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COMPARISON OF 2D AND 3D HOMOGENIZATION PROCESSES FOR MICROMECHANICS ANALYSIS OF UNIDIRECTIONAL COMPOSITES

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ABSTRACT

Multiscale modeling of composite materials has become quite popular for analysis of composite structures. Progressive failure analysis of composites is one area where micromechanics based approaches are widely used. Micromechanics approach requires the modeling of the smallest repetitive volume, also called as the Representative Volume Element (RVE), such that volume fraction of the RVE must be in accordance with the volume fraction of the composite material. Current study aims to show both 2D and 3D RVE applications through a complete homogenization process of the 3D model of the unidirectional composite material. Comparisons of the elastic moduli determined by the 2D and 3D RVEs are formed and compared. The applicability of the 2D RVE in micromechanics analysis of a 3D macro structure is investigated.

INTRODUCTION

Mechanical analysis performed with a general finite element software mainly depends on the homogeneous material models. Homogenization process is the generation of this homogeneous equivalent (or better to say "approximate") of a heterogeneous material such as composite materials [Aboudi J., 1991; Aboudi et al., 2012], polycrystals [Gurses et al., 2011], concrete etc. [Maekawa et al., 2003]. Unidirectional composite materials are one of the basic models that micromechanics have been conducted for [Torquato, S., 2002; Miehe et al., 2002].

Homogenization process can provide initial properties of the material to start an analysis with, as well as it can be coupled to the macro model throughout the analysis to update material properties at every iteration to include nonlinearities like plastification and damage. Various applications can be found on the so called micro-to-macro coupling ie. FE^2 [Feyel, F. and Chaboche, J. L. , 2000].

Current study is a preliminary study on the calculation of the homogenized properties for unidirectional composites. In order to obtain the complete set of material information, one needs to have directional variables when the material is not isotropic. To achieve this, in every direction representative volume element is tested with known input strain and calculated output stress results need to be integrated over the domain in order to calculate the average properties such that moduli.

Micromechanics approach mainly depends on 2D RVE's since they are quite popular due to shorter

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modeling and finite element solution times. In this study, both 2D and 3D RVE's are used to calculate the 3D homogenized material properties and compare them from different perspectives. In the 2D RVE case, results obtained from two different action planes, as shown in Figures 1 and 2, are combined together to produce a set of complete material properties. On the other hand, in 3D RVE case, there is only one model providing the homogenized material properties of the unidirectional composites.

REPRESENTATIVE VOLUME ELEMENT and BOUNDARY CONDITIONS

Representative Volume Element (RVE) is defined as a tool of micromechanics by [Hill, R., 1963] and similarly used by many following researchers [Hashin, Z., 1983]. RVE is a material model that is large enough to contain every variation and specification of the actual heterogeneous material whereas small enough for efficient calculations. Usually, it is required to perform a survey on the RVE size, in order to make sure that the average properties collected from that RVE's converged with respect to the size of the RVE.

RVE's are conditioned and used by predefined boundary conditions [Miehe, C., 2003; Temizer, I., 2010; Cioranescu, D. and Donato, P. , 1998]. There are a number of boundary condition methods essentially based on the Hill's Energy Condition [Hill, R., 1963]. Among these methods, Periodic Boundary Condition (PBC) is the most famous and accurate one especially for periodic structures. In the current study PBC is used in the finite element analyses of the RVE.

FORMATION of the 3D MATERIAL MODEL

For the calculation of the homogenized properties of the unidirectional composite, composite material properties are chosen as it was suggested by Miehe [Miehe et al., 2002]. Matrix material has a bulk modulus of 1740 N/mm^2 and shear modulus of 800 N/mm^2 and the fiber has 100 times higher properties than the matrix material. Geometrically, RVE has fiber volume fraction of 0.1257. 2D studies are performed by 4-noded-quadrilateral elements with plane strain formulation. 3D RVE analyses are performed using 10-noded-tetrahedral elements. Analyses are performed by an in-house FEM code written in FORTRAN 90.

2D RVE Results

2D RVE study is performed in two different cut directions of the actual unidirectional composite material configuration. XZ (or YZ) plane is visualized with a centered fiber layer where as the XY plane has a circular fiber inclusion in the center.

Summary of strain inputs used in the 2D RVE study $\bar{\varepsilon}_{11}, \bar{\varepsilon}_{22}$ and $\bar{\varepsilon}_{12}$. Here 1 and 2 directions are local axes of each 2D models. They are properly matched with the 3D axes (which are named as X, Y, Z) later in the Table 3.

2D RVE with Centered Rectangular Fiber: is shown in Figure 1 with a sample mesh configuration. One may easily notice that RVE model is created with proper fiber volume fraction adjustment to the geometric value of 0.1257. In Miehe's paper [Miehe et al., 2002], it was modeled as a cut through fiber center with a bigger fiber section which yields fiber volume fraction of 0.3, approximately. Since the aim of the current study is to combine two different models, they required to be consistent in terms of volume fraction at first glance.

Analytical results and results of the current study, for the RVE with centered rectangular fiber layer, obtained using the periodic boundary condition are given in Table 1. In Table 1, results of current study are summarized for 7 by 7 (C_1), 12 by 12 (C_2) and 21 by 21 (C_3) linear quadrilateral element meshes.

2D RVE with Centered Cylindrical Fiber: is given in Figure 2. For the circular inclusion case, conforming mesh with linear quadrilateral elements is prepared for the finite element analysis.

Results obtained for the in-plane elastic moduli are presented for different mesh sizes in Table 2 where $C_1 - C_4$ correspond to edgewise mesh densities of 12, 20, 40 and 80 elements, respectively.

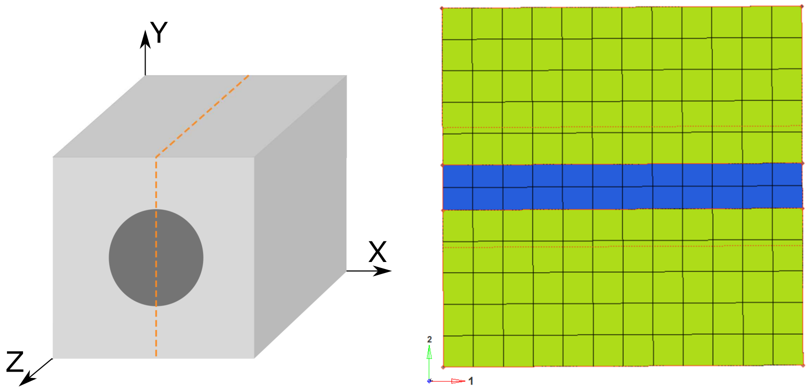

Figure 1: 2D RVE with Centered Rectangular

Table 1: Moduli for the 2D RVE with Centered Rectangular Fiber

	Voigt Bound	Reuss Bound	Hashin Shtrikman		Current Study PBC Results		
			(+)	(-)	C_1	C_2	C_3
C_{1111}	86528	3795	38278	4382	31352	31352	31352
C_{2222}	86528	3795	38278	4382	3206	3206	3206
C_{1122}	32022	1405	13078	1590	1378	1378	1378
C_{1212}	27253	1195	12600	1396	914	914	914
fiber vol. frac.	0.1257	0.1257	0.1257	0.1257	0.1257	0.1257	0.1257
$C_1 - C_3$ for edgewise mesh densities of 7, 12 and 21 respectively							

Sample deformation distribution of the 2D RVE with cylindrical fiber inclusion for pure shear strain loading with periodic boundary condition is given in Figure 3. As it is seen in the figure, deformed shapes of opposing edges are same. In this way, boundary condition enforces edges to behave as there are repeating models in every direction. Main advantage of this method is the elimination of the stress concentrations near edges and so the reduction in the necessity of using bigger models with more fiber inclusions.

In the present study, results of the two 2D RVEs, with rectangular and cylindrical fiber layer and inclusion, are combined in an attempt to recover the 3D homogenized material properties. In order to understand how the results are combined, it is better to assign 3D axes definitions in a 3D RVE and match those axes to their 2D counterparts. Definition of the axes in the 3D RVE is given in Figure 4. According to the axis definitions given in Figure 4, degrees of freedom of the two 2D RVE models are

Table 2: Moduli for the 2D RVE with Centered Cylindrical Fiber

	Voigt Bound	Reuss Bound	Hashin Shtrikman		Current Study PBC Results			
			(+)	(-)	C_1	C_2	C_3	C_4
C_{1111}	34001	2899	13885	3068	3396	3397	3399	3399
C_{2222}	34001	2899	13885	3068	3394	3397	3399	3399
C_{1122}	12583	1073	4753	1126	1396	1402	1405	1406
C_{1212}	10709	913	4566	971	960	959	959	959
fiber vol. frac.	0.1257	0.1257	0.1257	0.1257	0.1223	0.1240	0.1249	0.1253
$C_1 - C_4$ for edgewise mesh densities of 12, 20, 40 and 80, respectively								

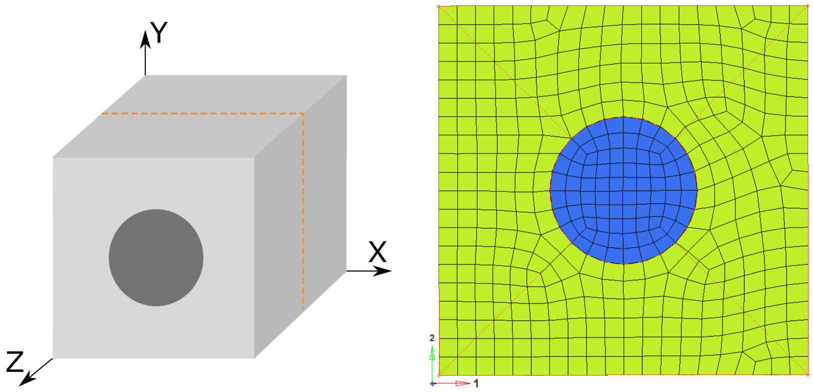

Figure 2: 2D RVE with Centered Cylindrical Fiber Inclusion

Table 3: 2D data summary with 3D axes equivalents matched

		3D Elastic Moduli						
		C_{xxxx}	C_{yyyy}	C_{xxyy}	C_{xyxy}	C_{xzxz}	C_{zzzz}	C_{xxzz}
Centered Rectangular Fiber Inclusion	C_{1111}						31352	
	C_{2222}		*3206*					
	C_{1122}							1378
	C_{1212}					914		
Centered Cylindrical Fiber Inclusion	C_{1111}	3399						
	C_{2222}		3399					
	C_{1122}			1406				
	C_{1212}				959			
		Assume $\mathrm{C}_{yzyz} = C_{xzxz}; C_{yyzz} = C_{xxzz}$						

matched with the 3D equivalents, as given in Table 3.

In recovering the 3D homogenized properties from the two 2D RVEs, transverse properties are taken from results of the 2D RVE with centered cylindrical inclusion. On the other hand, axial properties are taken from the results of the 2D RVE with the centered rectangular layer. It should be noted that for the 2D RVE with centered rectangular fiber layer, fiber layer is modeled like it has rectangular cross section such that its width goes as deep as the matrix, even though it has a cylindrical cross section. It is assumed that this modeling technique is fair enough as long as the actual volume fraction of the fiber is preserved as the 3D RVE. Assuming that the current examples are proper in terms of the volume fraction requirements, resultant 3D homogenized moduli are given by Equation 1.

$$C_{3D} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & & & \\ & C_{2222} & C_{2233} & & & \\ & & C_{3333} & & & \\ & & & C_{1212} & & \\ & & & & C_{2323} & \\ & & & & & C_{1313} \end{bmatrix} = \begin{bmatrix} 3399 & 1406 & 1378 & & & \\ & 3399 & 1378 & & & \\ & & 31352 & & & \\ & & & 959 & & \\ & & & & 914 & \\ & & & & & 914 \end{bmatrix}$$

[Eq. 1]

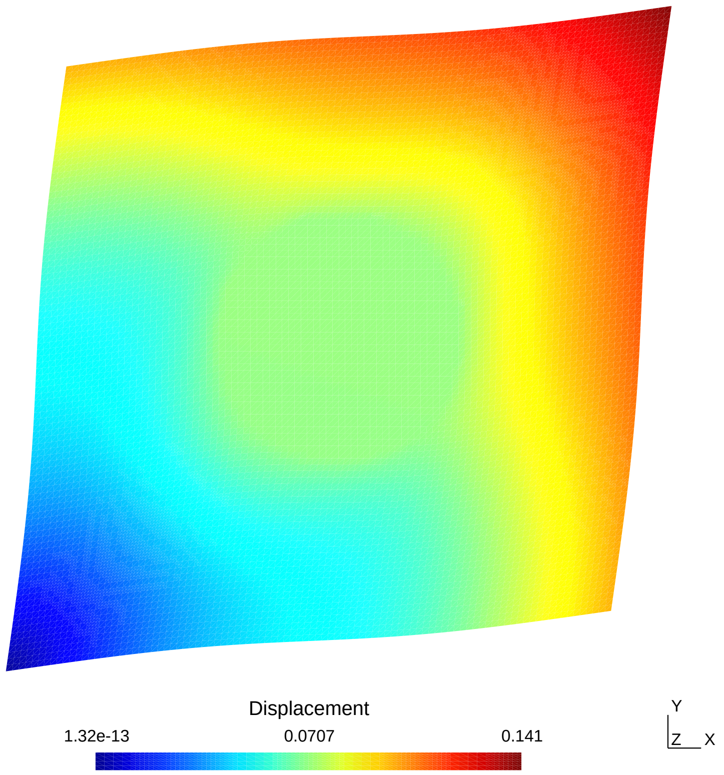

Figure 3: 2D RVE Deformation as a Result of Pure Shear Strain Loading with PBC

3D RVE Results

3D RVE solution is established by a single finite element model, again within the in-house-FEM code. 10-noded quadratic tetrahedral elements are used. Sample model is given in Figure 4.

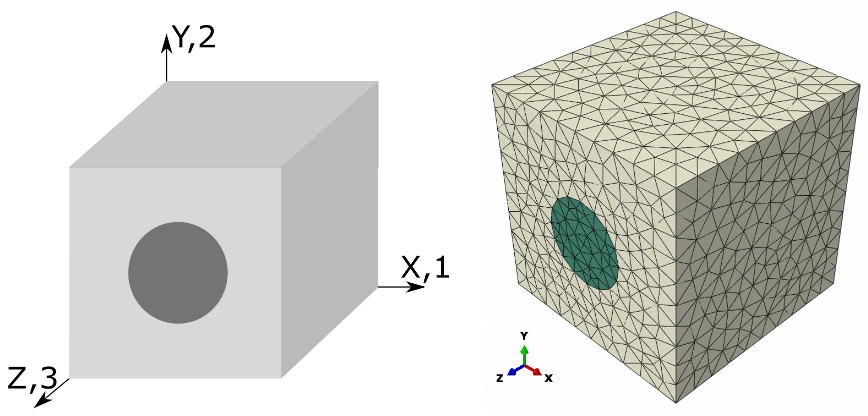

Figure 4: Axes Definition on a 3D RVE with Centered Circular Fiber and 3D RVE FEM Modal

Six different strain inputs are applied on finite element model of the 3D RVE. Strain inputs are ε_{11}, ε_{22}, ε_{33}, ε_{12}, ε_{23} and ε_{13}. In the 3D RVE case, four different mesh densities are used for convergence study. Elastic moduli calculated for each case is presented in Table 4 where the edgewise element densities are 2, 5, 10 and 20, respectively. In Table 4, fiber volume fractions are also calculated using the finite element models of the 3D RVEs for four different mesh sizes. It is seen that as the mesh size is reduced, cylindrical fiber inclusion is better approximated with the tetrahedral elements used in the 3D RVE model, and the fiber volume fraction of the finite element model approaches to the

Table 4: Moduli for the 3D RVE with Centered Cylindrical Fiber

	Voigt Bound	Reuss Bound	Hashin Shtrikman		Current Study PBC Results			
			(+)	(-)	C_1	C_2	C_3	C_4
C_{1111}	37734	3206	15471	3395	3304.4	3365.1	3386.2	3395.8
C_{2222}	37734	3206	15471	3395	3304.4	3350.1	3386.2	3395.7
C_{3333}	37734	3206	15471	3395	23726.2	26246.0	28160.6	28619.8
C_{1122}	16223	1378	6301	1451	1390.6	1401.5	1419.4	1423.9
C_{2233}	16223	1378	6301	1451	1406.4	1423.6	1439.0	1443.3
C_{1133}	16223	1378	6301	1451	1406.4	1423.6	1439.0	1443.3
C_{1212}	10755	914	4585	972	958.5	953.3	956.9	958.2
C_{2323}	10755	914	4585	972	998.5	1007.3	1019.8	1023.1
C_{1313}	10755	914	4585	972	1001.3	1013.8	1019.8	1023.1
fiber vol. frac.	0.1257	0.1257	0.1257	0.1257	0.1021	0.1131	0.1224	0.1246

$C_1 - C_4$ for edgewise mesh densities of 2, 5, 10 and 20, respectively

actual fiber volume fraction of 0.1257.

For the fine mesh case, homogenized material properties obtained by the finite element analysis of the 3D RVE are be organized in the matrix form as shown in Equation 2.

$$C_{3D} = \begin{bmatrix} 3396 & 1424 & 1443 & & & \\ & 3396 & 1443 & & & \\ & & 28620 & & & \\ & & & 958 & & \\ & & & & 1023 & \\ & & & & & 1023 \end{bmatrix} \quad \text{[Eq. 2]}$$

Sample deformation distribution of the 3D RVE with cylindrical fiber inclusion for pure shear strain loading with periodic boundary condition is given in Figure 5.

COMPARISON of RESULTS and CONCLUSION

In the present study, it is aimed to combine the material properties obtained from the homogenization of two 2D RVEs to generate the 3D elastic coefficient matrix which is also independently obtained by the 3D RVE. The main motivation for the use of 2D RVEs is the significant reduction in the computation time required to generate the homogenized material properties which are required in many applications in multiscale modeling and analysis of composites via FE^2 approach. In this study, it is aimed to investigate how reliable is it to combine the elastic coefficients obtained from the analysis of two 2D RVEs to generate the 3D elastic coefficient matrix for a simple unidirectional fiber reinforced composite material configuration which essentially behaves as transversely isotropic.

In 2D RVE results, first obvious outcome is that at all different mesh density solutions of Centered Rectangular Fiber, resultant Moduli is exactly the same. This fact emphasizes the volume fraction effect. On the other hand, in 2D RVE applications, applicant assumes constant cross section through that view. There is no possibility to define constant section through the thickness in the first model (centered layer) of 2D applications as seen. One may modify this section according to his/her own wishes but in any other section selection, it still will not represent the all section but maybe one part of it. In this study, Centered Rectangular Fiber model is modified and formed such that fiber volume fraction is consistent and equivalent to the geometric one.

2D RVE results are calculated quite close to the 3D RVE results. 3D results are converging to a higher values as the fiber volume fraction increases and at last step it is decided to stop, while fiber

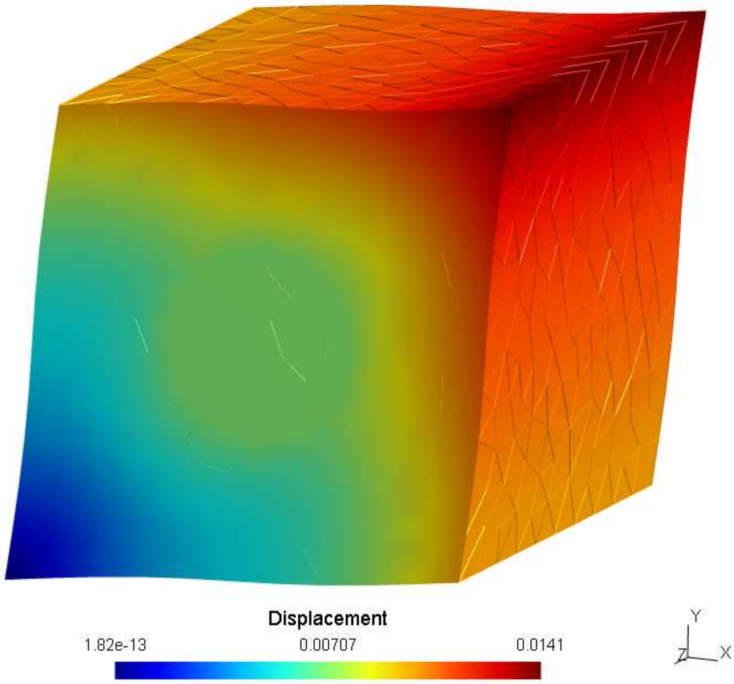

Figure 5: 3D RVE Deformation on Shear Strain Loading with PBC

volume fraction is just 0.1246 which is still less then actual fiber fraction. According to this fact, 3D RVE results might get even closer to the 2D RVE results.

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