A Constructive Approach for Heterogeneous Material Modeling and Analysis

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ABSTRACT

In this paper, we apply the Constructive Solid Analysis (CSA) method developed recently to heterogeneous material modeling and analysis. The key idea in the methodology is that the hierarchy in the description of the geometry is mirrored by an identical hierarchy in the analysis fields guided by the appropriate governing equations. It is shown that the method is ideal for handling the multi-phases in the heterogeneous material microstructure, especially when the microstructure is subject to iterative change which, arises during microstructure design. The effective elastic properties of various 2D composites and porous material microstructures, including random microstructures, are evaluated to verify the procedure. The results are in good agreement with those obtained using the finite element method.

Keywords: heterogeneous material, composites, porous material, constructive solid geometry, constructive solid analysis.

1. INTRODUCTION

Heterogeneous materials such as porous materials, fiber reinforced composites and particle reinforced composites have been used extensively in engineering applications due to their excellent properties. Typically, the analysis of these materials is through the decomposition of the problem into a macro-scale problem and a micro-scale problem based on the assumption that there exists a Representative Volume Element (RVE) that can describe the periodic microstructure. The effective properties are determined by a homogenization procedure. The heterogeneous structure is then replaced by an equivalent homogeneous material having the calculated effective properties. The analytical/semi-analytical models, such as the self consistent model, for determining the effective properties often yield inaccurate results when the volume fractions of second phase are high or the difference between the properties of the second phase and the matrix is large. This is due to the fact that the analytical model considers the volume fractions of the various phases in the material and ignores the detailed microstructure of the material. To overcome the limitations of analytical methods, the finite element method is applied with either a unit cell representation (see for example [17]) or homogenization theory [2],[5] to solve the microscale problem. The homogenization theory is known to give more accurate results than the unit cell method [6], but the unit cell method is more popular due to its simplicity, adequate accuracy for most applications and compatibility with the existing finite element software.

The material microstructure design is an inverse homogenization problem that seeks optimized microstructure of the material to achieve given property values. In the literature, the design of the microstructure of the heterogeneous material is in general formulated as a topology optimization of the RVE. [4],[8],[13],[16] The microstructure obtained through topology optimization may be very complex, and therefore very difficult to manufacture. Very few studies have addressed shape optimal design at microscale. Thus, at present there appear to be no solutions to the problem of determining the optimal position, shape, size and orientation of inclusions or voids in a matrix to achieve a required effective property.

A critical computational challenge to microstructure design is the need for iterative changes to the geometry and position of the microstructural phases such as inclusions and voids followed by reanalysis. The conventional finite element analysis procedure is poorly integrated with the design problem and, the design techniques don't take cognizance of the analysis problem; they assume that an efficient analysis procedure exists to evaluate any design regardless of the complexity of the design. If the finite element method were to be applied to analyze and thereby design the

microstructure, they would require a large number of elements to capture the rapidly changing fields in the microstructure due to the heterogeneity, which results in a high computational cost. This is even worse during microstructure design, which requires iterative modification of the microstructures until the optimal one is determined. Any changing of the microstructure, such as resizing or relocating the particles, often needs a re-meshing of the whole microstructure and a complete re-analysis.

In this paper, we apply a recently developed hierarchical analysis method termed Constructive Solid Analysis (CSA) [12] to heterogeneous material modeling and analysis. Firstly, we describe the CSA method. The key idea in the methodology is that the hierarchy in the description of the geometry is mirrored by an identical hierarchy in the analysis fields guided by the appropriate governing equations. The method is implemented with a NURBS based meshless, field discretization. We then apply the method to model and analyze microstructures of heterogeneous material. It is shown that the Boolean operations implemented in the CSA procedure can very naturally handle changes in size and locations of the inclusions and voids in the heterogeneous material microstructures. The developed methodology is finally verified by evaluating the effective elastic properties of various 2D composites and porous material microstructures, including random microstructures.

2. CONSTRUCTIVE SOLID ANALYSIS

At the present time, a naturally hierarchical procedure, namely Constructive Solid Geometry (CSG) is well established for the creation of geometry [10],[15]. The constructive procedure describes a complex object through Boolean operations on the primitives. But, the analysis (commonly through the finite element method) is carried out only on the final geometry, in other words, the discretized analysis fields such as displacement fields are defined over the complex design domain. Therefore, a change in the geometry of even one primitive necessitates the reconstruction of the final geometry and remeshing of the final geometry.

The CSA method achieves an integration of design and analysis by emulating (during analysis) the hierarchical procedure used in Constructive Solid Geometry. The analysis on the final complex entity is decomposed into analyses on simple primitives. Since the analysis is carried out on the fields defined over the primitives, modifications to the final geometry do not require remeshing of the final geometry. A brief description of the CSA algorithm is presented in the following subsection. A more detailed description of the methodology can be found in [11],[12].

2.1 Problem statement

The boundary value problem formulated through CSA is defined as follows:

Given:

Design domain Ω,

Design boundary Γ,

Boundaries Γ_t and Γ_u

Boundary conditions on fields u and t as $u_{\Gamma_u} = \tilde{u}$ and $t_{\Gamma_t} = \tilde{t}$

Find:

Field variable $\tilde{u}_\Omega$ over the domain Ω

Such that:

$u = \{u_1, u_2, \cdots, u_n\}$, where $u_i, i = 1, \cdots, n$ are fields defined over the primitives Ω_i constituting the final geometry and $\{\}$ refers to the set operations on all u_i constituting u. The domains Ω_i satisfy the property $\Omega = \Omega_1 * \Omega_2 * \cdots * \Omega_n$, where $*$ represents a regularized Boolean operation:

$\bigcup$ (Union), $\bigcap$ (Intersection), and $-$ (Subtraction)

Subject to:

Field variable displacement u or traction t constraints across primitive interfaces.

2.2 Algorithm Outline

An outline of the algorithmic steps involved in the analysis procedure are as follows:

1. From the geometry construction step, determine n primitives $\Omega_i, i = 1, \cdots, n$, such that $\Omega = \Omega_1 * \Omega_2 * \cdots * \Omega_n$.
2. Given Ω_i and the Boolean operations on them, determine Γ in terms of the boundaries of each primitives
3. Formulate the mechanics (boundary value) problem
   a) Form individual boundary value problem for each Boolean operation
   b) Combine to formulate the system level analysis problem
4. For each Ω_i, discretize the field over the domain
5. Form the matrix system for system level solution.
6. Solve

2.3 Governing Equations

The balance of mechanical energy for a static system (neglecting the kinetic energy term) in the rate form is:

$$\dot{W} = P_E \tag{1}$$

where,

$$\dot{W} = \int_\Omega \sigma \dot{\varepsilon} d\Omega \tag{2}$$

$$P_E = \int_\Gamma t\dot{u} d\Gamma + \int_\Omega b\dot{u} d\Omega \tag{3}$$

are the rate of internal energy and the power of external work respectively.

For the union problem, the balance of mechanical energy for the static problem can be stated as:

$$\begin{aligned} W_{P-Q} &= P_{E_{P-Q}} \\ W_{Q-P} &= P_{E_{Q-P}} \\ W_{P\cap Q} &= P_{E_{P\cap Q}} \end{aligned} \tag{4}$$

Since the analysis is carried out on the primitives rather than the final geometry, the field associated with the complex entity needs to be defined in terms of the fields associated with the primitives. Thus, a key to the CSA method is the definition of the field over the composite entity in terms of primitives as (see Figure 1):

$$u_{P\cup Q} = u_P \cup u_Q = \begin{cases} u_P & \text{in } \Omega_{P-Q} \\ u_{P\cap Q} = c_P u_P + c_Q u_Q & \text{in } \Omega_{P\cap Q} \\ u_Q & \text{in } \Omega_{Q-P} \end{cases} \tag{5}$$

Here, c_P, c_Q are constants to be selected and u_P and u_Q are the field definitions for the domains P and Q respectively. It can be shown that

$$\begin{aligned} c_P + c_Q &= 1 \\ 0 \le c_P, c_Q &\le 1 \end{aligned} \tag{6}$$

Since the balance of mechanical energy is satisfied at every instant, and since it is required for the power of external work at the boundaries of $\Omega_{P\cap Q}$ to be equal and opposite to that at the corresponding boundaries of Ω_{P-Q} and Ω_{Q-P}, an approximate statement can be constructed as:

$$\min \int_0^{\tau_0} (\dot{W}_{P-Q} + \dot{W}_{P\cap Q} + \dot{W}_{Q-P} - \int_{\Gamma_{PoutQ}} t_P \dot{u}_P d\Gamma - \int_{\Gamma_{QoutP}} t_Q \dot{u}_Q d\Gamma) d\tau$$

$$\text{Subject to: } \begin{aligned} u_{P\cap Q} &= u_P \quad \text{on } \Gamma_{QinP} \\ u_{P\cap Q} &= u_Q \quad \text{on } \Gamma_{PinQ} \end{aligned} \tag{7}$$

where τ is the time step duration. The body force has been neglected for simplicity.

We consider the intersection problem as a special case of subtraction problem: $P \bigcap Q = P - (P - Q)$. For the subtraction problem, the intersection region Ω_{P-Q} is eliminated:

$$\dot{W}_{P\cap Q} = 0 = P_{E_{P\cap Q}} \tag{8}$$

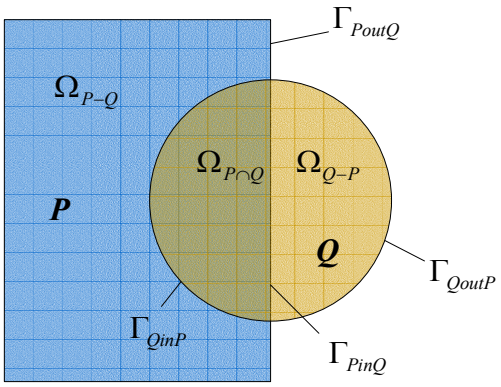

Figure 1. The definitions of domains and boundaries for the Boolean operation.

Carrying out the time integration, we get the governing equations for linear elastic static case in variational form. For a generalized union problem involving two overlapping primitives P and Q, the variational problem can be stated as:

$$\min W_{P-Q} + W_{P\cap Q} + W_{Q-P} - \int_{\Gamma_{PoutQ}} t_P u_P d\Gamma - \int_{\Gamma_{QoutP}} t_Q u_Q d\Gamma$$

$$\text{Subject to } \begin{aligned} u_{P\cap Q} &= u_P \quad \text{on } \Gamma_{QinP} \\ u_{P\cap Q} &= u_Q \quad \text{on } \Gamma_{PinQ} \end{aligned} \tag{9}$$

The variational statement for the subtraction problem can similarly be written as:

$$\min W_P - \int_{\Gamma_{PoutQ}} t_P u_P d\Gamma - \int_{\Gamma_{QoutP}} t_Q u_Q d\Gamma$$

$$\text{Subject to } W_{P\cap Q} = 0 \tag{10}$$

The details of the procedure can be found in [12]. Note that this approach is philosophically and fundamentally different from domain decomposition techniques for parallel finite element analysis (see for example [3]). The goal in domain decomposition approaches is to decompose a mesh defined over the domain into sub-meshes for parallel solution and therefore these procedures do not address the challenge of analyzing iteratively changing geometries.

2.4 NURBS Discretization

The CSA procedure is independent of the discretization scheme employed for numerical solution. In our implementation, a NURBS (Non-Uniform Rational B-Spline) representation is used to define the primitive geometries as well as the analysis fields and material fields defined on the primitives. NURBS are currently the most general mathematical representation available for parametric curves and surfaces. Due to the efficiency of its polynomial basis, NURBS can represent complex geometries with a very small number parameters [14]. A NURBS surface is defined as:

$$\mathbf{S}(u,v)=\sum_{i=0}^{n}\sum_{j=0}^{m}\frac{N_{i,p}(u)N_{j,q}(v)}{\sum_{i=0}^{n}\sum_{j=0}^{m}N_{i,p}(u)N_{j,q}(v)w_{ij}}w_{ij}\mathbf{P_{ij}} \tag{11}$$

$$N_{i,p}(u)=\frac{u-u_i}{u_{i+p}-u_i}N_{i,p-1}(u)+\frac{u_{i+p+1}-u}{u_{i+p+1}-u_{i+1}}N_{i+1,p-1}(u) \tag{12}$$

$$N_{i,0}(u)=\begin{cases}1 & u_i\le u<u_{i+1}\\ 0 & otherwise\end{cases}$$

On the spans of non-decreasing knots $u\in[u_i,u_{i+1})$ and $v\in[v_i,v_{i+1})$

$$U=\left\{\underbrace{0,\ldots,0}_{p+1},u_{p+1}\ldots u_{m-p-1},\underbrace{1,\ldots,1}_{p+1}\right\}$$

$$V=\left\{\underbrace{0,\ldots,0}_{q+1},v_{q+1}\ldots v_{m-q-1},\underbrace{1,\ldots,1}_{q+1}\right\} \tag{13}$$

Where P_{ij} and w_{ij} are the *ij*th control point vector and the weight associated with the control point. The above expression can be recast in the following form:

$$u(\xi,\eta)=\sum_I N_I(\xi,\eta)\mathbf{P}_I \tag{14}$$

Where

$$N_I(\xi,\eta)=\sum_{i=0}^{n}\sum_{j=0}^{m}\frac{N_{i,p}(\xi)N_{j,q}(\eta)}{\sum_{i=0}^{n}\sum_{j=0}^{m}N_{i,p}(\xi)N_{j,q}(\eta)w_{ij}}w_{ij} \tag{15}$$

P_I are the set of control points used to discretize the field with the index I taking on all possible values of the combination of indices. This discretization leads to a meshless analysis, and compare very favorably to element free Galerkin approaches [1]. Furthermore, NURBS are more flexible in representing local variations of the geometry as well as the field variables.

2.5 Formulation of the Discretized Solution System

The application of the boundary conditions in finite elements or boundary elements employing the standard Lagrangian interpolation is simple since nodes can be placed at the point of application of the boundary condition. However, in the case of a NURBS representation, the control points need not coincide with the boundary. Also, unlike in finite elements, the value of the shape function corresponding to a control point is not unity at that node. Thus, even if the control point were to be coincident with the location of the boundary condition, direct application of the boundary condition is not possible since the specified field value will be distributed to control points influencing the point under consideration. The same is true for the constraints that arise due to Boolean operations on the primitive fields in Constructive Solid Analysis. A Lagrange multiplier scheme is adopted for the application of the constraints on the primitives as well as the boundary conditions. For the sake of simplicity, only the methodology implemented for linear elastic problems is illustrated here. Discretizing the displacement and Lagrange multipliers over Ω and Γ_u as:

$$\tilde{u}=\sum_I N_I u_I \tag{16}$$

$$\tilde{\lambda}=\sum_K \phi_K \lambda_K \tag{17}$$

where, N_I are the NURBS basis functions for the displacement field, and ϕ_K are the NURBS basis for discretization of the Lagrange multipliers. $B=dN/d(u,v)$ is the strain displacment matrix, and further $\varepsilon=\sum_I B_I u_I$. Stationarity of the problem Lagrangian with respect to λ and u gives:

$$\begin{bmatrix}K & -G^T\\ G & 0\end{bmatrix}\begin{pmatrix}u\\ \lambda\end{pmatrix}=\begin{pmatrix}f\\ d\end{pmatrix} \tag{18}$$

Where:

$$K_{IJ}=\int_\Omega B_I^T D B_J d\Omega$$
$$G_{KI}=\int_{\Gamma_u}\phi_K^T N_I d\Gamma \tag{19}$$

$$f_I = \int_{\Omega} N_I^T b d\Omega + \int_{\Gamma_t} N_I^T \tilde{t} d\Gamma$$

$$d_K = \int_{\Gamma_u} \phi_K^T \tilde{u} d\Gamma$$

The solution to the union problem involves the application of displacement constraints on $\Gamma_{P\cap Q}$. Insight into the formulation of the solution system for this problem can be obtained from the discretized form of the first order necessary conditions for the problem. Ignoring the applied boundary conditions for clarity:

$$\begin{bmatrix} K_{P-Q} + c_P^2 K_{P\cap Q}^P & c_P c_Q K_{P\cap Q}^{PQ} & -G_{PP}^T & G_{QP}^T \\ c_P c_Q K_{P\cap Q}^{PQ} & K_{Q-P} + c_Q^2 K_{P\cap Q}^Q & G_{PQ}^T & -G_{QQ}^T \\ G_{PP} & -G_{PQ} & 0 & 0 \\ -G_{QP} & G_{QQ} & 0 & 0 \end{bmatrix} \times \begin{pmatrix} u_P \\ u_Q \\ \lambda_P' \\ \lambda_Q' \end{pmatrix} = \begin{pmatrix} f_P \\ f_Q \\ 0 \\ 0 \end{pmatrix} \tag{20}$$

where,

$$K_{P\cap Q}^P = \int_{\Omega_{P\cap Q}} B_P^T D B_P d\Omega$$

$$K_{P\cap Q}^Q = \int_{\Omega_{P\cap Q}} B_Q^T D B_Q d\Omega$$

$$K_{P\cap Q}^{PQ} = \int_{\Omega_{P\cap Q}} B_P^T D B_Q d\Omega$$

$$G_{PP} = \int_{\Gamma_{QinP}} \phi_P^T N_P d\Gamma, G_{PQ} = \int_{\Gamma_{QinP}} \phi_P^T N_Q d\Gamma$$

$$G_{QP} = \int_{\Gamma_{PinQ}} \phi_Q^T N_P d\Gamma, G_{QQ} = \int_{\Gamma_{PinQ}} \phi_Q^T N_Q d\Gamma \tag{21}$$

The subscripts P and Q refer to the primitives to which the discretizations belong. The subscripts on the stiffness terms K_{P-Q} refer to the domain of integration and the subscripts on λ refer to the domain on which the constraint is imposed.

3. MICROSTRUCTURE MODELING AND ANALYSIS THROUGH CSA

We now apply CSA to model and analyze micro-structure of heterogeneous materials. We define material/analysis dominated union as: (Figure 2)

$P \cup Q$ (P dominated): $c_P = 1, c_Q = 0$, Material in intersection region is identical to that in P

$P \cup Q$ (Q dominated): $c_P = 0, c_Q = 1$, Material in intersection region is identical to that in Q

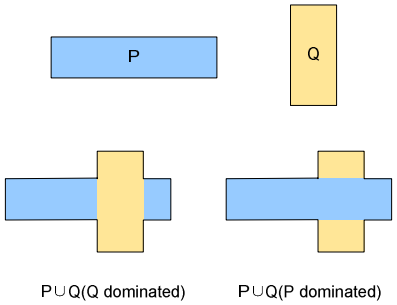

Figure 2. Material/analysis dominated union

The voids in the matrix can be modeled by CSA subtraction operation while the inclusions in the matrix can be modeled by an inclusion dominated union between the matrix and the inclusions (Figure 3). The CSA procedure can naturally model the heterogeneous material even if the second phase is random in size, shape and location. An example of constructing a complex composite RVE through CSA is illustrated in Figure 4. CSA method can be coupled with either unit cell method or homogenization theory to evaluate the properties of the RVE. Note that with CSA method, any modification of the microstructure does not necessitate re-meshing and the re-analysis is only necessary on the primitives affected by the changing microstructure.

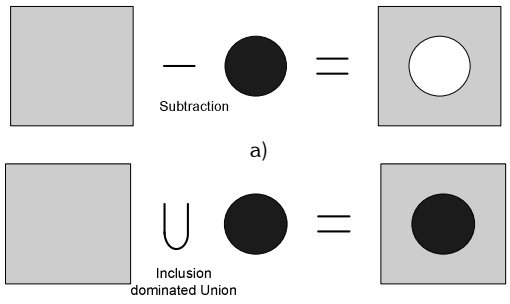

Figure 3. Modeling RVE through CSA. a) Use subtraction to model voids in matrix b) use inclusion dominated union to model inclusions in matrix

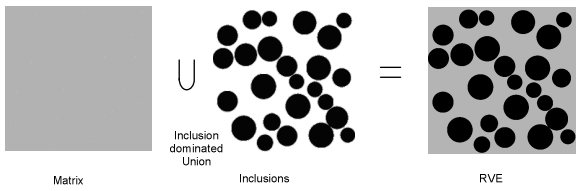

Figure 4. Construction of a complex RVE of composites through inclusion dominated union

4. NUMERICAL EXAMPLES

For simplicity, the unit cell method is coupled with the CSA method to predict the effective elastic properties of microstructures. Plane stress condition is assumed in all the numerical examples. Four pairs of microstructures are simulated and the results obtained by CSA are compared with that obtained by FEA. jNURBS [18] is applied to carryout the CSA analysis. jNURBS is a design-analysis integrated CAD framework that uses NURBS representation of the fields for meshless analysis. CSA method is implemented as an extension package in jNURBS. Object-Oriented Finite Elements [9], an image-based finite element analysis software package for material microstructure simulation developed at NIST, is applied to carry out the finite element analysis. The images used by OOF were generated using MATLAB.

In each problem, the effective Young's modulus in x and y direction were evaluated for both particle reinforced composites and the corresponding porous material with the particles replaced by voids. The volume fractions of the second phase, which is particles for composites and voids for porous materials, are 40%. The material properties are: $E_{matrix} = 72GPa$, $v_{matrix} = 0.3333$, $E_{inclusion} = 400GPa$, $v_{inclusion} = 0.3$. The first pair of problems are the square edge packed composite/porous material with circular second phase (Figure 5). The control point distributions for each case are illustrated in Figures 6 and Figure 7. Note that the control points arrangements on the primitives are independent of each other. In the second pair of problems, composites/porous material with rectangular edge packed elliptical second phase are considered. (Figure 8) The ratio between the long axis and the short axis is 2:1 and the ratio between the width and the height of the RVE is 4:3. In the third problem, microstructures with the circular inclusions/voids random in size and locations are analyzed (Figure 9), while in the fourth pair of microstructure, the elliptical inclusions/voids are random in size, direction and location. (Figure 10)

The simulation results of the composites microstructure are listed in Table 1 and the simulation results of the porous material microstructures are listed in Table 2. The results obtained by FEA and CSA are in very good agreement. For microstructures with rectangular packed elliptical second phase, the effective properties are very different in x and y direction, but the effective properties are almost identical in x and y direction if the elliptical second phase is random (the fourth pair of microstructures). In the third and fourth pair of microstructures, it is shown that CSA can naturally handle complex microstructures with multiple, random inclusions/voids. This is essentially important for material microstructure design because the microstructure design requires iterative modification of size, location and shape of the second phase. Our next step is to apply CSA method to material microstructure design.

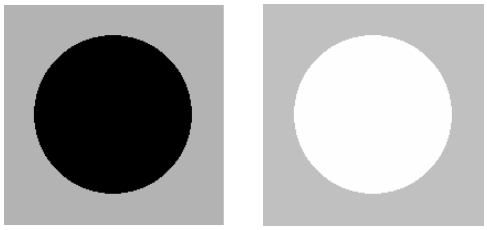

Figure 5. RVEs for square edge packed composites/porous material with circular particles/voids

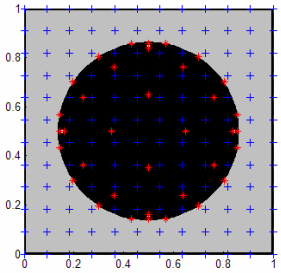

Figure 6. Control points distribution in RVE for square edge packed composite with circular inclusions. The blue '+'s are control points for the matrix while the red '*'s are the control points for the inclusion.

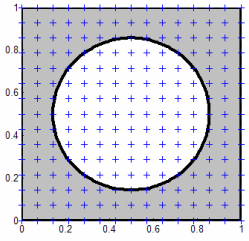

Figure 7. Control points distribution in RVE for square edge packed porous material with circular voids. The blue '+'s are the control points.

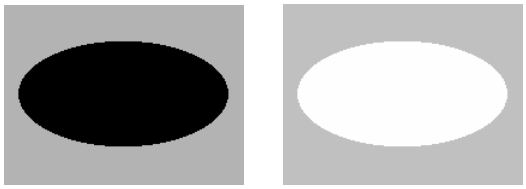

Figure 8. RVEs for rectangular edge packed composites/porous material with elliptical particles/voids

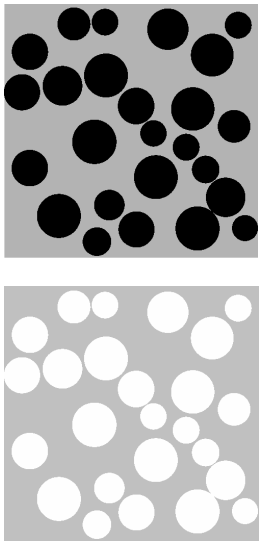

Figure 9. RVEs for random packed composites/porous material with circular particles/voids

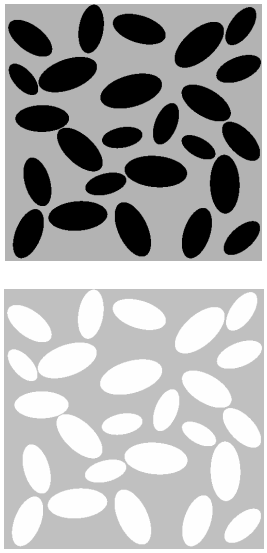

Figure 10. RVEs for random packed composites/porous material with elliptical particles/voids

Microstructure	E_x/E_y *(FEA method)*	E_x/E_y *(CSA method)*
Composite with square edge packed circular particles	125GPa/ 125GPa	125GPa/ 125GPa
Composite with rectangular edge packed elliptical particles	146GPa/ 117GPa	145GPa/ 117GPa
Composite with random packed circular particles	124GPa/ 122GPa	121GPa/ 125GPa
Composite with random packed elliptical particles	123GPa/ 125GPa	122GPa/ 121GPa

Tab. 1. Simulation results of composites

Microstructure	E_x/E_y *(FEA method)*	E_x/E_y *(CSA method)*
Porous material with square edge packed circular voids	28.2GPa/ 28.2GPa	28.2GPa/ 28.2GPa
Porous material with rectangular edge packed elliptical voids	36.5GPa/ 16.5GPa	36.6GPa/ 16.6GPa
Porous material with random packed circular voids	19.5GPa/ 17.8GPa	20.1GPa/ 18.0GPa
Porous material with random packed elliptical voids	18.3GPa/ 16.4GPa	18.7GPa/ 16.7GPa

Tab. 2. Simulation results of porous material

4. SUMMARY

In the present paper, we applied Constructive Solid Analysis (CSA) method to heterogeneous material modeling and analysis. It was shown that CSA method can naturally handle the multi-phases in the heterogeneous material. The effective elastic properties of various 2D microstructures include composites and porous material with random particles and voids were evaluated and the results are excellent agreement with those obtained by finite element method. Our next step is to apply the method to microstructural design.

5. ACKNOWLEDGEMENT

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