Mapping method for sensitivity analysis of composite material property

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Abstract Composite properties are dependent on the microstructure of materials, which is depicted with a base cell. The parameters for representing the microstructure should include the shape parameters of the base cell and those used to describe the distribution of materials in the base cell. The goal of material design optimization is to find appropriate values of these parameters to make the materials have specific properties. Design optimization needs the sensitivity information of the material properties with respect to the shape parameter of the base cell and the material distribution parameters. Moreover, sensitivity calculation is often expensive. Thus, it is very important to develop an efficient sensitivity analysis method. In this paper, a mapping method is proposed for predicting the material properties and computing their sensitivities with respect to the shape parameters of the base cell. Through mapping transformation, solutions to the micro-scale homogenization problem defined on the domain of a base cell can be obtained by solving a homogenization problem defined on an initial given domain. The composite properties and their sensitivities with respect to the shape parameters of the base cell are explicitly expressed in terms of the properties and their sensitivities of a virtual material with respect to the distribution parameters. This virtual material has an initially given base cell domain. Thus re-meshing for discretizing the problem is avoided and computing cost savings are realized. Numerical examples show that the proposed method is accurate and efficient in both the prediction of material properties and sensitivity calculation.

Key words mapping method, sensitivity analysis, homogenization, composite materials

1 Introduction

Composite material has been used widely in many areas because of its special features. According to particular application environments or special demands, the composite material needs to be designed precisely. For example, in order to meet the requirements of thermal geometry stability of a structure, it is always desired to design the material to exhibit zero thermal expansion coefficients. Another example is the design problem of a functionally gradient material, where the basic idea is to design the distribution of the material microstructure to make the different surface exhibit different properties and the material properties change continuously along the gradient direction (cf. Sata 1988; Cheng and Liu 1994).

Topology optimization is an increasingly powerful tool and can be used to optimize the material arrangement in a structural system to achieve a wide variety of performance objectives, including minimal compliance, optimal strength, viscoelastic damping, and compliant mechanisms (Bendsseen and Kikuchi 1988), etc. The effective properties of the materials are evaluated by use of the homogenization theory, the detail of which can be found in many papers (e.g. Guedes and Kikuchi 1990; Liu et al. 1998). Thus, the concepts and methods of topology optimization can be effectively applied to material design. The formulation of the design optimization of materials with specific properties has been investigated in the literature (cf. Sigmund 1995; Liu et al. 1998). To solve the material design optimization problem, the most important step is to calculate the sensitivity of the effective properties of the materials. In fact, the sensitivity information of an optimization problem is generally thought of as the basis of efficient optimization algorithms. Sensitivity information is also very important for structural identification, model synthesis, random finite element method and the solution of inverse problems.

The most direct way to obtain sensitivity is the overall finite difference method. In this method, the effective elastic properties of the material D for a given design $d = (d_1, d_2, \ldots, d_M)^T$, which includes material distribution parameters and the shape parameters of the base cell, are evaluated by the homogenization method.
The design is perturbed by a small increment $\Delta d_i$ of a certain design variable $d_i$ and a neighbouring design $d' = (d_1, d_2, \ldots, d_i + \Delta d_i, \ldots, d_M)^T$ is obtained. For this neighbouring design, the effective properties of the material are calculated and the sensitivity of $D$ with respect to $d_i$ is approximated by finite difference, i.e.

$$\frac{\partial D}{\partial d_i} \approx \frac{D(d') - D(d)}{\Delta d_i}. \quad (1)$$

This method is easily implemented, but has two drawbacks. To obtain sensitivities of the effective elastic properties of the materials with respect to $M$ design variables at one particular design point, we need to solve $M + 1$ micro-homogenization problems for predicting the effective properties. This is a huge computation for a large-scale structure. Furthermore, in the iteration process of the design optimization, the size and the shape of the base cell will change. The evaluation of the sensitivity with respect to shape parameters of the base cell needs to solve a changing definition-domain problem for prediction of the material properties, and remeshing modelling must be done. Another problem is the selection of the perturbation size $\Delta d_i$. Too large $\Delta d_i$ introduces a large truncating error, too small $\Delta d_i$ causes conditional errors because $D(d') - D(d)$ is the difference between two big numbers which are close to each other.

In this paper, a mapping method is proposed for predicting the material properties and computing the sensitivity of composites with respect to the shape parameters of base cell. Through mapping transformation, the solving of the micro-scale homogenization problem defined on a changed domain of a base cell can be obtained by solving a homogenization problem defined on an initial given domain. The composite properties and their sensitivities with respect to shape parameters of the base cell are explicitly expressed in terms of the properties and their sensitivities of a virtual material with respect to the distribution parameters. This virtual material has an initially given base cell domain. Thus remeshing for discretizing the problem is avoided and computing cost saving is realized. Numerical examples show that the proposed method is accurate and efficient in both the prediction of material properties and sensitivity calculation.

### Mapping method for predicting the effective properties of composites

Composite properties depend strongly on the shape of the base cell, thus, the design variables should include the shape parameters of the base cell. In this case, the shape of the base cell changes in the iteration process of material design optimization. The change of the base cell's shape leads to the change of the solution domain because the material property prediction problem is defined on the domain of the base cell. Thus, there are some difficulties in calculating the sensitivities with respect to shape parameters. For solving this problem the coordinate mapping method (for short: mapping method) is introduced to make the sensitivity computing process easy. The mapping method takes the initial mesh of cell as the original fixed mesh for each intermediate step. So the base cell need not be remeshed. The following explains the main idea of the mapping method in detail.

It is assumed that the initially given region of the base cell is $Z$ and the current region in some iteration step is $Y$, as shown in Fig. 1. These two regions have the same meshing forms. It is supposed that the current region $Y$ and the initial region $Z$ have the following mapping relation:

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}. \quad (2)$$

The effective properties of the material are evaluated by use of homogenization method that was presented in the literature (e.g. Cheng and Liu 1994; Bendsse and Kikuchi 1988; Guedes and Kikuchi 1990). Thus the equivalent material coefficients (e.g. the elastic properties) can be written as

$$E^H_{ijkl} = \frac{1}{|Y|} \int_Y \left( E_{ijkl} - E_{ijmp} \frac{\partial \phi^k_m}{\partial y_p} \right) \, dy,$$  \quad (3)

where $\phi^k_m$ is the periodic solution of the following equation:

$$\int_Y \left( E_{ijkl} - E_{ijmp} \frac{\partial \phi^k_m}{\partial y_p} \right) \frac{\partial \psi^l_n}{\partial y_j} \, dy = 0, \quad \forall v \in V. \quad (4)$$
The above equation can be written in matrix form

$$\int_{V} \varepsilon_{y}^{T}(v)[D - D\varepsilon_{y}(\phi)] dy = 0,$$  \hspace{1cm} (5)

where D is the elastic coefficients matrix of the material in the base cell domain, and \(\varepsilon_{y}(\cdot)\) is the strain calculator in the y-coordinate system,

\[
\begin{bmatrix}
E_{1111} & E_{1112} & E_{1112} \\
E_{1222} & E_{2222} & E_{2222} \\
\text{sym.} & E_{1212} & E_{1212}
\end{bmatrix},
\]

\[
\varepsilon_{y}(\cdot) = \begin{bmatrix}
\frac{\partial}{\partial y_{1}} & 0 & \frac{\partial}{\partial y_{2}} \\
0 & \frac{\partial}{\partial y_{2}} & \frac{\partial}{\partial y_{1}}
\end{bmatrix}^{T},
\]

\(\phi = (\phi^{11}, \phi^{22}, \phi^{12})\), \(\Phi^{a} = (\Phi_{1}^{a}, \Phi_{2}^{a})^{T}\), \(a = (11, 22, 12)\).  \hspace{1cm} (6)

By use of the coordinate transformation expressed by (2), we obtain the expression of the strain calculator in the y-coordinate system, \(\varepsilon_{y}(\cdot)\), in terms of the strain calculator in the z-coordinate system, \(\varepsilon_{z}(\cdot)\)

\[
\varepsilon_{y}(\cdot) = K\varepsilon_{z}(\cdot)K_{1},
\]

where

\[
K = \begin{bmatrix}
\frac{1}{\lambda_{1}} & 0 & 0 \\
0 & \frac{1}{\lambda_{2}} & 0 \\
0 & 0 & \frac{1}{(\lambda_{1}\lambda_{2})}
\end{bmatrix}, \quad K_{1} = \begin{bmatrix}
\lambda_{1} & 0 \\
0 & \lambda_{2}
\end{bmatrix}.
\]

(7)

Defining generalized displacement vectors \(\nabla\) and \(\bar{\phi}\) as

\(\nabla = K_{1}v\) and \(\bar{\phi} = K_{1}\phi\),

\[\varepsilon_{y}(v) = K\varepsilon_{z}(\nabla), \quad \varepsilon_{y}(\bar{\phi}) = \varepsilon_{z}(\bar{\phi}).\]  \hspace{1cm} (8)

Substituting (10) into (5) yields

\[
\int_{Z} \varepsilon_{z}^{T}(\nabla)K\left([D - DK\varepsilon_{z}(\phi)]\right) dz = 0,
\]

or

\[
\int_{Z} \varepsilon_{z}^{T}(\nabla)DK\varepsilon_{z}(\phi) dz = \int_{Z} \varepsilon_{z}^{T}(\nabla)KD\varepsilon_{z}(\phi) dz. \hspace{1cm} (11)
\]

Note \(K^{T} = K\). Defining \(\bar{D} = KDK\), we obtain

\[
\int_{Z} \varepsilon_{z}^{T}(\nabla)\bar{D}\varepsilon_{z}(\phi) dz = \int_{Z} \varepsilon_{z}^{T}(\nabla)KDz. \hspace{1cm} (12)
\]

By assuming \(\phi^{(1)}\) is the solution of the following equation:

\[
\int_{Z} \varepsilon_{z}^{T}(\nabla)\bar{D}\varepsilon_{z}(\phi^{(1)}) dz = \int_{Z} \varepsilon_{z}^{T}(\nabla)KDz,
\]

the solution of (13) has the form

\[\bar{\phi} = \phi^{(1)}K^{-1} \hspace{1cm} (13)\]

Comparing (14) with (5) we find that they have the same form except material properties matrix \(D\) has taken the place of \(\bar{D}\). We name the problem corresponding to (14) as the dual problem of the original problem corresponding to (5); \(\bar{D}\) is called as the elastic matrix of the dual material. According to (3), the macro-elastic matrix can be described as

\[
\bar{D}^{H} = \frac{1}{|Y|} \int_{Y} [\bar{D} - \bar{D}\varepsilon_{y}(\phi)] dy.
\]

(16)

Thus, the macro-elastic matrix of the dual problem has the following definition:

\[
\bar{D}^{H} = \frac{1}{|Z|} \int_{Z} \left[\bar{D} - \bar{D}\varepsilon_{z}(\phi^{(1)})\right] dz.
\]

(17)

Following the above equations, the relation between \(D^{H}\) and \(\bar{D}^{H}\) can be derived as follows:

\[
D^{H} = \frac{1}{|Y|} \int_{Y} [D - D\varepsilon_{y}(\phi)] dy =
\]

\[
\frac{1}{|Z|} \int_{Z} \left[D - DK\varepsilon_{z}(\phi)\right] dz =
\]

\[
\frac{1}{|Z|} \int_{Z} \left[D - DK\varepsilon_{z}(\phi^{(1)}K^{-1})\right] dz =
\]

\[
K^{-1} \left\{\frac{1}{|Z|} \int_{Z} \left[KDK - KD\varepsilon_{z}(\phi^{(1)})\right] dz\right\} K^{-1} =
\]

\[
K^{-1} \left\{\frac{1}{|Z|} \int_{Z} \left[\bar{D} - \bar{D}\varepsilon_{z}(\phi^{(1)})\right] dz\right\} K^{-1}.
\]

(18)

Considering the definition expressed by (17), the following relation is obtained:

\[
D^{H} = K^{-1}\bar{D}^{H}K^{-1}.
\]

(19)

From the above equation, it is obtained that the original problem's macro-elastic properties can be expressed by the dual problem's equivalent properties. This observation initiates a method, called the mapping method, for predicting the material properties. The main steps are summarized as follows.

1. Mesh the original domain Z.
2. Define and confirm the conversion matrix K defined by (9).
3. Compute the material properties of the dual problem in domain Z by \(\bar{D} = KDK\).
4. Solve the dual problem (14).
5. Calculate the macro-material properties of the dual problem, $\mathbf{D}^H$, by use of (17).
6. Calculate the macro-material properties $\mathbf{D}^H$ of the original problem, $\mathbf{D}^H = K^{-1} \mathbf{D}^H K^{-1}$.

3 Mapping method of sensitivity analysis

In the previous section, a dual problem was derived by introducing the mapping method and doing some coordinate translation. The material properties can be determined explicitly in terms of the material properties of the dual problem. This dual problem is defined on an initially given domain which remains unchanged in the iteration process. Thus, re-meshing is not needed to calculate the material properties with a changed base cell domain in the iteration domain, and the computing cost is saved. This advantage will be demonstrated significantly when the mapping method is applied in the sensitivity analysis.

The macro properties of the materials are associated with the shape and material distribution parameters. Next, we consider the sensitivities of the material properties with respect to these two kinds of parameters, separately. Firstly, the variation of distribution parameters will cause the relevant change of material properties which constitute the base cell, whereas the cell domain will not change. Therefore, the formulation of the sensitivity of macro-material properties with respect to distribution parameters can be easily derived as follows.

Based on the homogenization method, the macro-elastic properties of materials are given by

$$\mathbf{D}^H = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} [\mathbf{D} - \mathbf{D}_\varepsilon_y(\Phi)] \, dy,$$

where the generalized displacement parameter, $\Phi$, is defined by (7) and should be the periodic solution of (5).

Considering this nature of $\Phi$, the following series equations should be satisfied:

$$\mathbf{D}^H = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} [\mathbf{D} - \mathbf{D}_\varepsilon_y(\Phi)] \, dy -$$

$$\frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \varepsilon_y^T(\Phi) [\mathbf{D} - \mathbf{D}_\varepsilon_y(\Phi)] \, dy =$$

$$\frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \left\{ [\mathbf{D} - \mathbf{D}_\varepsilon_y(\Phi)] - \varepsilon_y^T [\mathbf{D} - \mathbf{D}_\varepsilon_y(\Phi)] \right\} \, dy =$$

$$\frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \left[ I - \varepsilon_y^T(\Phi) \right] D \left[ I - \varepsilon_y(\Phi) \right] \, dy.$$

Thus, the material properties can be rewritten as

$$\mathbf{D}^H = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \left[ I - \varepsilon_y(\Phi) \right]^T \mathbf{D} \left[ I - \varepsilon_y(\Phi) \right] \, dy.$$  (22)

Differentiation of the above equation with respect to a material distribution parameter, $\beta$, yields

$$\frac{\partial \mathbf{D}^H}{\partial \beta} = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \left[ I - \varepsilon_y(\Phi) \right]^T \frac{\partial \mathbf{D}}{\partial \beta} \left[ I - \varepsilon_y(\Phi) \right] \, dy -$$

$$\frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \left[ I - \varepsilon_y(\Phi) \right]^T \mathbf{D} \varepsilon_y \left( \frac{\partial \phi}{\partial \beta} \right) \, dy.$$  (23)

Considering (5) and the characteristics of $\phi$ and $\partial \phi / \partial \beta$, which are all $Y$-periodic possible displace functions, the last two items of the former equation are zero. Thus, the sensitivities of material elastic properties with respect to distribution parameter are written as

$$\frac{\partial \mathbf{D}^H}{\partial \beta} = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \left[ I - \varepsilon_y(\Phi) \right]^T \frac{\partial \mathbf{D}}{\partial \beta} \left[ I - \varepsilon_y(\Phi) \right] \, dy.$$  (24)

The above equation shows that the sensitivity with respect to the distribution parameter depends on the general displacement parameter and the derivative of the elastic properties with respect to $\beta$.

The above equation is not suitable for evaluation of the sensitivity with respect to the shape parameter which will change the original cellular domain $\mathcal{Y}$. In the following, a mapping method will be presented for determining the sensitivity with respect to the shape parameter of the base cell. The base cell is assumed to be rectangular, because a rectangular period, maybe not the minimum period, can be found for any kind of microstructure of materials. The ratio of the length of the base cell to its width is taken as a shape parameter and design variable, $x_1 = a$. By calculating the differential of (19), we obtain

$$\frac{\partial \mathbf{D}^H}{\partial a} = \frac{\partial K^{-1}}{\partial a} \mathbf{D}^H K^{-1} +$$

$$K^{-1} \frac{\partial \mathbf{D}^H}{\partial a} K^{-1} + K^{-1} \mathbf{D}^H \frac{\partial K^{-1}}{\partial a}.$$  (25)

Taking note that matrix $K$ and variable $a$ are relational results in

$$\mathbf{K} = \begin{bmatrix} 1/a^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1/a \end{bmatrix}, \quad \mathbf{K}^{-1} = \begin{bmatrix} a^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & a \end{bmatrix},$$  (26)
and
\[
\frac{\partial \mathbf{K}}{\partial a} = \begin{bmatrix}
-2/a^2 & 0 & 0
0 & 0 & 0
0 & 0 & -1/a^2
\end{bmatrix}
= \frac{1}{a^2} \begin{bmatrix}
2/a & 0 & 0
0 & 0 & 0
0 & 0 & 1
\end{bmatrix}.
\] (27)

Furthermore
\[
\frac{\partial \mathbf{K}^{-1}}{\partial a} = \begin{bmatrix}
2a & 0 & 0
0 & 0 & 0
0 & 0 & 1
\end{bmatrix}.
\] (28)

Hereinafter the sensitivity about \( \mathbf{D}^H \) will be discussed. It is obvious that the shape of current unit-cell domain \( Z \) is stationary with regard to variable \( a \). At the same time the variation of \( a \) will change the material properties \( \mathbf{D}^H \). The sensitivity of \( \mathbf{D}^H \) can be written via (24) as
\[
\frac{\partial \mathbf{D}^H}{\partial a} = \frac{1}{|Z|} \int_{Z} \left[ \mathbf{I} - \mathbf{\varepsilon}_z(\Phi) \right]^T \frac{\partial \mathbf{D}}{\partial a} \left[ \mathbf{I} - \mathbf{\varepsilon}_z(\Phi) \right] \, dz, \] (29)
where
\[
\frac{\partial \mathbf{D}}{\partial a} = \frac{\partial \mathbf{K}}{\partial a} \mathbf{K} + \mathbf{K} \frac{\partial \mathbf{K}}{\partial a}.
\] (30)

According to the above discussion can we summarize that the general procedure for calculating the sensitivity of macro-material properties with respect to the shape parameter of a unit-cell by using the mapping method has the following steps.

1. Compute the equivalent material coefficients \( \mathbf{D}^H \) of the dual problem and \( \mathbf{H} \mathbf{D}^H \) of the original problem.
2. Calculate the sensitivity of \( \mathbf{K} \) and \( \mathbf{K}^{-1} \) using (27) and (28).
3. Compute the sensitivity of dual material coefficients, \( \partial \mathbf{D}/\partial a \), by use of (30).
4. Calculate the sensitivity of equivalent material coefficients \( \mathbf{D}^H \) of the dual problem, \( \partial \mathbf{D}^H /\partial a \), via (29).
5. Obtain \( \partial \mathbf{D}^H /\partial a \), the sensitivity of equivalent material coefficients \( \mathbf{D}^H \) by use of (25).

4 Numerical results

For verifying the correctness of the mapping method in computing equivalent material properties and their sensitivities, a porous material of aluminum \((E = 6.958 \times 10^4 \text{ Mpa}, \mu = 0.1348)\) with uniformly distributed rectangular holes is considered. The periodic microstructure and a base cell are shown in Fig. 2. The aspect ratio of the rectangular base cell, \( k = a/b \) is chosen as the shape parameter.

The elastic property of this porous aluminum with the aspect ratio \( k = 1.5 \) is computed by use of the numerical homogenization method, and by the mapping method proposed in this paper in the case that the initial given as-

| Table 1 Sensitivities of the elastic properties of material when \( b = 1 \), \( k = a/b = 1 \) |
|---|---|---|---|---|---|
| \( k = 1.000 \) | \( k = 1.010 \) | \( k = 1.00 \) | \( \Delta k = 0.010 \) | \( \Delta k = 0.001 \) | \( \Delta k = 0.001 \) |
| \( D_{11} \) | 39606.28 | 39640.41 | 39609.69 | 3413.0 | 3410.0 | 3410.2 |
| \( D_{22} \) | 39606.28 | 39572.54 | 39602.87 | -3374.0 | -3410.0 | -3410.2 |
| \( D_{12} \) | 8286.173 | 8286.162 | 8286.173 | -1.1 | 0.0 | 0.0 |
| \( D_{33} \) | 7450.181 | 7449.736 | 7450.177 | -44.5 | -4.0 | -4.0 |
The sensitivities of the elastic properties of the material with respect to the shape parameter $k$ (aspect ratio) are evaluated when the aspect ratio is 1 and 1.5, and the porous fraction is 25%. The results are compared with sensitivities obtained by use of the finite difference method. The sensitivities of the elements of the elastic matrix agree well with the data obtained by finite differential method with 0.001 of the perturbation of the aspect ratio, see Tables 1 and 2. Finite difference method needs to compute the material properties for a perturbed shape parameter, thus, re-meshing work of the domain with changed shape must be done. Besides, it is always difficult to select an appropriate perturbation step to obtain accurate sensitivity. By mapping method, the sensitivity analysis problem is defined on the initial given domain, the re-meshing work in saved. Thus, the mapping method is very effective in calculate the material properties and their sensitivity.

5 Conclusions

In this paper, a mapping method is proposed for computing the material properties and the sensitivities of the material properties with respect to the shape parameter of the base cell. This method converted a variable definition domain problem into fixed definition domain problem, which makes it easy to calculate the effective material properties and their sensitivities with respect to the shape parameters. Using this method to compute the sensitivity information can improve significantly the efficiency of the design optimization of materials with specific properties. A numerical example shows its effectiveness and accuracy.

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