

Micromechanics Simulation Challenge – Level 1

Micromechanics Simulation Challenge

Because of the inherent heterogeneity in composite materials, the field of micromechanics provides essential tools for the understanding and analysis of composite materials and structures. Micromechanics can be segregated into two main branches: homogenization or prediction of the behavior of an effective homogeneous continuum and de-homogenization or recovery of the local fields in the actual heterogeneous structure given the loading on the effective homogeneous continuum. Many micromechanical tools have been developed and codified, including many commercially-available software packages that offer micromechanical analyses as either a stand-alone tool or as part of a chain of analyses. However, with the increasing number of tools available, the practitioner must determine which tool(s) provides the most value for the problem at hand given budget, time and resource constraints. To date, simple benchmarking examples have been reported in the literature. The present suggests a series of such benchmarking exercises in the field of micromechanics against which such tools can be compared.

The exercise will consist of three levels. Microstructures examined in all three levels will consist of 2-dimensional idealizations of continuous fiber-reinforced composites, 3-dimensional representations of laminate microstructures, 3-dimensional representations of particle-reinforced microstructures, and 3-dimensional representations of short-fiber reinforced microstructures. The problems specified in Level 1 will be linear-elastic phase constituent behavior. The contrast between matrix and reinforcement properties will be varied. Prediction of effective properties (homogenization) and local field recovery within the microstructure are specified. Level 2 extends the challenge by introducing non-linear phase properties, including elastic-plastic constitutive relations, which may be of particular interest in short-fiber composites. Finally, in Level 3 damage and failure prediction are addressed for both aligned, continuous-fiber systems and short-fiber systems. Multi-physics calculations, including fatigue life prediction under combined mechanical loading and environmental effects will be included.

Of interest in all three levels is both homogenization and de-homogenization (local field recovery). In addition to effective properties and local fields along a specified path, the computational efficiency will be an important metric in comparing the tools. For each problem, results will be compared with numeric results obtained from finite element analysis (FEA) of the specified boundary value problem. Note this exercise is focusing on the effectiveness of homogenization and dehomogenization of micromechanics codes. We are aware that different failure or damage criterion might be used in different tools. When damage and failure are considered, we will chose the same criteria for fair comparison if possible. It is anticipated that the results from the challenge will compare the relative strengths and trade-offs of the participating tools and identify areas currently unaddressed by the micromechanics field at large.

Micromechanics Simulation Challenge – Level 1

Specification of Challenge Problems: Level 1

The problem set in Level 1 is restricted to composite microstructures of linearly-elastic phases. All the microstructures are idealized representation of real heterogeneous materials. Nevertheless, these idealization are continually used in the micromechanics field.

In each case, the complete set of effective properties are sought. For level 1 microstructures, the effective homogeneous continuum could be generally anisotropic. If some effective properties turn out to be at most orthotropic, then the results will be given in terms of the effective elastic constants: the Young's Moduli, E_1 , E_2 , E_3 , shear moduli, G_{12} , G_{13} , G_{23} , Poisson's ratios, ν_{12} , ν_{13} , ν_{23} , and coefficients of thermal expansion, α_1 , α_2 , α_3 . Volume fractions will be an independent variable specified for these cases. The heterogeneous fields will be recovered along paths specified in each problem statement. The deformation cases consist of constant (unit) strain in the x_1 direction, constant (unit) strain in the x_2 direction, shearing strain in the x_2 - x_3 plane and shearing strain in the x_1 - x_3 plane, and combined unit axial strain in the x_1 direction and shearing strain in the x_1 - x_3 plane. These load cases can be converted to traction loads if applying tractions are more natural for some tools using the effective properties computed by the corresponding tools. All results should be normalized by the prescribed strain. Computing time should be reported with the specifications (CPU and RAM) of the computer for both homogenization and dehomogenization results.

Micromechanics Simulation Challenge – Level 1

Case 1: Square and Hexagonal Pack Microstructure

The first microstructures consist of two equivalent representations of a square pack array with representative volume elements, RVEs, shown in Figure 1. It can be used to describe a continuous fiber reinforced composites. If needed, an appropriate 3D microstructure can be constructed corresponding to theory implemented in the corresponding tools.

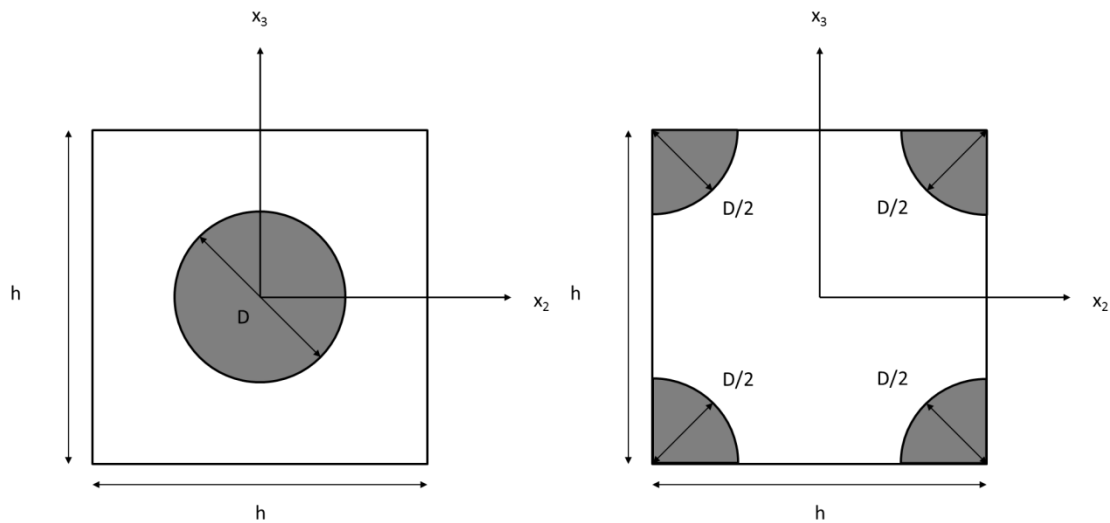


Figure 1: Circular fiber embedded in matrix. (Upper-Left) Case 1a; (Upper-Right) Case 1b; (Lower) Case 1c.

For the case of the circular fiber in the center of the RVE, Case 1a, the effective elastic constants are to be predicted at fiber volume fractions of 1%, 30%, 60% and 75%. The dilute 1% fiber volume fraction allows comparison with Eshelby's analytic solution [1]. Specifically, the Young's Moduli, E_1 , E_2 , E_3 , shear moduli, G_{12} , G_{13} , G_{23} , Poisson's ratios, ν_{12} , ν_{13} , ν_{23} , and coefficients of thermal expansion, α_1 , α_2 , α_3 are to be reported. For the case of the circular fibers at the four corners of the RVE, Case 1b, prediction of the above properties at a fiber volume fraction of 60% is sufficient. The predictions in Case 1a are to be carried out on the sets of material properties specified in Table 1. The predictions in Case 1b need be carried out for the first set of material properties specified in Table 1.

Micromechanics Simulation Challenge – Level 1

Table 1: Material properties for Case 1

	Set 1 Carbon/Epoxy		Set 2 (Low Contrast, Isotropic Fiber)	
Property	Matrix	Fiber	Matrix	Fiber
E_1 (GPa)	4.76	276	350	400
$E_2=E_3$ (GPa)	4.76	19.5	350	400
$\nu_{12}=\nu_{13}$	0.37	0.28	0.18	0.17
ν_{23}	0.37	0.70	0.18	0.17
$G_{12}=G_{13}$ (GPa)	1.74	70	148	171
G_{23} (GPa)	1.74	5.74	148	171
α_1 ($10^{-6}/^{\circ}\text{C}$)	64.8	-0.4	30	20
α_2 ($10^{-6}/^{\circ}\text{C}$)	64.8	5.6	30	20
α_3 ($10^{-6}/^{\circ}\text{C}$)	64.8	5.6	30	20

For local field recovery, all nontrivial stress components should be reported along the two paths defined by $x_3 = 0$ and $x_3 = -x_2$ for Cases 1a-b. For Case 1a, the local field recovery should be carried out at a fiber volume fraction of 75% and with both sets of material properties. For Case 1b, the local field recovery may be carried out at a fiber volume fraction of 60% and with only the first set of material properties.

Micromechanics Simulation Challenge – Level 1

Case 2: Three-Phase Interphase Microstructure

The second microstructure is a square pack array with a second reinforcement phase, representative of an interphase region between the fiber and matrix. The microstructure geometry is shown in Figure 2. If needed, an appropriate 3D microstructure can be constructed corresponding to the theory implemented in the corresponding tools.

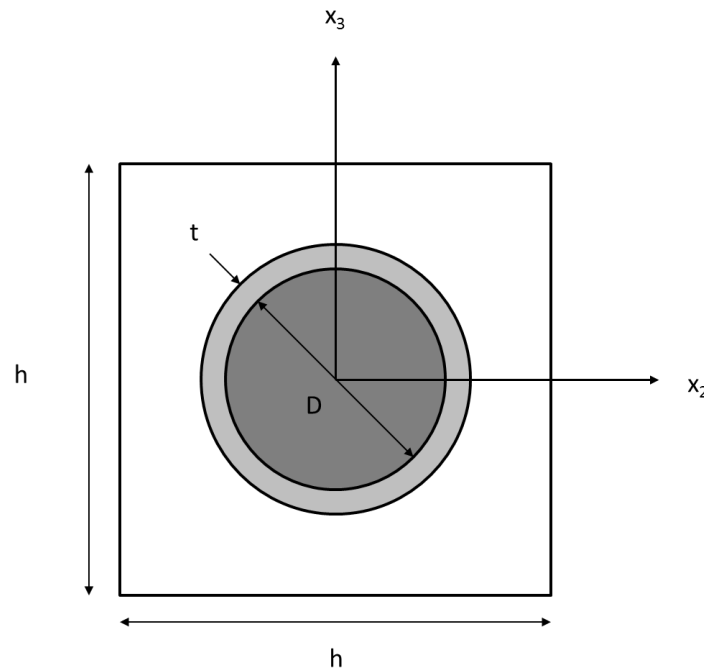


Figure 2: Case 2, circular fiber and interphase embedded in matrix.

Here the fiber is defined by diameter D and the interphase region by thickness, t . For the prediction of effective elastic constants, let the volume fraction of the fiber phase be 60% and vary the volume fraction of the interphase. Specifically, the effective elastic constants are to be predicted at interphase volume fractions of 1%, 5% and 10%. One set of fiber, matrix and interphase properties, representative of a generic CMC, is given in Table 2. Again, the Young's Moduli, E_1 , E_2 , E_3 , shear moduli, G_{12} , G_{13} , G_{23} , Poisson's ratios, ν_{12} , ν_{13} , ν_{23} , and coefficients of thermal expansion, α_1 , α_2 , α_3 are to be reported at each volume fraction.

For local field recovery, all nontrivial stress components should be reported along the two paths defined by $x_3 = 0$ and $x_3 = -x_2$. As with the prediction of effective properties, the local field recovery should be carried out at a fiber volume fraction of 60%, with interphase volume fraction of 5%, and with the material properties listed in Table 2.

Micromechanics Simulation Challenge – Level 1

Table 2: Material properties for Case 2

		Set 3 (CMC)	
Property	Matrix	Fiber	Interphase
E (GPa)	350	450	5.0
ν	0.18	0.17	0.22
G (GPa)	148	171	2.0
α_1 ($10^{-6}/^{\circ}\text{C}$)	64.8	-0.4	5.0
α_2 ($10^{-6}/^{\circ}\text{C}$)	64.8	5.6	5.0
α_3 ($10^{-6}/^{\circ}\text{C}$)	64.8	5.6	5.0

Micromechanics Simulation Challenge – Level 1
Case 3: 0/90 Microstructure

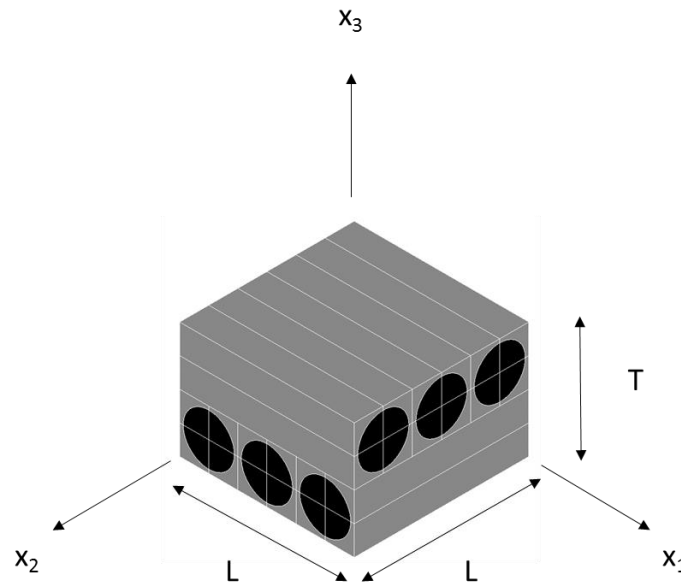


Figure 3: 0/90 microstructure

The third problem, shown in Figure 3, is a 0/90 microstructure characterized by two perpendicular rows of 3 fibers each, with fibers having diameter, $D = 5$ microns and volume fraction, V_f to be specified. This microstructure is assumed to be periodic in the x_1 and x_2 directions, representative of a 0/90 lamina interface. Though not representative of typical composite microstructures, boundary conditions on the x_3 faces are assumed to be periodic. The fiber volume fraction determines the thickness T and length L . Elastic properties for the fiber and matrix are given in Table 1, Set 1. Predict the elastic properties at fiber volume fractions of 30% and 60%. Specifically, the Young's Moduli, E_1 , E_2 , E_3 , shear moduli, G_{12} , G_{13} , G_{23} , Poisson's ratios, ν_{12} , ν_{13} , ν_{23} , and coefficients of thermal expansion, α_1 , α_2 , α_3 are to be reported.

For local field recovery, all nontrivial stress components should be reported along the paths defined by $(L/2, L/2, x_3)$, and by $(x_1, L/2, T/2)$. The local field recovery should be carried out at a fiber volume fraction of 30% and 60% with the material properties specified in Table 1, Set 1.

Micromechanics Simulation Challenge – Level 1
Case 4: Spherical Inclusions Microstructure

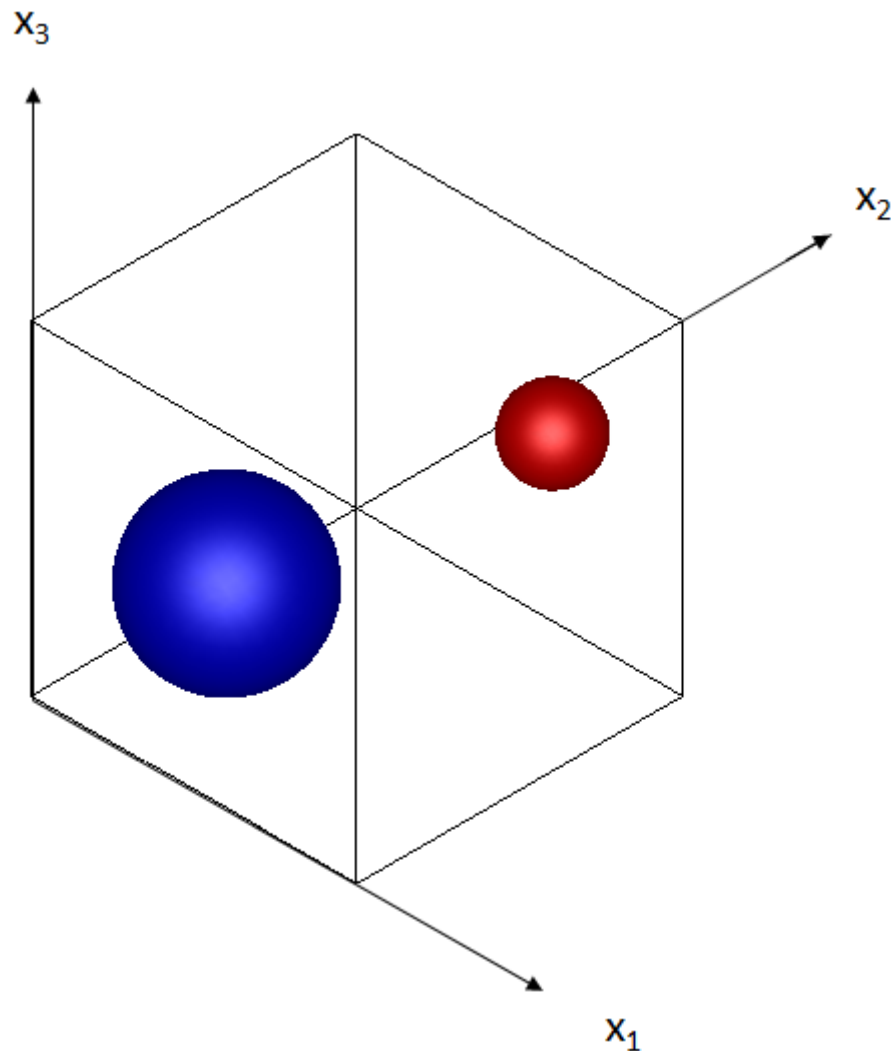


Figure 4: Spherical inclusions microstructure

A spherical-inclusion microstructure is shown in Figure 4. The spheres may represent particles or voids. The diameter of the 2 spheres is 1 micron and 0.5 microns, respectively. The dimensions of the RVE are 2x2x2 microns. The larger sphere is centered at (0.6, 0.6, 0.6) and the smaller sphere is centered at (1.5, 1.7, 1.3). The matrix elastic properties are listed in Table 3. For the case where the spheres represent particles, the elastic properties of the particles are listed in Table 3. For the case where the spheres represent voids, the moduli may all be assumed to vanish.

Predict the elastic properties of the microstructure for the case where the spheres represent particles, the case where the spheres represent voids and the case where the larger sphere represents

Micromechanics Simulation Challenge – Level 1

a particle and the smaller sphere represents a void. Specifically, the complete 6 x 6 stiffness matrix (C_{ij}) and thermal expansion coefficients (α_{ij}) should be reported.

Local field recovery should also be performed for the cases of spherical particles, spherical voids and the case where the larger sphere represents a particle and the smaller sphere represents a void. For local field recovery, all nontrivial stress components should be reported along the linear path from (0,0,0) to (2,2,2).

Table 3: Matrix and particle elastic properties

	Set 4 (Particle)	
Property	Matrix	Particle
E (GPa)	350	450
ν	0.18	0.17
G (GPa)	148	171
α_1 ($10^{-6}/^{\circ}\text{C}$)	64.8	-0.4

Micromechanics Simulation Challenge – Level 1
Case 5: Woven-fiber microstructure

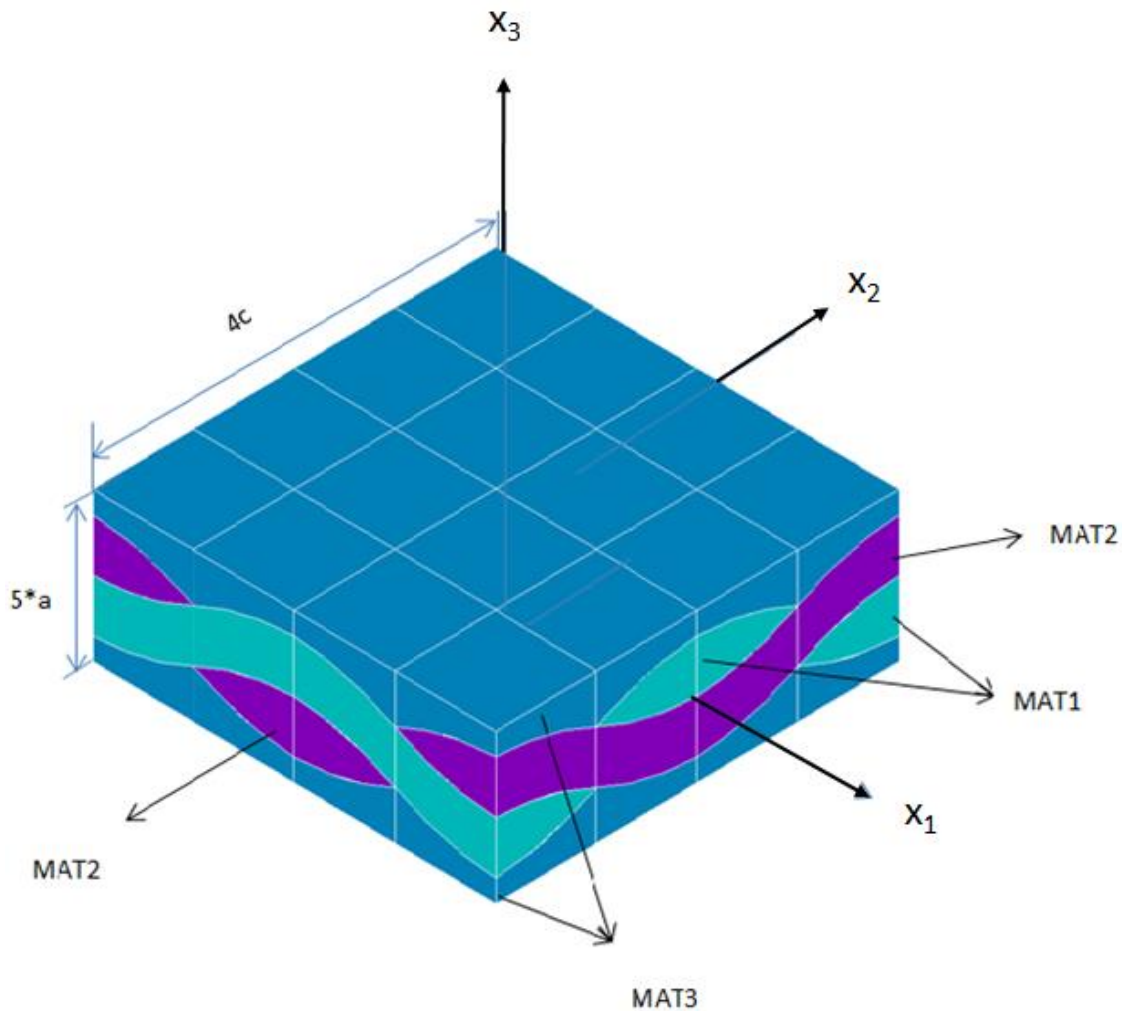


Figure 5: Woven-fiber microstructure

A woven-fiber microstructure is shown in Figure 5, representative of a plain weave fabric where the fibers are oriented along the x_1 and x_2 -directions. The elastic material properties of the fiber and matrix are listed in Table 1, Set 1. For this case, let both fibers have identical material properties. In Figure 5, MAT 3 denotes matrix and MAT2 and MAT1 denotes fibers. The specific weave geometry of the weave will be provided through the files WovenComposite.iges and WovenComposite.stp files.

Predict the elastic properties of the microstructure. Specifically, the complete 6×6 stiffness matrix (C_{ij}) and thermal expansion coefficients (α_{ij}) should be reported.

For local field recovery, all nontrivial stress components should be reported along the paths defined by $x_2=x_3=0$, by $x_1=x_2=0$.

Micromechanics Simulation Challenge – Level 1
Case 6: Short-fiber 3D “random” microstructure

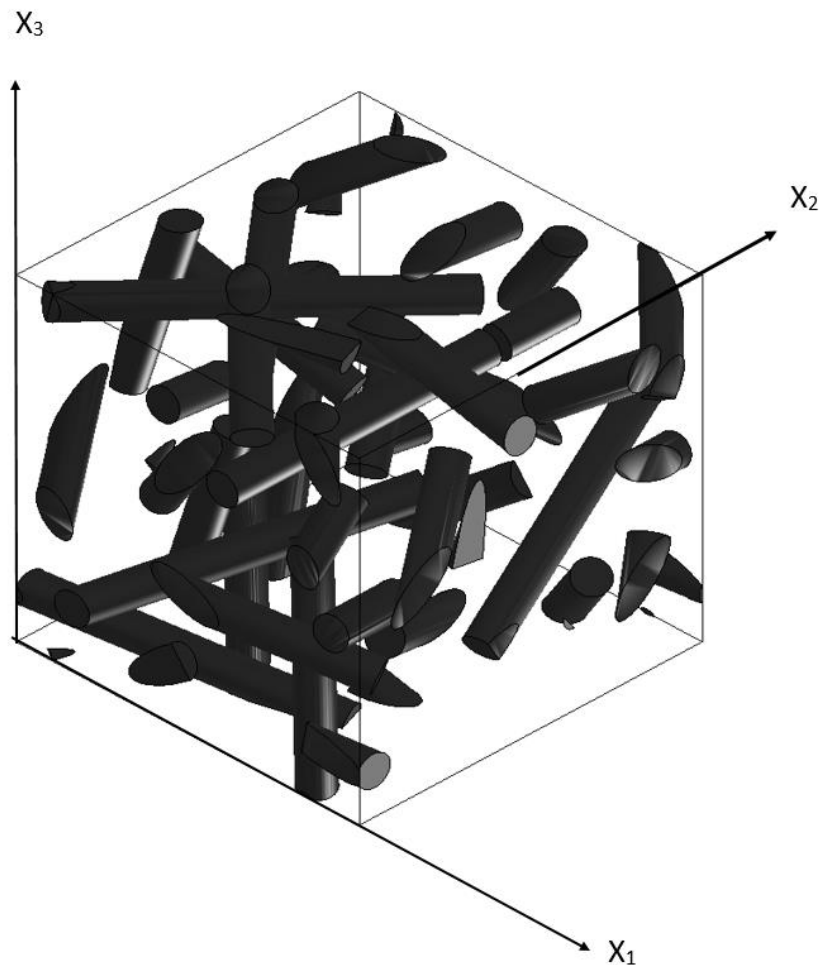


Figure 6: Short-fiber 3D random orientation microstructure

The final microstructure, shown in Figure 6, represents a complex 3-dimensional short-fiber microstructure. While much physical insight can be gained from simplification of realistic microstructures, the intent of the present microstructure is to challenge the simulation tool in treating relatively complex geometries. The geometry of the fibers and matrix is given in ShortFiber_phase1.stp and ShortFiber_phase2.stp, respectively, and both geometries are given in ShortFiber.igs.

A short-fiber microstructure is shown in Figure 6, where the fibers are “randomly” oriented by rotations in each of the coordinate directions. The length and diameter of each cylindrical fiber is 1.1 micron and 0.11 micron, respectively. There are a total of 16 fibers in the microstructure. The elastic material properties of the fiber and matrix are listed in Table 1, Set 1.

Micromechanics Simulation Challenge – Level 1

Predict the elastic properties of the microstructure. Specifically, the complete 6 x 6 stiffness matrix (C_{ij}) and thermal expansion coefficients (α_{ij}) should be reported.

For local field recovery, all nontrivial stress components should be reported along the linear paths from (0,0,0) to (L,L,L) and from (L/2,L/2,0) to (L/2,L/2,L).