Multiscale analysis of composite material reinforced by randomly-dispersed particles

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A multiscale analysis method is presented in which detailed information on the microscopic level is incorporated into macroscopic models capable of simulating damage evolution and ultimate failure. The composite considered is reinforced by randomly-dispersed particles, which reflects the statistical characteristics of real materials, such as cement-based materials. Specifically, a three-dimensional material body is decomposed into many unit cells. Each unit cell is reinforced by a cylindrical particle, the orientation of which is characterized by three Euler angles generated by the random number generator. Based on a detailed finite element analysis, the material properties of the representative volume element are obtained. As verification, the properties of the cylindrical particles are set equal to those of the matrix and the computed ‘composite’ properties reduce exactly to those of the ‘isotropic’ material, as expected. Through coordinate transformation, the effective material properties of each unit cell are calculated. The assembly of stiffness matrices of all unit cells leads to the stiffness matrix of the whole specimen. Under the simple tension loading condition, the initial damaged unit cell can be identified according to the von Mises yield criterion. The stiffness of the damaged unit cell will then be reduced to zero and it will cause stress redistribution and trigger further damage. It was found that the reinforcement is effective to mitigate and arrest the damage propagation, and therefore prolongs the material’s lifetime. These results suggest that the hierarchical coupling approaches used here may be useful for material design and failure protection in composites.

Keywords: multiscale analysis; random response; finite element method; representative volume element; Euler angle; damage propagation

1. Introduction

Composites make up a very broad and important class of engineering materials. Since materials have different properties, it seems sensible to make use of the beneficial properties of each single ingredient in a proper combination [1]. For example, a simple mixture of clay, sand and straw produced a composite building material which was used by the oldest known civilizations. The further development of non-metallic materials and composites has attracted the attention of scientists and engineers in various fields. Apart from their considerably low weight-to-strength ratio, some composites benefit from other desirable properties, such as sustainability, durability, toughness and lower cost [2]. Usually, a composite material consists of a matrix, which could be metal, polymeric (like plastics) or
ceramic, and a reinforcement, which could be particles or fibers of steel, aluminum, silicon, carbon nanotubes, etc.

It is generally accepted that composite materials can be prepared easily by dispersing the reinforcements into the matrix and stirring in order to mix them uniformly yet randomly. Therefore, a composite material, as an inhomogeneous material, has some degrees of uncertainty in terms of geometry or orientation of the reinforcement, which will greatly influence its material properties. To evaluate the reliability of a composite structure, the randomness of the microstructure must be investigated.

For this purpose, Bazant et al. [3] and Jirasek and Bazant [4] considered random geometrical configurations and locations of the particles. By using a triangular softening force–displacement diagram, they investigated the fracture behavior of composites with inter-particle links. Also, some results on the stochastic homogenization analysis have been reported by Sakata et al. [5,6]. They proposed a perturbation-based homogenization analysis method to solve the stochastic microscopic stress analysis problem with an assumed microscopic random variation. This method reduced the computational cost compared with the Monte Carlo simulation. Moreover, they proposed the inverse stochastic homogenization analysis method for identifying a microscopic random variation. In addition, the effect of particle clustering on stress distribution and fracture of composites has been discussed [7–9]. Interested readers are referred to the abovementioned articles.

The principal objective of this work was to study the macroscopic damage propagation and microscopic stress distribution in a composite, taking into account the randomness of the orientation of the reinforcements. A general purpose finite element program MECORAP (MEchanics of COmposites reinforced by RAndomly dispersed Particles) has been developed by the authors at George Washington University. An analysis of the effect of the microstructure on the strength and damage resistance of the material can be a basis for the improvement of a material’s durability and performance.

2. Multiscale analysis procedure

In this paper, we propose a multiscale analysis procedure. This procedure is divided into four stages, which are implemented sequentially. Figure 1 outlines the detailed relationships between the four stages.

Consider a three-dimensional (3D) composite specimen and divide it into many unit cells, as shown in Figure 2. Each unit cell is reinforced by a cylindrical particle, the orientation of which is characterized by three Euler angles, $\alpha$, $\beta$ and $\theta$. As shown in Figure 1, the random variables in this problem are the three Euler angles for each unit cell. Obviously, such composites show marked inhomogeneity and anisotropy, that is to say, the properties of the unit cells vary significantly when measured in different locations or directions.

However, it is almost ‘mission impossible’ to create the simulation model for this kind of composite, because the microstructures for different unit cells are different in the global $xyz$ coordinates. Even with the help of supercomputers, the computation time consumed is still a big problem to model and mesh all the unit cells. A natural way to overcome this difficulty is to choose the one with all three Euler angles equal to zero ($\alpha = \beta = \theta = 0^\circ$) as the representative volume element (RVE), and label the local $x'y'z'$ coordinates on it. All the unit cells can be represented by the RVE through the rotation from the local coordinates to the global coordinates. By changing the radius and the height of the cylinder, we can represent the effects of the morphology of the reinforcement on the mechanical properties of the composite. The damage propagation at the macroscopic level and the stress analysis at the microscopic level can be obtained from the following computational process.
At the first stage, we calculate the homogenized stiffness matrix for the RVE microstructure based on finite element (FE) analysis in Section 3. As shown in Figure 1, the purpose of the second stage is to obtain the stiffness matrices for all the unit cells through the Euler angles. This procedure will be described in Section 4. Then, the damage propagation analysis is performed at the macroscopic level. At the microscopic level, we further explore the microstructural stress distribution for any element. Sections 5 and 6 show the numerical results. The microscopic stress distribution depends not only on the microstructure but also on the macroscopic stresses obtained in Stage 3. This is one reason why a multiscale analysis is needed here.

3. Homogenized material properties of RVE

The FE method is used here to evaluate the effective material properties of the RVE. Figure 3 shows the FE models for the RVE. It is assumed that both the particle and the matrix are linear isotropic elastic continua, with given Young’s moduli and Poisson’s ratio.
Figure 3. Finite element models of (a) RVE, (b) half of RVE (cross-sectional view) and (c) the reinforcement.

The reinforcement is embedded in a softer matrix, e.g. aggregates embedded in cement paste (concrete) or fibers embedded in polymer (fiber-reinforced composite). It is also assumed that the two materials are perfectly bonded at the interface.

Notice that the tensor form of the constitutive relation [11] \( \sigma_{ij} = A_{ijkl}e_{kl} \) can be expressed in Voigt form \( \sigma_i = C_{ij}e_j \), i.e.

\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\tau_{23} \\
\tau_{31} \\
\tau_{12}
\end{pmatrix}
= \begin{pmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\
C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\
C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\
C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66}
\end{pmatrix}
\begin{pmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
2\varepsilon_{23} \\
2\varepsilon_{31} \\
2\varepsilon_{12}
\end{pmatrix}.
\tag{1}
\]

To determine all the coefficients in the stiffness matrix \( \mathbf{C} \), we need to consider six cases and solve them one by one. Table 1 illustrates the boundary conditions for the six cases. The first three are simple tension cases, and the last three are simple shear cases. The FE analysis of each case leads to six equivalent stresses which are the coefficients in the corresponding column in the stiffness matrix. For example, in the first case, let the applied strain \( \varepsilon_{11} = 1 \) and other five strains be zero, then the boundary conditions are set as \( x = (1 + \varepsilon_{11})x, \ y = y \) and \( z = z \), i.e. \( u_x = \varepsilon_{11}x, \ u_y = 0 \) and \( u_z = 0 \). The static case is considered here, and the governing equation can be expressed as \( \mathbf{Ku} = \mathbf{F} \). Then one may proceed to solve for the displacement field. It is noticed that, at the boundary where displacements are specified, one obtains the corresponding reactive forces. At each of the six surfaces of the cube (cf. Figure 3a), the equivalent stresses \( \sigma_{ij} \) are calculated from the summation of reactive forces over that surface divided by the area of that surface. Then \( C_{11} = \sigma_{11}/\varepsilon_{11}, \ C_{21} = \sigma_{22}/\varepsilon_{11}, \ C_{31} = \sigma_{33}/\varepsilon_{11}, \ C_{41} = \tau_{23}/\varepsilon_{11}, \ C_{51} = \tau_{31}/\varepsilon_{11} \) and \( C_{61} = \sigma_{12}/\varepsilon_{11} \).

As an example, consider the Al matrix reinforced by SiC particles. Young’s modulus and Poisson’s ratio are \( E_m = 73 \text{ GPa}, \nu_m = 0.345 \) for the matrix, and \( E_p = 485 \text{ GPa}, \nu_p = 0.165 \) for the particles. The geometric dimensions of the matrix are \( 2 \times 2 \times 2 \). The radius of the cylindrical particle is 0.5, and the height is 1.8. Therefore, the volume fraction of
Table 1. Boundary conditions for the six cases.

| Case No. | Boundary conditions |
|----------|---------------------|
| 1        | $\varepsilon_{11} = 1$, other $\varepsilon_{ij} = 0$ |
| 2        | $\varepsilon_{22} = 1$, other $\varepsilon_{ij} = 0$ |
| 3        | $\varepsilon_{33} = 1$, other $\varepsilon_{ij} = 0$ |
| 4        | $2\varepsilon_{23} = 1$, other $\varepsilon_{ij} = 0$ |
| 5        | $2\varepsilon_{31} = 1$, other $\varepsilon_{ij} = 0$ |
| 6        | $2\varepsilon_{12} = 1$, other $\varepsilon_{ij} = 0$ |

The particle is $\pi (0.5)^2 \times 1.8/2^3 \approx 18\%$. The numerical results of the stiffness matrix $C$ (in GPa) are obtained as:

$$
C = \begin{bmatrix}
137.2 & 66.02 & 63.64 & 0 & 0 & 0 \\
66.02 & 137.2 & 63.64 & 0 & 0 & 0 \\
63.64 & 63.64 & 153.2 & 0 & 0 & 0 \\
0 & 0 & 0 & 31.2 & 0 & 0 \\
0 & 0 & 0 & 0 & 31.2 & 0 \\
0 & 0 & 0 & 0 & 0 & 29.24
\end{bmatrix}
$$

It should be noted that the numerical results for the stiffness matrix turn out to be symmetric, and that it includes six independent constants. Also, the Cauchy condition $C_{1212} = \frac{1}{2}(C_{1111} - C_{1122})$ is not satisfied. This means the homogenized material is not exactly axis-symmetric. It is due to the fact that the FE mesh and the model, which is a cube, have $\frac{\pi}{4}$ rotational symmetry, not hexagonal symmetry.

For an isotropic material, material symmetry imposes restrictions on the coefficients of the stiffness matrix, thus further reducing the number of independent coefficients. This leads to the theoretical expression of the isotropic stiffness matrix as follows [10,11]:

$$
C = \begin{bmatrix}
\lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\
\lambda & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\
\lambda & \lambda & \lambda + 2\mu & 0 & 0 & 0 \\
0 & 0 & 0 & \mu & 0 & 0 \\
0 & 0 & 0 & 0 & \mu & 0 \\
0 & 0 & 0 & 0 & 0 & \mu \\
\end{bmatrix} \quad \text{(SYM)},
$$

where $\lambda = \frac{E_v}{(1+v)(1-2v)}$ and $\mu = \frac{E}{2(1+v)}$.

MECORAP can also be used to calculate the stiffness matrix for an isotropic material by changing the material constants of the particle to the constants of the matrix. The following numerical results match the theoretical results. This is a good validation of our computer code.

$$
C = \begin{bmatrix}
114.7 & 60.40 & 60.40 & 0 & 0 & 0 \\
60.40 & 114.7 & 60.40 & 0 & 0 & 0 \\
60.40 & 60.40 & 114.7 & 0 & 0 & 0 \\
0 & 0 & 0 & 27.14 & 0 & 0 \\
0 & 0 & 0 & 0 & 27.14 & 0 \\
0 & 0 & 0 & 0 & 0 & 27.14
\end{bmatrix}.
$$
4. Macroscopic material properties

One may carry out the transformation from a given Cartesian coordinate system to another by means of three successive rotations performed in a specific sequence. The Euler angles are then defined as the three successive angles of rotation. There are twelve distinct sets of rotational sequences [12,13]. The sequence employed here starts by rotating the coordinate \( xyz \) by an angle \( \alpha \) counterclockwise about the \( x' \) axis. Then, the coordinate \( x'y'z' \) is rotated about the \( y' \) axis counterclockwise by an angle \( \beta \). Finally, the coordinate \( x'y'z' \) is rotated counterclockwise by an angle \( \theta \) about the \( z' \) axis to produce the desired \( x'y'z' \) coordinate system. Figure 4 illustrates the three steps of the rotational sequence. The Euler angles \( \alpha, \beta \) and \( \theta \) thus completely specify the orientation of the \( x'y'z' \) system relative to the \( xyz \) system.

The transformation between the coordinate \( x'y'z' \) and the coordinate \( xyz \) can now be expressed as

\[
\mathbf{x} = \mathbf{R} \mathbf{x'}
\]

and the elements of the complete transformation matrix \( \mathbf{R} \) can be obtained by writing the matrix as the triple product of the separate rotation matrices, i.e.

\[
\mathbf{R} = \mathbf{R}(x; \alpha)\mathbf{R}(y; \beta)\mathbf{R}(z; \theta),
\]

where

\[
\mathbf{R}(x; \alpha) = \begin{bmatrix}
1 & 0 & 0 \\
0 & \cos \alpha & -\sin \alpha \\
0 & \sin \alpha & \cos \alpha
\end{bmatrix};
\]

\[
\mathbf{R}(y; \beta) = \begin{bmatrix}
\cos \beta & 0 & \sin \beta \\
0 & 1 & 0 \\
-\sin \beta & 0 & \cos \beta
\end{bmatrix};
\]

\[
\mathbf{R}(z; \theta) = \begin{bmatrix}
\cos \theta & -\sin \theta & 0 \\
\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{bmatrix}.
\]

An important aspect of the simulation is to use the random number generator to generate the three Euler angles for each unit cell. Actually, the homogenized material property of the RVE almost has axis symmetry, and therefore the third Euler angle \( \theta \) does not affect

![Figure 4. Three Euler angles: (a) \( \alpha \) (about \( x' \) axis); (b) \( \beta \) (about \( y' \) axis); (c) \( \theta \) (about \( z' \) axis).](image-url)
the results very much. For simplicity, we only generate two Euler angles $\alpha$ and $\beta$ for each unit cell. Figure 5 illustrates the distributions of the two Euler angles, which are generated randomly from 0 to $2\pi$.

Once we have the transformation between the two coordinates for each unit cell, we can evaluate the effective material properties for each unit cell based on the effective stiffness matrix of the RVE, i.e.

$$A_{abcd} = R_{ax} R_{by} R_{cy} R_{dx} A'_{a\beta y\delta},$$

(5)

where $A'$ is the stiffness matrix of the RVE and is equivalent to the $C$ matrix in Equation (1).

5. Macroscopic damage propagation

For the simple tension problem, there are two kinds of loading conditions, corresponding to two kinds of boundary conditions. One is force-specified, and the other is displacement-specified. Here, we use the second one to simulate an applied strain $\varepsilon_{xx} = 3\%$. Under the

Figure 6. The distribution of von Mises stress under simple tension.
uniformly-distributed displacement in the $x$ direction, i.e. $u_x$, the stress distribution can be obtained by MECORAP. Figure 6 shows the distribution of the von Mises stress. It should be noticed that the distribution is very random, not uniform, which is different from the case for homogenous material.

The von Mises criterion is employed to determine whether damage occurs or not. The damage was modeled by using the element elimination technique. This means the elements of which the von Mises stress exceed a critical value, namely the von Mises strength, are considered as damaged elements, and the Young’s modulus of these elements is set to be zero. As a consequence, the stresses in the entire specimen are redistributed. The specimen is then analyzed with a new set of stiffness matrices to determine if any further failure is
induced. If further failure does not occur, the load is increased to the level needed to cause the next failure. This incremental process continues until catastrophic failure occurs. The ultimate load-carrying capacity of the structure is then determined.

Now we demonstrate the capability of MECORAP in performing damage propagation analysis. Let us first consider the composite with $E_m/E_p = 73/485$. Figures 7 and 8 show the entire process of damage propagation and the curve of the applied strain versus the percentage of damage. The damaged elements are shown in gray, and the elements in white have negligibly low stresses.

In this case, we do not need to increase the applied loading. The initial damage will trigger further damage step by step, like dominos. This pattern is considered as a catastrophic case in engineering. As depicted in Figure 8, the cross represents the ultimate failure. At this step, the specimen has been broken into two pieces, and it can no longer bear any loading. Therefore, the elements in Figure 7f are either damaged or have zero stress.

To investigate the other pattern of the damage propagation, consider a second case, i.e. a composite with $E_m/E_p = 1/50$. Figure 9 illustrates the damaged elements at steps 1, 10, 14–16 and 18. One interesting phenomenon occurs from step 1 to step 10: the damaged elements randomly appear over the whole specimen. This is because the stiffness matrices for different elements are different. This phenomenon will never happen in a homogeneous material.

Figure 10 depicts the relationship between the applied strain and the percentage of damaged elements. After we identify the first damaged element, the externally applied loading needs to be increased in order to get the damage propagation process going. If we do not increase the external loading, the ultimate failure can be prevented. This is the difference between Case 1 ($E_m/E_p = 1/6.47$) and Case 2 ($E_m/E_p = 1/50$). From the comparison of the abovementioned two cases, we see a potential and considerable variety for material specification and material design.

6. Microscopic stress distribution

After the stress analysis at the macroscopic level, we can further explore the detailed stress analysis at the microscopic level for any unit cell. At this stage, the stress analysis is performed in the local coordinate system. At stage 3, we have obtained the six components of stress tensor in the global coordinate and we also have the three Euler angles. The stress
tensors in the global coordinate system $\sigma$ and in the local coordinate system $\sigma'$ are related to each other as

$$\sigma'_{mn} = R_{im}R_{jn}\sigma_{ij}. \quad (6)$$

The stress tensor $\sigma'$ is used to calculate the surface traction, which is converted to the force-specified boundary conditions acting on the RVE. Take the initial damaged element as an example, Figure 11 shows the detailed stress distribution in the microstructure. This is the case of which the applied strain is 1.35% (cf. Figure 8). It can be seen that the stresses in the reinforcement are higher than that in the matrix. This is because the load-carrying capability of the reinforcement is higher than that of the matrix.

Figure 9. Evolution of damage at various steps: steps 1, 10, 14–16 and 18.
Figure 10. The relationship between the applied strain and the percentage of damaged elements corresponding to the damage in Figure 9.

Figure 11. The distribution of von Mises stress (in GPa) (a) for the microstructure and (b) its cross-sectional view.

7. Conclusion

MECORAP is a general purpose finite element code which was developed for the analysis of composites reinforced by randomly-dispersed particles. Most commercial codes seem to be ineffective in dealing with this kind of composite, in that creating the material properties for all unit cells is too complicated, while MECORAP makes it possible to perform not only the stress analysis but also failure analysis. Currently, MECORAP is a static code. It can be developed to a new level so that it can be used to analyze dynamic problems.

Generally speaking, a composite material is a natural choice to enhance material properties, such as sustainability and durability. Our simulation results show that composite materials can mitigate and arrest the damage propagation effectively and prolong the material’s lifetime. Actually, we realize that one may choose the reinforcement and the matrix, and also one may design the reinforcement and the matrix for required mechanical properties and performance.
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