2^2 - \lambda_3^2)}{(\lambda_1^2 - \lambda_2^2)^2 (\lambda_1^2 - \lambda_3^2)^2} \right) \\ \frac{\partial P_{12}}{\partial \lambda_1} &= P_{12} \frac{\lambda_1^2 + \lambda_2^2}{\lambda_1 (\lambda_2^2 - \lambda_1^2)}, \frac{\partial P_{22}}{\partial \lambda_1} = P_{22} \frac{\lambda_1^3 + \lambda_1 (\lambda_2^2 - 2h^2)}{(\lambda_2^2 - \lambda_1^2) (\lambda_1^2 - h^2)} \\ \frac{\partial P_{32}}{\partial \lambda_1} &= P_{32} \frac{\lambda_1^3 + \lambda_1 (\lambda_2^2 - 2k^2)}{(\lambda_2^2 - \lambda_1^2) (\lambda_1^2 - k^2)}, \frac{\partial P_{13}}{\partial \lambda_1} = P_{13} \frac{\lambda_1^2 + \lambda_3^2}{\lambda_1 (\lambda_3^2 - \lambda_1^2)} \\ \frac{\partial P_{23}}{\partial \lambda_1} &= P_{23} \frac{\lambda_1^3 + \lambda_1 (\lambda_3^2 - 2h^2)}{(\lambda_3^2 - \lambda_1^2) (\lambda_1^2 - h^2)}, \frac{\partial P_{33}}{\partial \lambda_1} = P_{33} \frac{\lambda_1^3 + \lambda_1 (\lambda_3^2 - 2k^2)}{(\lambda_3^2 - \lambda_1^2) (\lambda_1^2 - k^2)}\end{aligned}$$

(41)

And the formulas of  $\frac{\partial P_{ij}}{\partial \lambda_2}$  are:

$$\begin{aligned}
 \frac{\partial P_{11}}{\partial \lambda_2} &= P_{11} \frac{\lambda_1^2 + \lambda_2^2}{\lambda_2 (\lambda_1^2 - \lambda_2^2)}, \quad \frac{\partial P_{21}}{\partial \lambda_2} = P_{21} \frac{\lambda_2^3 + \lambda_2 (\lambda_1^2 - 2h^2)}{(\lambda_1^2 - \lambda_2^2) (\lambda_2^2 - h^2)} \\
 \frac{\partial P_{31}}{\partial \lambda_2} &= P_{31} \frac{\lambda_2^3 + \lambda_2 (\lambda_1^2 - 2k^2)}{(\lambda_1^2 - \lambda_2^2) (\lambda_2^2 - k^2)} \\
 \frac{\partial P_{12}}{\partial \lambda_2} &= 2x_1 \left( \frac{(2\lambda_2^2 - h^2 - k^2)}{(\lambda_2^2 - \lambda_1^2) (\lambda_2^2 - \lambda_3^2)} - \frac{(2\lambda_2^2 - \lambda_1^2 - \lambda_3^2)(\lambda_2^2 - h^2)(\lambda_2^2 - k^2)}{(\lambda_2^2 - \lambda_1^2)^2 (\lambda_2^2 - \lambda_3^2)^2} \right) \\
 \frac{\partial P_{22}}{\partial \lambda_2} &= x_2 \left( \frac{4\lambda_2^4 - (3h^2 + 2k^2)\lambda_2^2 + h^2k^2}{(\lambda_2^2 - \lambda_1^2) (\lambda_2^2 - \lambda_3^2) (\lambda_2^2 - h^2)} - \frac{2\lambda_2^2(\lambda_2^2 - k^2)(2\lambda_2^2 - \lambda_1^2 - \lambda_3^2)}{(\lambda_2^2 - \lambda_1^2)^2 (\lambda_2^2 - \lambda_3^2)^2} \right) \\
 \frac{\partial P_{32}}{\partial \lambda_2} &= x_3 \left( \frac{4\lambda_2^4 - (2h^2 + 3k^2)\lambda_2^2 + h^2k^2}{(\lambda_2^2 - \lambda_1^2) (\lambda_2^2 - \lambda_3^2) (\lambda_2^2 - k^2)} - \frac{2\lambda_2^2(\lambda_2^2 - h^2)(2\lambda_2^2 - \lambda_1^2 - \lambda_3^2)}{(\lambda_2^2 - \lambda_1^2)^2 (\lambda_2^2 - \lambda_3^2)^2} \right) \\
 \frac{\partial P_{13}}{\partial \lambda_2} &= P_{13} \frac{\lambda_2^2 + \lambda_3^2}{\lambda_2 (\lambda_3^2 - \lambda_2^2)}, \quad \frac{\partial P_{23}}{\partial \lambda_2} = P_{23} \frac{\lambda_2^3 + \lambda_2 (\lambda_3^2 - 2h^2)}{(\lambda_3^2 - \lambda_2^2) (\lambda_2^2 - h^2)} \\
 \frac{\partial P_{33}}{\partial \lambda_2} &= P_{33} \frac{\lambda_2^3 + \lambda_2 (\lambda_3^2 - 2k^2)}{(\lambda_3^2 - \lambda_2^2) (\lambda_2^2 - k^2)}
 \end{aligned} \tag{42}$$

And the formulas of  $\frac{\partial P_{ij}}{\partial \lambda_3}$  are:

$$\begin{aligned}
 \frac{\partial P_{11}}{\partial \lambda_3} &= P_{11} \frac{\lambda_1^2 + \lambda_3^2}{\lambda_3 (\lambda_1^2 - \lambda_3^2)}, \quad \frac{\partial P_{21}}{\partial \lambda_3} = P_{21} \frac{\lambda_3^3 + \lambda_3 (\lambda_1^2 - 2h^2)}{(\lambda_1^2 - \lambda_3^2) (\lambda_3^2 - h^2)} \\
 \frac{\partial P_{31}}{\partial \lambda_3} &= P_{31} \frac{\lambda_3^3 + \lambda_3 (\lambda_1^2 - 2k^2)}{(\lambda_1^2 - \lambda_3^2) (\lambda_3^2 - k^2)}, \quad \frac{\partial P_{12}}{\partial \lambda_3} = P_{12} \frac{\lambda_2^2 + \lambda_3^2}{\lambda_3 (\lambda_2^2 - \lambda_3^2)} \\
 \frac{\partial P_{22}}{\partial \lambda_3} &= P_{22} \frac{\lambda_3^3 + \lambda_3 (\lambda_2^2 - 2h^2)}{(\lambda_2^2 - \lambda_3^2) (\lambda_3^2 - h^2)}, \quad \frac{\partial P_{32}}{\partial \lambda_3} = P_{32} \frac{\lambda_3^3 + \lambda_3 (\lambda_2^2 - 2k^2)}{(\lambda_2^2 - \lambda_3^2) (\lambda_3^2 - k^2)} \\
 \frac{\partial P_{13}}{\partial \lambda_3} &= 2x_1 \left( \frac{(2\lambda_3^2 - h^2 - k^2)}{(\lambda_3^2 - \lambda_1^2) (\lambda_3^2 - \lambda_2^2)} - \frac{(2\lambda_3^2 - \lambda_1^2 - \lambda_2^2)(\lambda_3^2 - h^2)(\lambda_3^2 - k^2)}{(\lambda_3^2 - \lambda_1^2)^2 (\lambda_3^2 - \lambda_2^2)^2} \right) \\
 \frac{\partial P_{23}}{\partial \lambda_3} &= x_2 \left( \frac{4\lambda_3^4 - (3h^2 + 2k^2)\lambda_3^2 + h^2k^2}{(\lambda_3^2 - \lambda_1^2) (\lambda_3^2 - \lambda_2^2) (\lambda_3^2 - h^2)} - \frac{2\lambda_3^2(\lambda_3^2 - k^2)(2\lambda_3^2 - \lambda_1^2 - \lambda_2^2)}{(\lambda_3^2 - \lambda_1^2)^2 (\lambda_3^2 - \lambda_2^2)^2} \right) \\
 \frac{\partial P_{33}}{\partial \lambda_3} &= x_2 \left( \frac{4\lambda_3^4 - (2h^2 + 3k^2)\lambda_3^2 + h^2k^2}{(\lambda_3^2 - \lambda_1^2) (\lambda_3^2 - \lambda_2^2) (\lambda_3^2 - k^2)} - \frac{2\lambda_3^2(\lambda_3^2 - h^2)(2\lambda_3^2 - \lambda_1^2 - \lambda_2^2)}{(\lambda_3^2 - \lambda_1^2)^2 (\lambda_3^2 - \lambda_2^2)^2} \right)
 \end{aligned}$$

$$(43)$$

## 5 TVCs with Ellipsoidal Inclusions/Voids

### 5.1 Trefftz Trial Displacement Fields for Different Types of Inhomogeneities

Consider a linear elastic solid undergoing infinitesimal elasto-static deformation. The governing equation can be written in terms of displacements, which is the Navier's equation:

$$(\lambda + \mu)\theta_{,i} + \mu\Delta u_i = 0 \quad (44)$$

The boundary conditions are:

$$u_i = \bar{u}_i \text{ at } S_u \quad (45)$$

$$n_j\sigma_{ij} = \bar{t}_i \text{ at } S_t \quad (46)$$

We consider that the domain  $\Omega$  is discretized into many Voronoi Cells  $\Omega^e$  with boundary  $\partial\Omega^e$ , each VC boundary can be divided into  $S_u^e, S_t^e, \rho^e$ , which are intersections of  $\partial\Omega^e$  with  $S_u, S_t$  and other VC boundaries respectively. For VCs developed in this study, an inclusion or void  $\Omega_c^e$  is present inside each VC, which satisfies  $\Omega_c^e \subset \Omega^e, \partial\Omega_c^e \cap \partial\Omega^e = \emptyset$ , see Fig. 1. We denote the matrix material in each VC as  $\Omega_m^e$ , such that  $\Omega_m^e = \Omega^e - \Omega_c^e, \partial\Omega_m^e = \partial\Omega^e + \partial\Omega_c^e$ .

When an elastic inclusion is considered, we denote the displacement field in  $\Omega_m^e$  and  $\Omega_c^e$  as  $u_i^m$  and  $u_i^c$ , the strain and stress fields corresponding to which are  $\varepsilon_{ij}^m, \sigma_{ij}^m$  and  $\varepsilon_{ij}^c, \sigma_{ij}^c$  respectively. We also denote the displacement field along  $\partial\Omega^e$  as  $\tilde{u}_i^m$ , which is inter-VC compatible, by using Barycentric coordinates as nodal shape functions. Then, in addition to  $u_i^c$  satisfying (44) in each  $\Omega_c^e$ ,  $u_i^m$  satisfying (44) in each  $\Omega_m^e$ , satisfying (46) at  $S_t^e$ ,  $\tilde{u}_i^m$  satisfying (45) at  $S_u^e$ , displacement continuity and traction reciprocity conditions at each  $\rho^e$  should be considered:

$$u_i^m = \tilde{u}_i^m \text{ at } \partial\Omega^e \quad (47)$$

$$(n_j\sigma_{ij}^m)^+ + (n_j\sigma_{ij}^m)^- = 0 \text{ at } \rho^e \quad (48)$$

Displacement continuity and traction reciprocity conditions at  $\partial\Omega_c^e$  should also be considered:

$$u_i^m = u_i^c \text{ at } \partial\Omega_c^e \quad (49)$$

$$-n_j\sigma_{ij}^m + n_j\sigma_{ij}^c = 0 \text{ at } \partial\Omega_c^e \quad (50)$$

where  $n_j$  is the unit outer-normal vector at  $\partial\Omega_c^e$ .

When a rigid inclusion is considered, because only rigid-body displacement is allowed for the inclusion, there is no need to assume  $u_i^c$ . The following conditions need to be satisfied at  $\partial\Omega_c^e$ :

$$u_i^m(\text{non - rigid - body}) = 0 \text{ at } \partial\Omega_c^e \quad (51)$$

$$\begin{aligned} \int_{\partial\Omega_c^e} n_j \sigma_{ij}^m dS &= 0 \\ \int_{\partial\Omega_c^e} e_{ghi} x_h n_j \sigma_{ij}^m dS &= 0 \end{aligned} \quad (52)$$

When a void is to be considered, for TVC-BVP,  $\tilde{u}_i^c$  is assumed only along  $\partial\Omega_c^e$ . The following displacement continuity and traction free conditions are to be satisfied:

$$u_i^m = \tilde{u}_i^c \text{ at } \partial\Omega_c^e \quad (53)$$

$$n_j \sigma_{ij}^m = 0 \text{ at } \partial\Omega_c^e \quad (54)$$

For TVC-C, on the other hand, there is no need to assume such a boundary field  $\tilde{u}_i^c$ . Only (54) needs to be satisfied at  $\partial\Omega_c^e$ .

It should be noted that, for a priori equilibrated displacement fields, condition (52) is a necessary condition of (50) or (54). Hence, for problems with elastic inclusion or voids, condition (52) is satisfied as long as conditions (50) or (54) are satisfied.

In TVCs derived in this study,  $u_i^m, u_i^c$  satisfy (44) as well as (52) a priori, and all other conditions as shown in (45)-(54) are satisfied using variational principles or using collocation method. Such displacement fields can be expressed in terms of Papkovitch-Neuber potentials. When an ellipsoidal inclusion or void is present, as shown in Fig. 5, a local Cartesian coordinate system is used, where the origin lies at the center of the ellipsoid, and the three axes  $x_1, x_2, x_3$  coincide with the three semi-axes  $a, b, c$  of the ellipsoid. Therefore, an ellipsoidal coordinate system  $\lambda_1 - \lambda_2 - \lambda_3$  is developed which corresponds to this local Cartesian system  $x_1 - x_2 - x_3$ . And the two types of ellipsoidal harmonics are used as Papkovitch-Neuber potentials for the displacements in the matrix material:

$$\begin{aligned} \mathbf{B}_{mp} &= \sum_{n=0}^M \sum_p \alpha_n^p \frac{E_n^p(\lambda_1)}{E_n^p(\lambda_{mp})} \frac{E_n^p(\lambda_2) E_n^p(\lambda_3)}{\gamma_n^p} \\ \mathbf{B}_{mk} &= \sum_{n=0}^N \sum_p \beta_n^p \frac{F_n^p(\lambda_1)}{F_n^p(\lambda_{mk})} \frac{E_n^p(\lambda_2) E_n^p(\lambda_3)}{\gamma_n^p} \end{aligned} \quad (55)$$

$\mathbf{B}_{mp}$  are ellipsoidal harmonics for the internal problems, which are non-singular in the whole domain. And  $\mathbf{B}_{mk}$  are ellipsoidal harmonics for the external problems, which are singular at the source point:

Two characteristic lengths  $\lambda_{mk}$  and  $\lambda_{mp}$  are defined.  $\lambda_{mk}$  is equal to the minimum  $\lambda_1$  between the source point  $S^e$  and any point in  $\Omega_m^e$ , therefore  $\frac{F_n^p(\lambda_1)}{F_n^p(\lambda_{mp})}$  is confined between 0 and 1 for any positive  $n$ . For an ellipsoidal inclusion/void, it is obvious that  $\lambda_{mk}$  is equal to  $a$ .

$\lambda_{mp}$  is equal to the maximum  $\lambda_1$  between the source point  $S^e$  and any point in  $\Omega_m^e$ , therefore  $\frac{E_n^p(\lambda_1)}{E_n^p(\lambda_{mp})}$  is confined between 0 and 1 for any positive  $n$ .

And the displacement field in the matrix material is express as:

$$\begin{aligned}\mathbf{u}_m &= \mathbf{u}_{mp} + \mathbf{u}_{mk} \\ \mathbf{u}_{mp} &= [4(1 - \nu_m)\mathbf{B}_{mp} + \mathbf{R} \cdot \nabla \mathbf{B}_{mp} - \mathbf{R} \nabla \cdot \mathbf{B}_{mp}] / 2G_m \\ \mathbf{u}_{mk} &= [4(1 - \nu_m)\mathbf{B}_{mk} - \nabla \mathbf{R}_{mk} \cdot \mathbf{B}] / 2G_m\end{aligned}\quad (56)$$

When an ellipsoidal elastic inclusion is considered,  $u_i^c$  can be express using the ellipsoidal harmonics for internal problems:

$$\begin{aligned}\mathbf{u}_c &= \mathbf{u}_{cp} = [4(1 - \nu_c)\mathbf{B}_{cp} + \mathbf{R} \cdot \nabla \mathbf{B}_{cp} - \mathbf{R} \nabla \cdot \mathbf{B}_{cp}] / 2G_c \\ \mathbf{B}_{cp} &= \sum_{n=0}^L \sum_p \chi_n^p \frac{E_n^p(\lambda_1)}{E_n^p(\lambda_{cp})} \frac{E_n^p(\lambda_2) E_n^p(\lambda_3)}{\gamma_n^p}\end{aligned}\quad (57)$$

$\lambda_{cp}$  is equal to the maximum  $\lambda_1$  between the source point  $S^e$  and any point in  $\Omega_c^e$ , therefore  $\frac{E_n^p(\lambda_1)}{E_n^p(\lambda_{cp})}$  is confined between 0 and 1 for any positive  $n$ .

When a rigid inclusion is considered,  $u_i^c$  does not need to be assumed. Assuming  $u_i^m$  is enough for developing TVCs.

When a void is considered, for TVC-BVP,  $\tilde{u}_i^c$  is assumed only at  $\partial\Omega_c$ . We assume

$$\begin{aligned}\tilde{\mathbf{u}}_c &= \tilde{\mathbf{u}}_{cp} = [4(1 - \nu_m)\tilde{\mathbf{B}}_{cp} + \mathbf{R} \cdot \nabla \tilde{\mathbf{B}}_{cp} - \mathbf{R} \nabla \cdot \tilde{\mathbf{B}}_{cp}] / 2G_m \\ \tilde{\mathbf{B}}_{cp} &= \sum_{n=0}^L \sum_p \chi_n^p \frac{E_n^p(\lambda_1)}{E_n^p(\lambda_{mp})} \frac{E_n^p(\lambda_2) E_n^p(\lambda_3)}{\gamma_n^p}\end{aligned}\quad (58)$$

It should be noted that, there are 6 modes in  $\frac{E_n^p(\lambda_1)}{E_n^p(\lambda_{mp})} \frac{E_n^p(\lambda_2) E_n^p(\lambda_3)}{\gamma_n^p}$  corresponding to the potentials of rigid-body displacement modes, and there are 6 modes in  $\frac{F_n^p(\lambda_1)}{F_n^p(\lambda_{mp})} \frac{E_n^p(\lambda_2) E_n^p(\lambda_3)}{\gamma_n^p}$  corresponding to the potentials of displacement modes which contribute to the resultant force and moment at  $\partial\Omega_c^e$ , these modes should be found out numerically and eliminated beforehand.

Now that the displacement fields are defined, the undetermined parameters can be related to nodal displacements of the VC using either multi-field boundary variational principles or using the collocation method, and leading to different methods of deriving stiffness matrices as shown in the next two sections.

It should be noted that, the displacement fields in this section are developed in a local coordinate system, thus the developed stiffness matrices should be transferred to the global coordinate system using well-known coordinate transfer techniques.

Moreover, the displacement assumptions considered in this section are all invariant with respect to change of coordinate systems. Therefore, the VC stiffness matrices developed from these displacement assumptions are invariant.

## 5.2 TVCs Using Multi-Field Boundary Variational Principles

In this section, TVCs are developed using multi-field boundary variational principles.

An inter-VC compatible displacement field  $\tilde{u}_i^m$  is assumed at  $\partial\Omega^e$  with Wachspres coordinates as nodal shape functions. Using matrix and vector notation, we have:

$$\tilde{\mathbf{u}}_m = \tilde{\mathbf{N}}_m \mathbf{q} \text{ at } \partial\Omega^e \quad (59)$$

The displacement field in  $\Omega_m^e$  and its corresponding traction field  $t_i^m$  at  $\partial\Omega_m^e, \partial\Omega_c^e$  as:

$$\begin{aligned} \mathbf{u}_m &= \mathbf{N}_m \alpha \text{ in } \Omega_m^e \\ \mathbf{t}_m &= \mathbf{R}_m \alpha \text{ at } \partial\Omega_m^e, \partial\Omega_c^e \end{aligned} \quad (60)$$

When an elastic inclusion is to be considered, the displacement field in the inclusion is independently assumed. We have:

$$\begin{aligned} \mathbf{u}_c &= \mathbf{N}_c \beta \text{ in } \Omega_c^e \\ \mathbf{t}_c &= \mathbf{R}_c \beta \text{ at } \partial\Omega_c^e \end{aligned} \quad (61)$$

Therefore, finite element equations can be derived using the following three-field boundary variational principle:

$$\begin{aligned} \pi_3(\tilde{u}_i^m, u_i^m, u_i^c) &= \sum_e \left\{ - \int_{\partial\Omega^e + \partial\Omega_c^e} \frac{1}{2} t_i^m u_i^m dS + \int_{\partial\Omega_m^e} t_i^m \tilde{u}_i^m dS - \int_{S_i^e} \bar{t}_i \tilde{u}_i^m dS \right\} \\ &+ \sum_e \left\{ \int_{\partial\Omega_c^e} t_i^m u_i^c dS + \int_{\partial\Omega_c^e} \frac{1}{2} t_i^c u_i^c dS \right\} \end{aligned} \quad (62)$$

This leads to finite element equations:

$$\delta \begin{Bmatrix} \mathbf{q} \\ \beta \end{Bmatrix}^T \begin{bmatrix} \mathbf{G}_{\alpha q}^T \mathbf{H}_{\alpha\alpha}^{-1} \mathbf{G}_{\alpha q} & \mathbf{G}_{\alpha q}^T \mathbf{H}_{\alpha\alpha}^{-1} \mathbf{G}_{\alpha\beta} \\ \mathbf{G}_{\alpha\beta}^T \mathbf{H}_{\alpha\alpha}^{-1} \mathbf{G}_{\alpha q} & \mathbf{G}_{\alpha\beta}^T \mathbf{H}_{\alpha\alpha}^{-1} \mathbf{G}_{\alpha\beta} + \mathbf{H}_{\beta\beta} \end{bmatrix} \begin{Bmatrix} \mathbf{q} \\ \beta \end{Bmatrix} = \delta \begin{Bmatrix} \mathbf{q} \\ \beta \end{Bmatrix}^T \begin{Bmatrix} \mathbf{Q} \\ \mathbf{0} \end{Bmatrix} \quad (63)$$

where

$$\begin{aligned} \mathbf{G}_{\alpha q} &= \int_{\partial\Omega^e} \mathbf{R}_m^T \tilde{\mathbf{N}}_m dS \\ \mathbf{G}_{\alpha\beta} &= \int_{\partial\Omega_c^e} \mathbf{R}_m^T \mathbf{N}_c dS \\ \mathbf{H}_{\alpha\alpha} &= \int_{\partial\Omega^e + \partial\Omega_c^e} \mathbf{R}_m^T \mathbf{N}_m dS \\ \mathbf{H}_{\beta\beta} &= \int_{\partial\Omega_c^e} \mathbf{R}_c^T \mathbf{N}_c dS \\ \mathbf{Q} &= \int_{S_i^e} \tilde{\mathbf{N}}_m^T \bar{\mathbf{t}} dS \end{aligned} \quad (64)$$

This equation can be further simplified by static-condensation.

When the inclusion is rigid,  $u_i^c$  does not need to be assumed, and we use the following variational principle:

$$\pi_4(\tilde{u}_i^m, u_i^m) = \sum_e \left\{ - \int_{\partial\Omega^e + \partial\Omega_c^e} \frac{1}{2} t_i^m u_i^m dS + \int_{\partial\Omega_m^e} t_i^m \tilde{u}_i^m dS - \int_{S_i^e} \bar{t}_i \tilde{u}_i^m dS \right\} \quad (65)$$

The corresponding finite element equations are:

$$\sum_e (\delta \mathbf{q}^T \mathbf{G}_{\alpha q}^T \mathbf{H}_{\alpha\alpha}^{-1} \mathbf{G}_{\alpha q} \mathbf{q} - \delta \mathbf{q}^T \mathbf{Q}) = 0 \quad (66)$$

When the VC includes a void instead of an elastic/rigid inclusion,  $\tilde{u}_i^c$  is merely assumed at  $\partial\Omega_c^e$ . We have:

$$\tilde{\mathbf{u}}_c = \tilde{\mathbf{N}}_c \gamma \text{ at } \partial\Omega_c^e \quad (67)$$

We use the following variational principle:

$$\begin{aligned} \pi_5(\tilde{u}_i^m, u_i^m, \tilde{u}_i^c) &= \sum_e \left\{ - \int_{\partial\Omega^e + \partial\Omega_c^e} \frac{1}{2} t_i^m u_i^m dS + \int_{\partial\Omega_m^e} t_i^m \tilde{u}_i^m dS - \int_{S_i^e} \bar{t}_i \tilde{u}_i^m dS \right\} \\ &\quad + \sum_e \int_{\partial\Omega_c^e} t_i^m \tilde{u}_i^c dS \end{aligned} \quad (68)$$

The corresponding finite element equations are:

$$\delta \begin{Bmatrix} \mathbf{q} \\ \gamma \end{Bmatrix}^T \begin{bmatrix} \mathbf{G}_{\alpha q}^T \mathbf{H}_{\alpha\alpha}^{-1} \mathbf{G}_{\alpha q} & \mathbf{G}_{\alpha q}^T \mathbf{H}_{\alpha\alpha}^{-1} \mathbf{G}_{\alpha\gamma} \\ \mathbf{G}_{\alpha\gamma}^T \mathbf{H}_{\alpha\alpha}^{-1} \mathbf{G}_{\alpha q} & \mathbf{G}_{\alpha\gamma}^T \mathbf{H}_{\alpha\alpha}^{-1} \mathbf{G}_{\alpha\gamma} \end{bmatrix} \begin{Bmatrix} \mathbf{q} \\ \gamma \end{Bmatrix} = \delta \begin{Bmatrix} \mathbf{q} \\ \gamma \end{Bmatrix}^T \begin{Bmatrix} \mathbf{Q} \\ \mathbf{0} \end{Bmatrix} \quad (69)$$

where

$$\mathbf{G}_{\alpha\gamma} = \int_{\partial\Omega_c^e} \mathbf{R}_m^T \mathbf{N}_c dS \quad (70)$$

Similarly, this equation can be further simplified by static-condensation.

It should be pointed out that TVC-BVPs developed in this section, with ellipsoidal voids/inclusions, are plagued by LBB conditions, because all these multi-field boundary variational principles involve Lagrange multipliers. Similarly, because the VCFEMs developed by Ghosh and his coworkers involve Lagrange multipliers, they are also plagued by LBB conditions. For detailed discussion of LBB conditions, see [Babuska (1973); Brezzi (1974); Rubinstein, Punch and Atluri (1983); Punch and Atluri (1984); Xue, Karlovitz and Atluri (1985); Dong and Atluri (2011a)]. TVC-Cs without involving LBB conditions are developed in section 5.3, by using collocation method to enforce the compatibility between independently assumed fields.

In addition, the VCFEMs developed by Ghosh and his coworkers are based on Hybrid-Stress variational principle of Pian, and involve only equilibrated stresses which are forced to satisfy compatibility conditions through the variational principles. Thus the hybrid-stress VCFEMs of Ghosh et al. involve volume integrals as wells as surface integrals in the development of the stiffness matrices. However, only surface integrals are involved in developing TVC-BVP, as well as the TVC-C in section 5.3. Therefore, TVCs developed in this study are computationally more efficient.

Moreover, the TVCs developed in this study are based on a well-known complete trial displacement field. Therefore, TVCs can obtain more accurate solutions of stress/strains than the VCFEMs developed by Ghosh and his coworkers, because the completeness of Airy and Maxwell stress functions in a multiply connected domain is of question.

### 5.3 Trefftz TVCs Using Collocation and a Primitive Field Boundary Variational Principle

In this section, we develop 3D TVCs with ellipsoidal inclusions/voids using collocation method and a primitive field variational principle, in a similar fashion to its 2D versions as shown in [Dong and Atluri (2012a)], and its 3D version with spherical inclusions/voids in [Dong and Atluri (2012b)].

A finite number of collocation points are selected along  $\partial\Omega^e$  and  $\partial\Omega_c^e$ , denoted as  $x_i^{mp} \in \partial\Omega^e, p = 1, 2, \dots$ , and  $x_i^{cq} \in \partial\Omega_c^e, q = 1, 2, \dots$ .

Collocations are carried out in the following manner:

**1.** When an elastic inclusion is considered, we enforce the following conditions at corresponding collocation points:

$$\begin{aligned} u_i^m(x_j^{mp}, \alpha) &= \tilde{u}_i^m(x_j^{mp}, \mathbf{q}) \quad x_j^{mp} \in \partial\Omega^e \\ u_i^m(x_j^{cq}, \alpha) - u_i^c(x_j^{cq}, \beta) &= 0 \quad x_j^{cq} \in \partial\Omega_c^e \\ wt_i^m(x_j^{cq}, \alpha) + wt_i^c(x_j^{cq}, \beta) &= 0 \quad x_j^{cq} \in \partial\Omega_c^e \end{aligned} \quad (71)$$

$\alpha, \beta$  are related to  $\mathbf{q}$  in the following way:

$$\begin{aligned} \alpha &= \mathbf{C}_{\alpha q}^1 \mathbf{q} \\ \beta &= \mathbf{C}_{\beta q}^1 \mathbf{q} \end{aligned} \quad (72)$$

**2.** When the inclusion is rigid, there is no need to assume  $u_i^c$ , and the following collocations are considered:

$$\begin{aligned} u_i^m(x_j^{mp}, \alpha) &= \tilde{u}_i^m(x_j^{mp}, \mathbf{q}) \quad x_j^{mp} \in \partial\Omega^e \\ u_i^m(\text{non-rigid-body}, x_j^{cq}, \alpha) &= 0 \quad x_j^{cq} \in \partial\Omega_c^e \end{aligned} \quad (73)$$

We obtain:

$$\alpha = \mathbf{C}_{\alpha q}^2 \mathbf{q} \quad (74)$$

**3.** When a void is considered instead of a inclusion, there is no need to assume  $u_i^c$  or  $\tilde{u}_i^c$ . The following conditions are enforced:

$$\begin{aligned} u_i^m(x_j^{mp}, \alpha) &= \tilde{u}_i^m(x_j^{mp}, \mathbf{q}) \quad x_j^{mp} \in \partial\Omega^e \\ wt_i^m(x_j^{cq}, \alpha) &= 0 \quad x_j^{cq} \in \partial\Omega_c^e \end{aligned} \quad (75)$$

By solving (75), we have:

$$\alpha = \mathbf{C}_{\alpha q}^3 \mathbf{q} \quad (76)$$

It should be noted that, in (71) and (75), a parameter  $w$  is used to weigh the collocation equations for tractions, so that they have the same order of importance as collocation equations for displacements. For displacement fields assumed in section 5.1, it is obvious that a proper choice of  $w$  is  $w = a/2G_m$ . It should also be

pointed out that, for the over-determined system of equations obtained using either (71), (73), or (75), the least square solution as discussed in [Dong and Atluri (2012b)] is obtained.

Now that the interior displacement field is related to nodal displacements, finite element equations can be derived from the following primitive-field boundary variational principle:

$$\pi_2(u_i) = \sum_e \left\{ \int_{\partial\Omega^e} \frac{1}{2} t_i u_i dS - \int_{S_i^e} \bar{t}_i u_i dS \right\} \quad (77)$$

Substituting corresponding displacement fields into (77), we obtain finite element equations:

$$\sum_m (\delta \mathbf{q}^T \mathbf{C}_{\alpha q}^s{}^T \mathbf{M}_{\alpha\alpha} \mathbf{C}_{\alpha q}^s \mathbf{q} - \delta \mathbf{q}^T \mathbf{Q}) = 0, \quad s = 1, 2 \text{ or } 3 \quad (78)$$

$$\mathbf{M}_{\alpha\alpha} = \int_{\partial\Omega^e} \mathbf{R}_m^T \mathbf{N}_m dS$$

When  $s$  is equal to 1, 2, and 3,  $\mathbf{C}_{\alpha q}^s{}^T \mathbf{M}_{\alpha\alpha} \mathbf{C}_{\alpha q}^s$  is the stiffness matrix for TVCs with an elastic inclusion, a rigid inclusion, and a void respectively.

Because in the development of TVC-C, integration of only one matrix  $\mathbf{M}_{\alpha\alpha}$  along the outer boundary is needed, and collocation along the inner boundary require less points where the Trefftz trial functions are evaluated, TVC-C is expected to be computationally more efficient than TVC-BVP. Also, as explained previously, TVC-C does not suffer from LBB conditions, which is a tremendous advantage of TVC-C over TVC-BVP.

## 6 Numerical Examples

Firstly, we illustrate the reason why we use characteristic lengths to scale the Trefftz trial functions. See Fig. 5 for the geometry of the VC. Material properties of the matrix are  $E_m = 1, \nu_m = 0.25$ . Three kinds of heterogeneities are considered: an elastic inclusion with  $E_c = 2, \nu_c = 0.3$ , a rigid inclusion, and a void. Stiffness matrices of TVC-C are computed, with and without using characteristic lengths to scale Trefftz trial functions. Condition numbers of the coefficient matrix of equations (71)(73)(75) are shown in Tab. 1. We can clearly see that by scaling the Trefftz functions using characteristic lengths, the resulting systems of equations have significantly smaller condition number. Although not shown here, scaling Trefftz trial functions using characteristic lengths also has similar effect on TVC-BVP.

We also compare the CPU time required for computing the stiffness matrix of the VC shown in Fig. 5, using different TVCs. The CPU time required is shown in

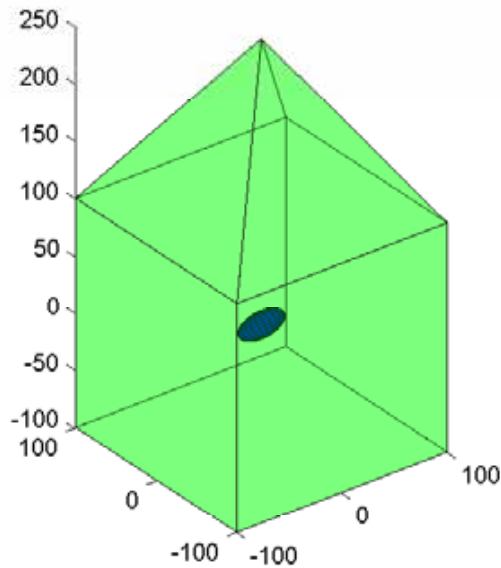


Figure 5: A VC with an ellipsoidal inclusion/void used for condition number test, eigenvalue test, and patch test

Table 1: Condition number of coefficient matrices of equations used to relate  $\alpha, \beta$  to  $\mathbf{q}$  using the collocation method with/without using characteristic lengths to scale Trefftz Trial functions for the VC shown in Fig. 5

|                       | Elastic Inclusion  |                      | Rigid Inclusion   |                      | Void              |                      |
|-----------------------|--------------------|----------------------|-------------------|----------------------|-------------------|----------------------|
| Characteristic Length | Scaled             | Not scaled           | Scaled            | Not scaled           | Scaled            | Not scaled           |
| Condition number      | $1.31 \times 10^3$ | $2.3 \times 10^{31}$ | $2.1 \times 10^3$ | $3.3 \times 10^{31}$ | $3.1 \times 10^3$ | $2.5 \times 10^{31}$ |

Tab. 2. As can be seen, TVC-C needs less time for computing one VC than that for TVC-BVP. The computational time for either of these two types of TVCs should

be much less than VCFEMs developed in [Ghosh and Moorthy (2004)], although a non-optimized MATLAB code is used for computation.

Table 2: CPU time required for computing the stiffness matrix of the VC in Fig. 7

| CPU Time<br>(seconds) | TVC-BVP | TVC-C |
|-----------------------|---------|-------|
|                       | 15.5    | 10.1  |

Using the same VC, we compute the eigenvalues of stiffness matrices of different TVCs. This is conducted in the original and rotated global Cartesian coordinate system. Experimental results are shown in Tab. 3-5

As can clearly be seen, these VCs are stable and invariant, because additional zero energy modes do not exist, and eigenvalues do not vary with respect to change of coordinate systems. However, this does not mean that LBB conditions are satisfied by TVC-BVP for an arbitrary Voronoi Cell

We also conduct the patch test. The same VC is considered. The materials of the matrix and the inclusion are the same, with material properties  $E = 1, \nu = 0.25$ . A uniform traction is applied to the upper faces. The displacements in the lower face are prescribed to be the exact solution.

The exact solution is:

$$\begin{aligned}
 u_1 &= -\frac{P\nu}{E}x_1 \\
 u_2 &= -\frac{P\nu}{E}x_2 \\
 u_3 &= \frac{P}{E}x_3
 \end{aligned} \tag{79}$$

The numerical result of different VCs is shown in Tab. 6, with error defined as:

$$Error = \frac{\|\mathbf{q} - \mathbf{q}^{exact}\|}{\|\mathbf{q}^{exact}\|} \tag{80}$$

As can be seen, TVC-BVP can pass the patch test with errors equal to or less than an order of  $10^{-7}$ . Although the error for TVC-C is larger, but still in an order of  $10^{-3}$ . We consider the performance of all TVCs to be satisfactory in this patch test.

In order to evaluate the overall performances of different TVCs for modeling problems with inclusions or voids, we consider the following problem: an infinite medium with an ellipsoidal elastic/rigid inclusion or void in it. Exact solution of all

Table 3: Eigenvalues of stiffness matrices of different TVCs when an elastic inclusion is considered

| Eigenvalues<br>Rotation=0°&45° | TVC-BVP  | TVC-C    |
|--------------------------------|----------|----------|
| 1                              | 234.0298 | 234.7411 |
| 2                              | 108.8477 | 110.2444 |
| 3                              | 108.1132 | 109.1381 |
| 4                              | 84.1480  | 84.4025  |
| 5                              | 84.1361  | 84.3963  |
| 6                              | 83.5074  | 77.0706  |
| 7                              | 62.6870  | 61.6714  |
| 8                              | 61.6146  | 60.5611  |
| 9                              | 60.0356  | 60.1607  |
| 10                             | 60.0351  | 60.1564  |
| 11                             | 55.2950  | 53.7224  |
| 12                             | 54.0791  | 52.9699  |
| 13                             | 54.0783  | 52.9693  |
| 14                             | 50.3029  | 50.4278  |
| 15                             | 29.8491  | 29.6434  |
| 16                             | 25.1172  | 25.4681  |
| 17                             | 25.1168  | 25.4678  |
| 18                             | 19.1535  | 18.3437  |
| 19                             | 19.1508  | 18.3437  |
| 20                             | 16.9186  | 17.3702  |
| 21                             | 12.1886  | 13.2283  |
| 22                             | 0.0000   | 0.0000   |
| 23                             | 0.0000   | 0.0000   |
| 24                             | 0.0000   | 0.0000   |
| 25                             | 0.0000   | 0.0000   |
| 26                             | 0.0000   | 0.0000   |
| 27                             | 0.0000   | 0.0000   |

Table 4: Eigenvalues of stiffness matrices of different TVCs when a rigid inclusion is considered

| Eigenvalues<br>Rotation=0°&45° | TVC-BVP  | TVC-C    |
|--------------------------------|----------|----------|
| 1                              | 234.3199 | 235.0434 |
| 2                              | 109.0337 | 110.4286 |
| 3                              | 108.3032 | 109.3291 |
| 4                              | 84.3204  | 84.5869  |
| 5                              | 84.2409  | 84.5144  |
| 6                              | 83.5379  | 77.1085  |
| 7                              | 62.7570  | 61.6943  |
| 8                              | 61.6410  | 60.5849  |
| 9                              | 60.0685  | 60.2163  |
| 10                             | 60.0628  | 60.2009  |
| 11                             | 55.3055  | 53.7417  |
| 12                             | 54.0904  | 52.9710  |
| 13                             | 54.0860  | 52.9706  |
| 14                             | 50.3309  | 50.4484  |
| 15                             | 29.8729  | 29.6766  |
| 16                             | 25.1264  | 25.4732  |
| 17                             | 25.1251  | 25.4720  |
| 18                             | 19.1552  | 18.3436  |
| 19                             | 19.1510  | 18.3435  |
| 20                             | 16.9205  | 17.3723  |
| 21                             | 12.1893  | 13.2290  |
| 22                             | 0.0000   | 0.0000   |
| 23                             | 0.0000   | 0.0000   |
| 24                             | 0.0000   | 0.0000   |
| 25                             | 0.0000   | 0.0000   |
| 26                             | 0.0000   | 0.0000   |
| 27                             | 0.0000   | 0.0000   |

Table 5: Eigenvalues of stiffness matrices of different TVCs when a void is considered

| Eigenvalues<br>Rotation=0°&45° | TVC-BVP  | TVC-C    |
|--------------------------------|----------|----------|
| 1                              | 233.5479 | 233.3206 |
| 2                              | 108.7508 | 108.7786 |
| 3                              | 108.0065 | 107.8411 |
| 4                              | 87.1961  | 86.1117  |
| 5                              | 84.2842  | 84.1957  |
| 6                              | 84.2553  | 84.1538  |
| 7                              | 64.2478  | 64.6534  |
| 8                              | 61.9575  | 61.7710  |
| 9                              | 60.6613  | 59.6460  |
| 10                             | 60.6404  | 59.6236  |
| 11                             | 57.5684  | 55.6119  |
| 12                             | 57.5653  | 55.6104  |
| 13                             | 56.4398  | 55.1562  |
| 14                             | 51.0058  | 51.3416  |
| 15                             | 30.2436  | 30.0702  |
| 16                             | 25.4234  | 26.2632  |
| 17                             | 25.4185  | 26.2587  |
| 18                             | 19.8318  | 18.6557  |
| 19                             | 19.8309  | 18.6548  |
| 20                             | 17.2973  | 18.3053  |
| 21                             | 12.5848  | 12.2776  |
| 22                             | 0.0000   | 0.0000   |
| 23                             | 0.0000   | 0.0000   |
| 24                             | 0.0000   | 0.0000   |
| 25                             | 0.0000   | 0.0000   |
| 26                             | 0.0000   | 0.0000   |
| 27                             | 0.0000   | 0.0000   |

Table 6: Performances of different TVCs in patch test

| Error | TVC-BVP              | TVC-C                |
|-------|----------------------|----------------------|
|       | $3.6 \times 10^{-7}$ | $5.6 \times 10^{-3}$ |

of these three problems found using Eshelby's solution and the equivalent inclusion method. For details of the exact solution, see [Eshelby (1957); Nemat-Nasser and Hori (1999)].

The material properties of the matrix are  $E_m = 1, v_m = 0.25$ . When an elastic inclusion is considered, the material properties of the inclusion are  $E_c = 2, v_c = 0.3$ . The magnitude of the remote tension  $P$  in the direction of  $x_3$  is equal to 1. The semi-axes of the ellipsoid are 1/5, 1/7.5, 1/10 respectively. For numerical implementation, the infinite medium is truncated to a finite cube. The length of each side of the truncated cube is equal to 2. For all three cases with an elastic/rigid inclusion or a void, only one VC is used. Traction boundary conditions are applied to the outer-boundary of the VC. Least number of nodal displacements are prescribed to the exact solution.

We compare the computed  $\sigma_{11}$  along axis  $x_3$ ,  $\sigma_{33}$  along axis  $x_1$ , to that of the exact solution. As shown in Fig. 7-9, no matter an elastic inclusion, a rigid inclusion, or a void is considered, TVCs always give very accurate computed stresses, even though only one VC is used. For this reason, we consider TVCs very efficient for micromechanical modeling of heterogeneous materials.

We also use the TVCs developed in this study to study the stiffness of heterogeneous materials. A Unit Cell model of Al/SiC material is considered. The material properties are:  $E_{Al} = 74GPa, v_{Al} = 0.33, E_{SiC} = 410GPa, v_{SiC} = 0.19$ . The volume fraction of SiC is 20%. This model was studied in [Chawla, Ganesh, Wunsch (2004)], using around 76,000 ten-node tetrahedral elements with ABAQUS. However, in this study, we use just one TVC, see in Fig. 10. The TVCs developed in [Dong and Atluri(2012b)] was used to study this Unit Cell model with a spherical inclusion. For the TVCs developed in this study, a quasi-sphere with aspect ratios 1.1:1.05:1.0 is used as the inclusion. As shown in Tab. 7, although only one VC is used, the homogenized Young's modulus is quite close to what is obtained by using round 76,000 ten-node tetrahedral elements with ABAQUS.

We also study a RVE of Al/SiC material, with 125 randomly distributed ellipsoidal

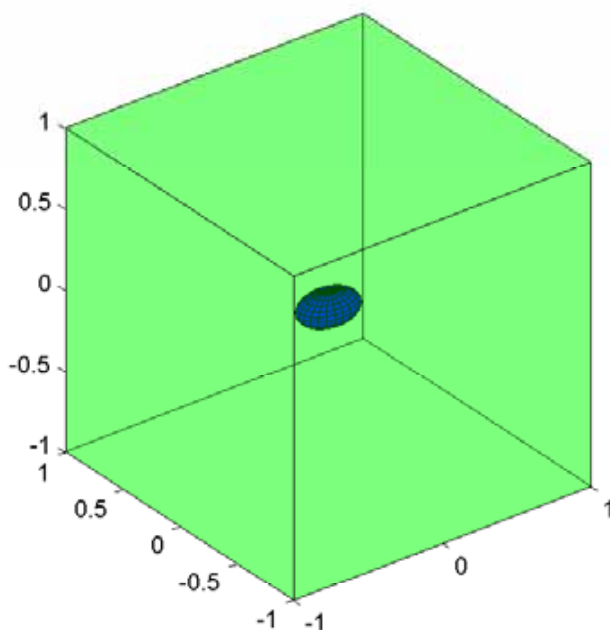


Figure 6: An ellipsoidal elastic/rigid inclusion or hole under remote tension

SiC particles. The RVE is shown in Fig. 11, discretized with 125 TVCs developed in this study. The material properties of Al and SiC are taken the same as those in the last example. The size of the RVE is  $100\ \mu\text{m} \times 100\ \mu\text{m} \times 100\ \mu\text{m}$ . A uniform tensile stress of  $100\ \text{MPa}$  is applied in the  $x_3$  direction. Both TVC-BVP and TVC-C are used to study the microscopic stress distribution in the RVE. However, because very similar results are obtained by these two types of TVCs, only the results obtained by TVC-BVP are shown here. The maximum principal stress is plotted in Fig. 12, and the strain energy density is shown in Fig. 13. While the inclusions are presenting a relative uniform stress state, the maximum principal stress and the strain energy density in the matrix material show high concentration. To be more specific, high stress and strain energy concentration is observed near the tip of the long axes of the inclusions, and in the direction which is parallel to the direction of loading. On the other hand, in the direction which is perpendicular to the direction of loading, very low stress values and strain energy density are observed. This gives us the idea at where damages are more likely to initiate and develop, for materials reinforced by stiffer particles.

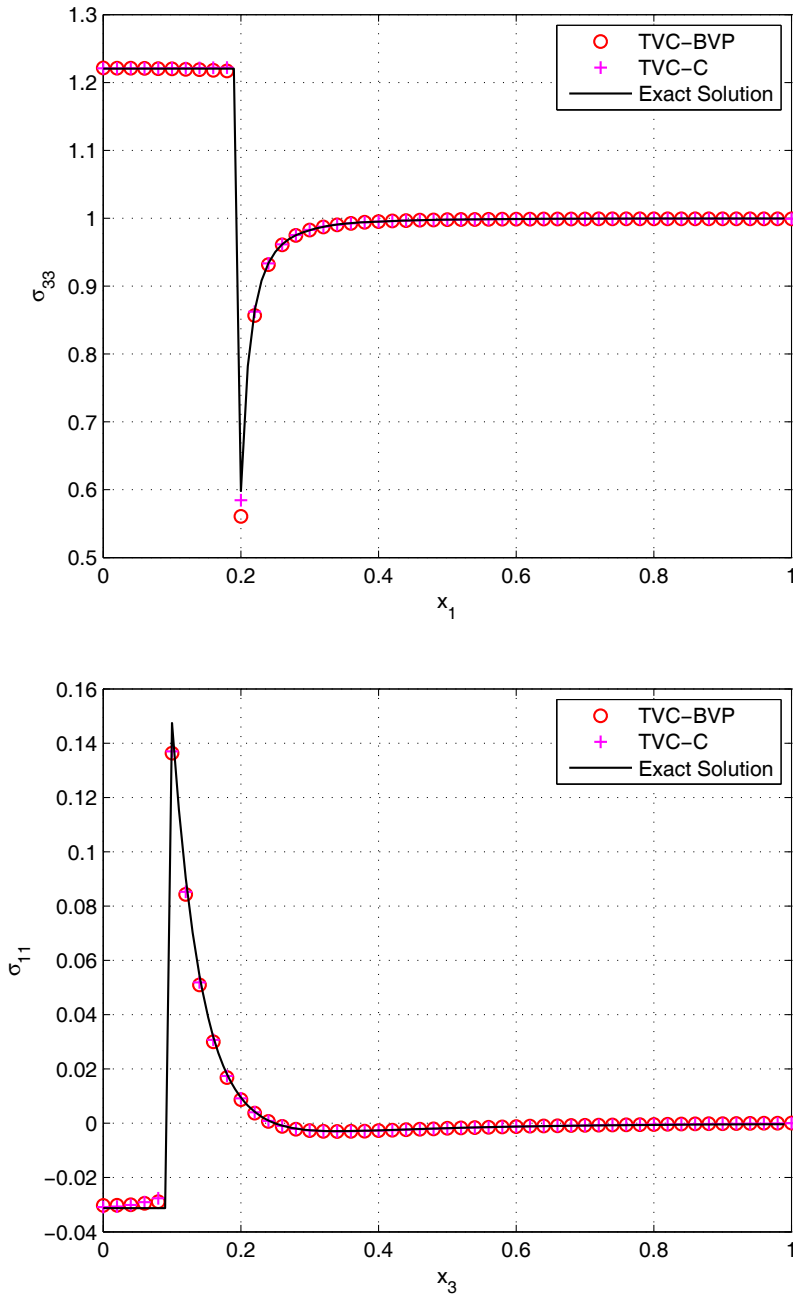


Figure 7: Computed  $\sigma_{11}$  along axis  $x_3$ ,  $\sigma_{33}$  along axis  $x_1$  for the problem with an elastic inclusion

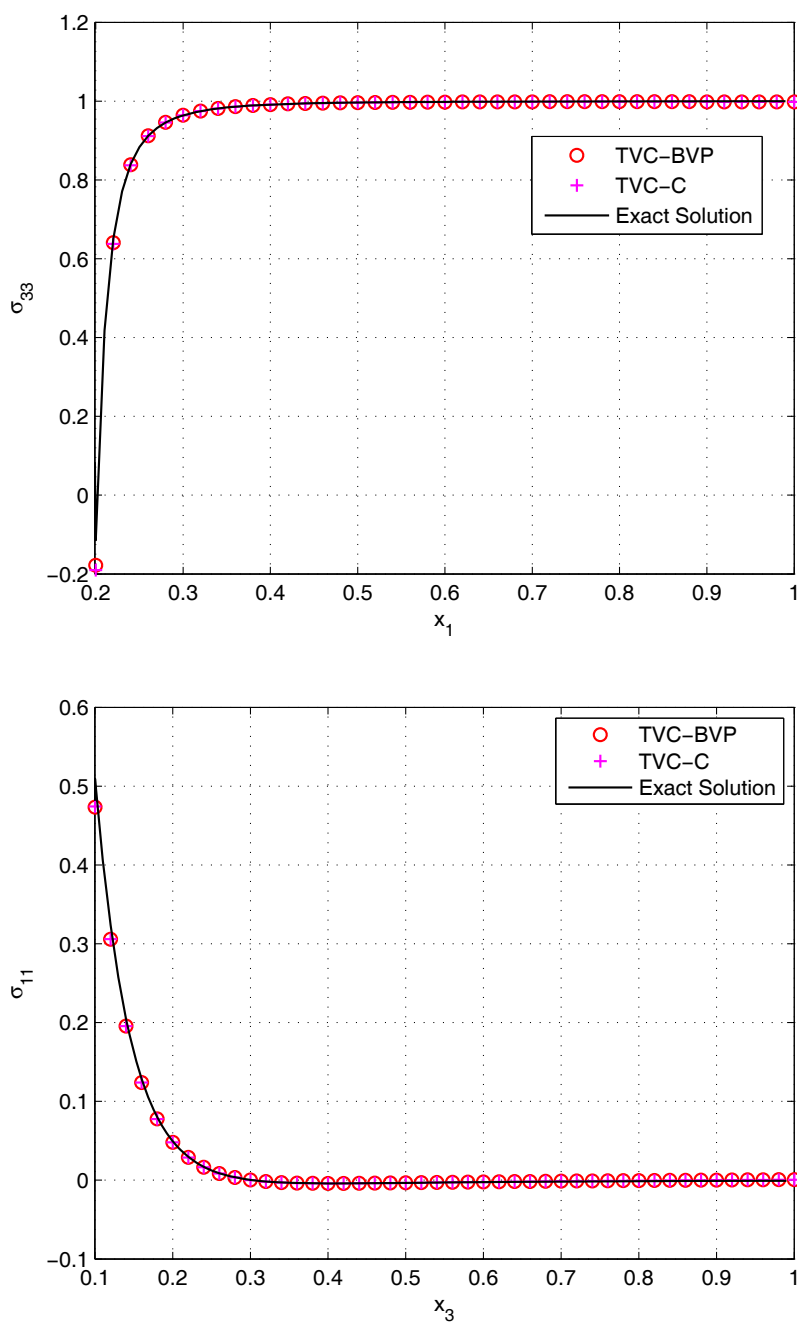


Figure 8: Computed  $\sigma_{11}$  along axis  $x_3$ ,  $\sigma_{33}$  along axis  $x_1$  for the problem with a rigid inclusion

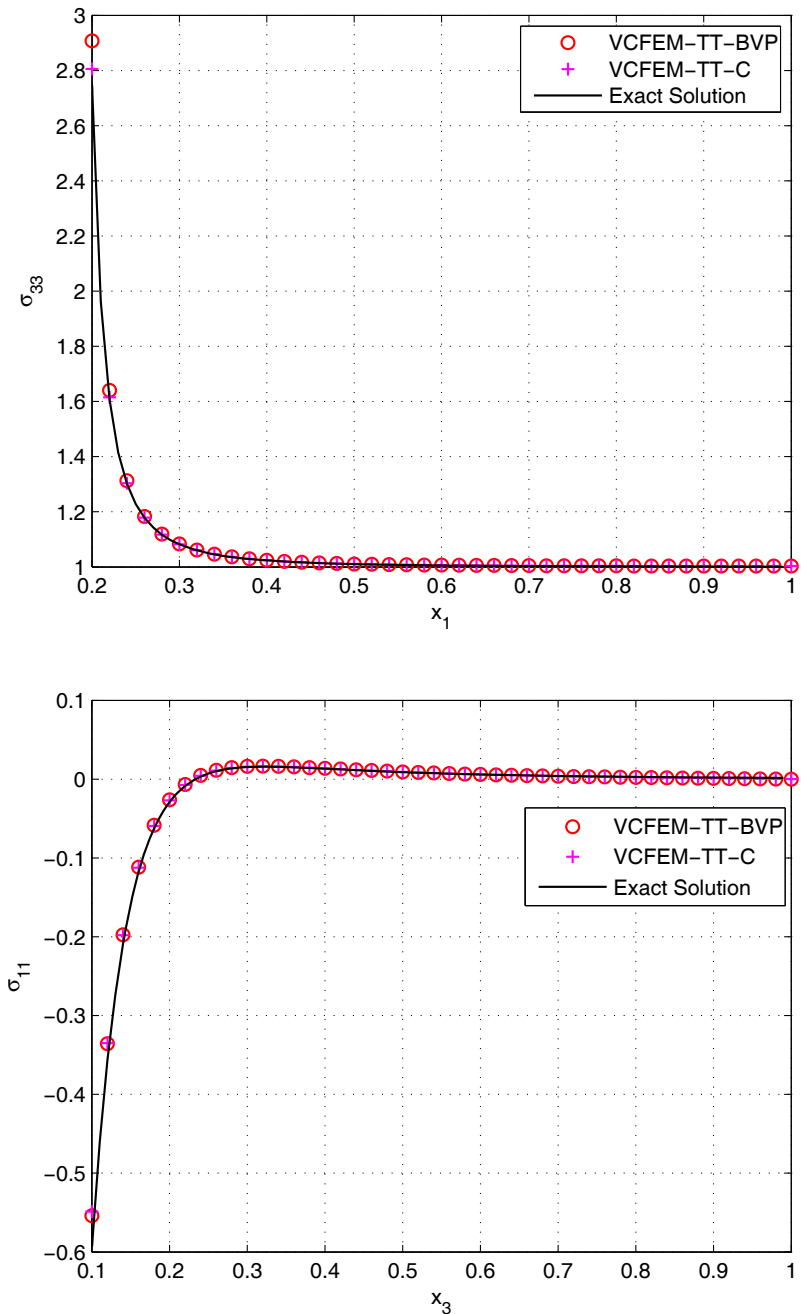


Figure 9: Computed  $\sigma_{11}$  along axis  $x_3$ ,  $\sigma_{33}$  along axis  $x_1$  for the problem with a void

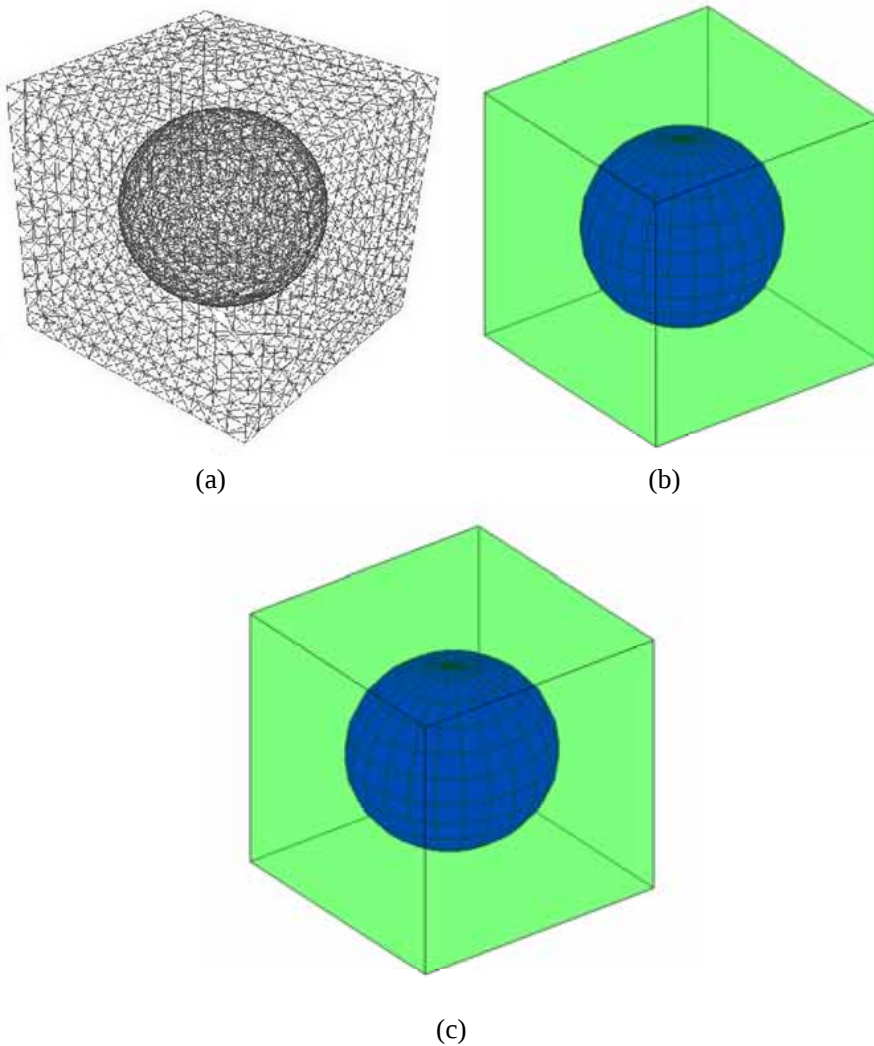


Figure 10: The mesh of an Al/SiC Unit Cell model using: (a) around 76,000 ten-node tetrahedral elements with ABAQUS in the study of [Chawla, Ganesh, Wunsch (2004)]; (b) one TVC with a spherical inclusion; (c) one TVC with a quasi-sphere ellipsoidal inclusion

Table 7: Homogenized Young's modulus using different methods

| Method              | Young's Modulus (GPa) |
|---------------------|-----------------------|
| TVC-BVP (sphere)    | 103.8                 |
| TVC-C (sphere)      | 98.8                  |
| TVC-BVP (ellipsoid) | 102.8                 |
| TVC-C (ellipsoid)   | 98.3                  |
| ABAQUS              | 100.0                 |

We also use the same RVE as shown in Fig. 11, to study porous PZT ceramic material. The RVE includes 125 ellipsoidal voids. The material properties of the matrix material are:  $E = 165\text{GPa}$ ,  $\nu = 0.22$ . Only the results obtained by TVC-BVP are shown here. The maximum principal stress is plotted in Fig. 14, and the strain energy density is shown in Fig. 15. The stress and energy density concentration is showing a different pattern as the Al/SiC material, of which SiC particles are stiffer inclusions. For PZT material with ellipsoidal pores, high stress and strain energy density concentration is observed near the long axes of the cavities, and in the direction which is perpendicular to the direction of loading. On the other hand, in the direction which is parallel to the direction of loading, very low stress values and strain energy density are observed. This gives us the idea at where damage is more likely to initiate and develop for porous materials.

## 7 Conclusions

Three-dimensional Trefftz Voronoi Cells (TVCs) with ellipsoidal inclusions/voids, are developed. For each VC, a compatible displacement field along the VC outer-boundary is assumed, with Barycentric coordinates as nodal shape functions. Independent displacement fields in the VC are assumed as characteristic-length-scaled Trefftz trial functions. Papkovitch-Neuber solution is used to construct the Trefftz trial displacement fields. The Papkovitch-Neuber potentials are linear combinations of ellipsoidal harmonics. Two approaches are used alternatively to develop stiffness

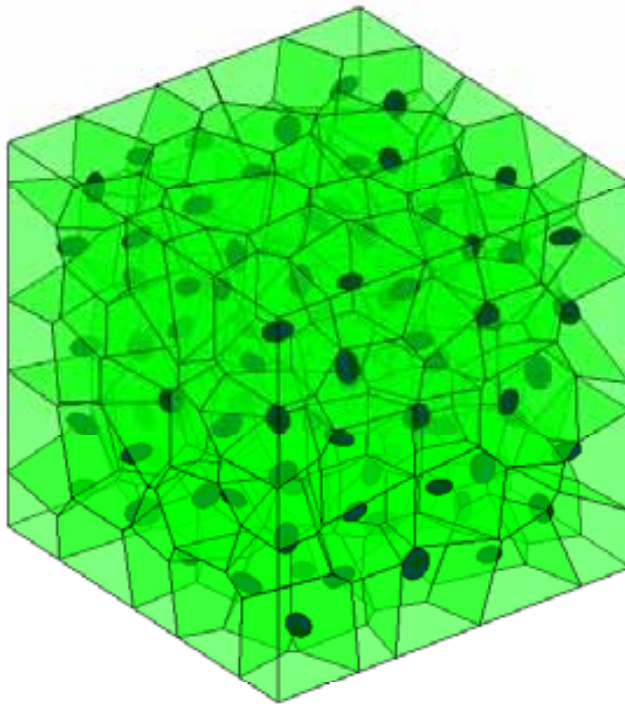


Figure 11: A RVE with 125 ellipsoidal inclusions/voids

matrices. TVC-BVP uses multi-field boundary variational principles to enforce all the conditions in a variational sense. TVC-C uses the collocation method to relate independently assumed displacement fields to nodal displacements, and develop a linear system of equations based on a primitive-field boundary variational principle. Through numerical examples, we demonstrate that TVCs developed in this study can capture the stress concentration around ellipsoidal voids/inclusion quite accurately, and the time needed for computing each VC is much less than that for the hybrid-stress version of TVCs in [Ghosh and Moorthy (2004)]. TVCs developed in this study are also used to estimate the overall material properties of heterogeneous materials, as well as to compute the microscopic stress distribution. It is observed that, for composite materials with stiffer second-phase inclusions, high stress concentration in the matrix is shown near the long axis of the inclusion, in the direction of which is parallel to the direction of loading. However, for materials with ellipsoidal cavities, high stress concentration is observed in the direction which is perpendicular to the direction of loading.

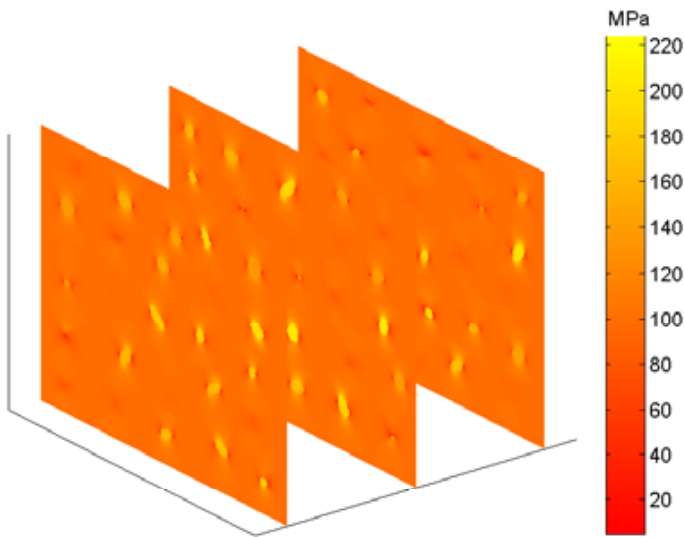


Figure 12: Distribution of maximum principal stress in the RVE of Al/SiC material modeled by 125 TVC-Cs, each VC includes an ellipsoidal inclusion

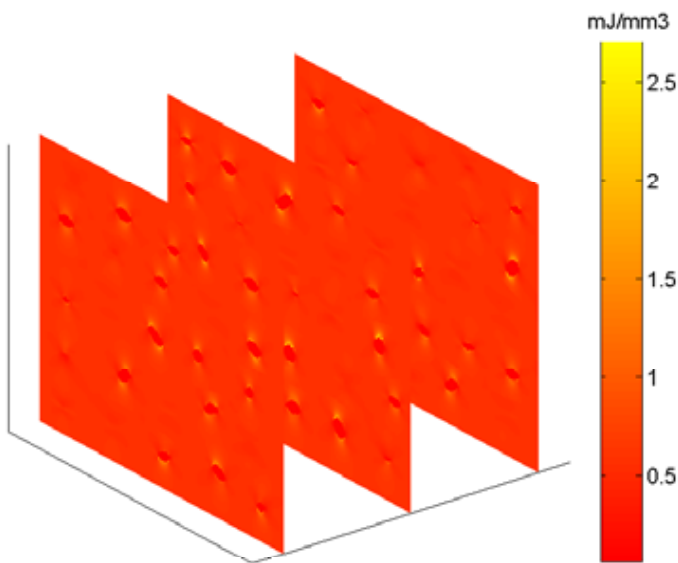


Figure 13: Distribution of strain energy density in the RVE of Al/SiC material modeled by 125 TVC-Cs, each VC includes an ellipsoidal inclusion

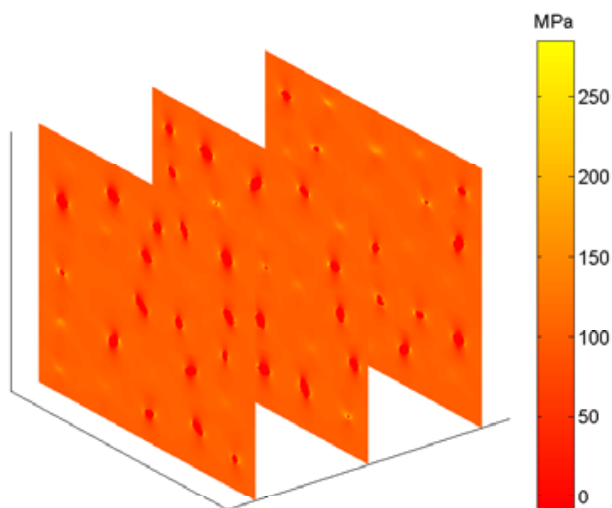


Figure 14: Distribution of maximum principal stress in the RVE of porous PZT ceramic material modeled by 125 TVC-Cs, each VC includes an ellipsoidal void

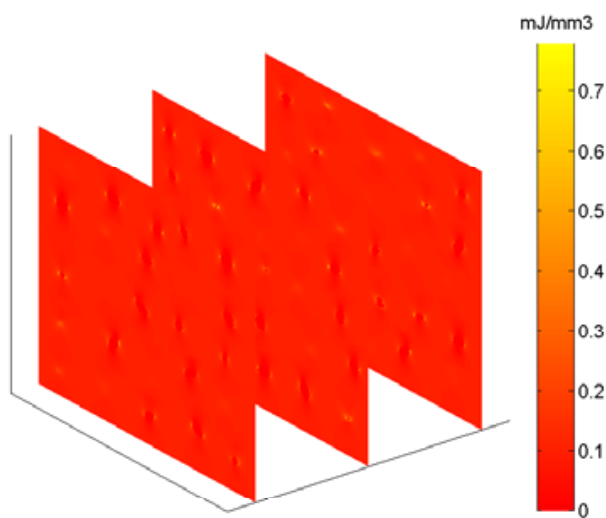


Figure 15: Distribution of strain energy density in the RVE of porous PZT ceramic material modeled by 125 TVC-Cs, each VC includes an ellipsoidal void

Because of their accuracy and efficiency, we consider that the 3D TVCs developed in this study are suitable for micromechanical modeling of heterogeneous materials. Moreover, because they can efficiently and accurately capture the micro-scale stress distribution around inclusions/voids, they can be used to study the damage of materials, in combination of tools to model micro-crack initiation and fatigue.

We also would like to point out that, 3D TVCs with arbitrary shaped voids/inclusions will be presented in future studies.

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