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INVERSE STOCHASTIC HOMOGENIZATION OF A PARTICLE REINFORCED COMPOSITE MATERIAL WITH A FUNCTION APPROXIMATION APPROACH

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Abstract. *This paper describes a new computational methodology for the inverse stochastic homogenization problem. The inverse stochastic homogenization analysis will be performed for identifying a microscopic random variation in a microstructure of a heterogeneous material such as a composite material from a set of observed probabilistic characteristics of the homogenized material properties. In the previous paper, the Monte-Carlo simulation-based approach has been proposed, but it takes a high computational cost. For this problem, a function-approximation based inverse stochastic homogenization analysis is proposed in this paper. With employing a single point approximation called the perturbation approach or a multi point approximation called the polynomial based response function approach, an inverse stochastic homogenization problem for a particle reinforced composite material is solved. From the numerical results, accuracy and effectiveness of the proposed approach will be discussed.*

Keywords: *Inverse Stochastic Homogenization, Polynomial Approximation, Perturbation, Particle Reinforced Composite Material, Homogenization Method.*

1. INTRODUCTION

Since a microscopic random variation of a component material of a heterogeneous material causes a random response of a homogenized material property or a microscopic stress field, influence of the microscopic random variation on each scales should be investigated. From this reason, the stochastic homogenization analysis has been studied [1][3][8]. In order to improve accuracy of the analysis, the approximation based approaches have been also reported [2][4]. In addition, some results on the multiscale stochastic stress analysis of a composite material considering a microscopic random variation have been reported recently[5][6].

It can be recognized that a microscopic random variation will have an influence on a macroscopic and microscopic stress field, and therefore it will be very important in reliability evaluation of a composite structure. In the previous reports, numerical analysis has been performed with assuming a degree and the kind of microscopic random variation, but it will be difficult to be identified in practical.

From this reason, an inverse stochastic homogenization analysis procedure will be needed for identifying a random variation in a microstructure. Sakata et al proposed the concept of the inverse stochastic homogenization problem[7]. In the previous report, the authors proposed an inverse stochastic homogenization analysis method with employing the Monte-Carlo simulation and the function mapping technique. However, in case of using the homogenization method with the finite element method which can be applied to a complex microstructure or multiscale stress analysis problem, it will take a high computational cost, and therefore a new methodology for identifying a microscopic random variation at a lower cost will be needed.

In this study, a new approach for the inverse stochastic homogenization analysis of a particle reinforced composite material considering a random variation of an elastic property of a component material is developed. A new proposed method employs a function approximation technique, and it enables to reduce a computational effort to estimate a microscopic random variation. In this presentation, outline and detailed procedure for the proposed method are introduced.

Several approaches, for example, based on a single-point approximation with the perturbation method or multipoint approximation with a polynomial regression will be presented.

With the numerical results, accuracy and effectiveness of each proposed method for the inverse stochastic homogenization problem will be discussed.

2. INVERSE STOCHASTIC HOMOGENIZATION PROBLEM

A microscopic random variation of a microscopic stress field in a composite material will be caused by random variations of both macroscopic quantities as shape and size of a structure or boundary conditions like loading conditions or displacement conditions and microscopic quantities as geometry or material properties of component materials.

The stochastic homogenization analysis aims to reveal influence of a microscopic random variation on a homogenized material property, namely, a macroscopic quantity. A random variation of a homogenized material property will cause a random variation of a macroscopic response such as a displacement or strain field, this analysis will be important for reliability evaluation or the validation and verification process in computational mechanics for a composite structure.

Since the microscopic stress filed will also take an influence of a microscopic random variation, the multiscale stochastic stress analysis will be also very important. However, in general, a random variation of a microscopic quantity will be difficult to be measured especially after manufacturing. From this reason, a methodology for identifying a microscopic random variation of a composite structure from a known property will be needed.

Figure 1 illustrates outline of a (direct) stochastic homogenization, multiscale stochastic stress analysis and the inverse stochastic homogenization problem. As shown in Fig.1, in a general stochastic homogenization problem or a multiscale stochastic stress analysis problem, a degree and the kind of the microscopic random variation is assumed to be known quantity.

On the other hand, in the inverse stochastic homogenization problem, it is assumed that the random variation of the macroscopic quantities are known and the microscopic random variation is an unknown variable to be identified.

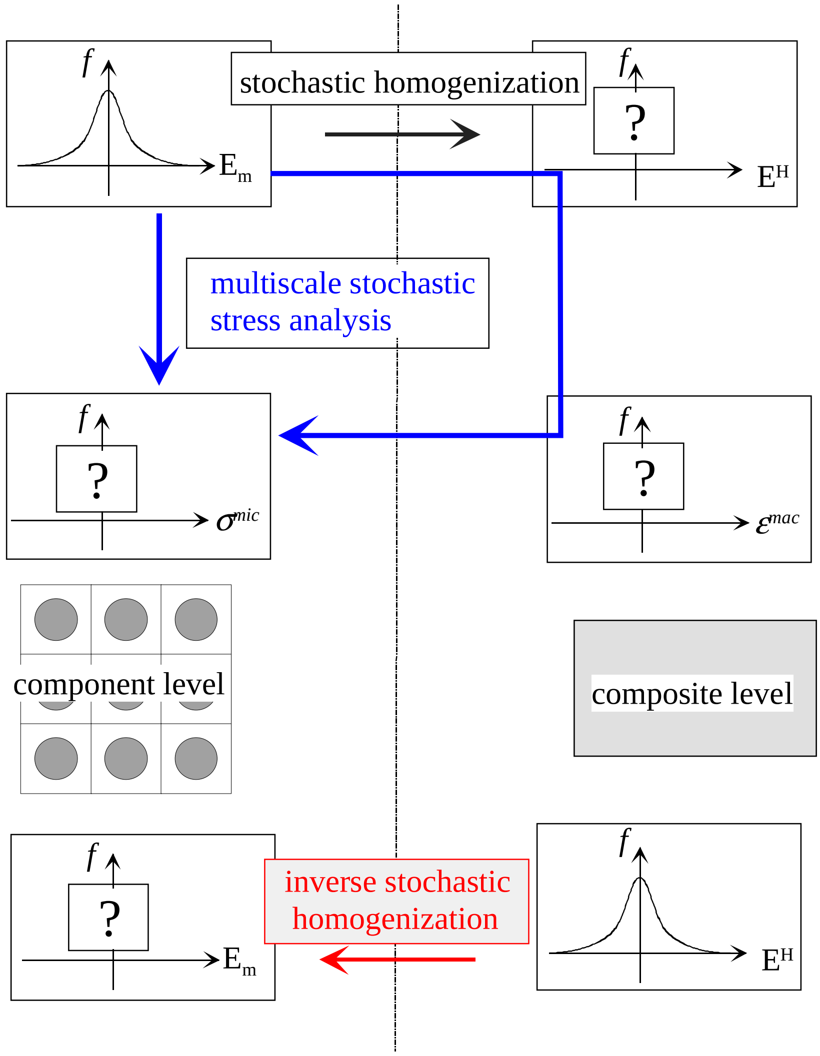

Figure 1. Outline of the direct and inverse stochastic homogenization and multiscale stochastic stress analysis problems

3. FUNCTION APPROXIMATION-BASED INVERSE STOCHASTIC HOMOGENIZATION

3.1. Function approximation-based Stochastic homogenization

It is assumed that a microscopic quantity such as an elastic property or geometry of a microstructure have a random variation, and the observed value of the microscopic quantity X^* can be expressed with its expected value X^0 and a normarized random variable α as follows.

$$X^* = X^0(1+\alpha). \tag{1}$$

In this case, with the perturbation theory, the observed value of the homogenized material property (the elastic tensor in this case) will be expressed as the following form.

$$E^{H*} \approx E^{H0} + E^{H1}\alpha + E^{H2}\alpha^2 + \cdots + E^{Hi}\alpha^i + \cdots \tag{2}$$

where the superscript *H* shows the homogenized property and the superscript *i* shows the *i*th perturbation term. With the perturbation-based approach, each order perturbation term can be obtained as each order derivative with respect to the random variable at an expansion point.

If the random variable α distributes according to the Gaussian distribution, one can use the *i*-th order approximation-second moment method. In this case, the expected value $\mathrm{Exp}[\ ]$ and variance $\mathrm{Var}[\ ]$ can be estimated with the following form.

$$\mathrm{Exp}\left[E^H\right] = E^{H0} + \sum_i \sum_j E^{H2}{}_{ij} \operatorname{cov}\left[\alpha_i, \alpha_j\right] + \cdots. \tag{3}$$

$$\begin{aligned}\mathrm{Var}\left[E^H\right] = \sum_i \sum_j E^{H1}{}_i E^{H1}{}_j \operatorname{cov}\left[\alpha_i, \alpha_j\right] + \sum_i \sum_j \sum_k \sum_l E^{H2}{}_{ij} E^{H2}{}_{kl} \\ \times \left(\mathrm{E}\left[\alpha_i, \alpha_j, \alpha_k, \alpha_l\right] - \operatorname{cov}\left[\alpha_i, \alpha_j\right] \operatorname{cov}\left[\alpha_k, \alpha_l\right]\right) + \cdots\end{aligned}. \tag{4}$$

where cov means the covariance and $\mathrm{E}[\ ]$ shows each order probabilistic moment.

Since eq.(2) can be regarded as a polynomial approximation of the stochastic response of the homogenized elastic tensor with respect to the random variable α, each coefficient can be also determined with a function approximation approach such as the least square method.

When the least square method is employed, the following problem will be solved for determining the surrogate model of the response function.

$$\left.\begin{array}{ll} \text{find} & E^H{}_{p_1 p_2 \cdots p_m} \\ \text{to minimize} & f = \displaystyle\sum_{j=1}^{ns} \left(E^{H*}\left(\boldsymbol{\alpha}_j\right) - \widehat{E^{H*}}\left(\boldsymbol{\alpha}_j\right)\right)^2 \\ \text{s.t.} & \widehat{E^{H*}}\left(\boldsymbol{\alpha}\right) = \sum E^H{}_{p_1 p_2 \cdots p_m} \alpha_1{}^{p1} \alpha_2{}^{p2} \cdots \alpha_m{}^{p_m} \end{array}\right\}. \tag{5}$$

where *ns* shows the number of samples. If only one random variation is taken into account, eq.(5) can be simply rewritten as

$$\left.\begin{array}{ll} \text{find} & E^{H0}, E^{H1}, E^{H2} \cdots \\ \text{to minimize} & f = \displaystyle\sum_{j}^{ns} \left(E^{H*}\left(\boldsymbol{\alpha}_j\right) - \widehat{E^{H*}}\left(\boldsymbol{\alpha}_j\right)\right)^2 \\ \text{s.t.} & \widehat{E^{H*}}\left(\boldsymbol{\alpha}\right) = \displaystyle\sum_i E^{Hi} \alpha^i \end{array}\right\}. \tag{6}$$

In order to minimize the objective function f showing the difference between the exact and approximated response of the homogenized quantity for the microscopic random variation, a general optimization algorithm such as the mathematical programming or a heuristic method can be employed.

From the viewpoint of the function approximation, the perturbation-based approach can be regarded as the single point approximation, while the latter approaches can be classified as the multi-point approximation.

3.2. Inverse Stochastic homogenization with a function approximation

With the above-mentioned approximation-based stochastic homogenization approaches, namely the perturbation based approach or the polynomial response function approach, each order coefficients (perturbation terms) can be determined. From the assumption on the problem setting, namely the variance of the homogenized elastic property is known, the CV (coefficient of variance) can be estimated with the following procedure.

To simplify, it is considered the case that only one microscopic quantity has a random variation. In this case, at first, from the first order second moment method, the CV of the microscopic random variation can be simply computed as follows.

$$\mathrm{cov}[\alpha,\alpha]=\frac{\mathrm{Var}\left[E^{H}\right]}{\left(E^{H1}\right)^{2}}. \tag{7}$$

In case of using a higher order approximation, the following optimization problem can be solved for estimating the CV of the microscopic quantity.

$$\left.\begin{array}{ll} \text{find} & \mathrm{cov}[\alpha,\alpha] \\ \text{to minimize} & \left(\mathrm{Var}\left[E^{H}\right]-\widehat{\mathrm{Var}}\left[E^{H}\right]\right)^{2} \end{array}\right\}. \tag{8}$$

where $\widehat{\mathrm{Var}}[\ ]$ is the estimated variance with the approximated response function and ith-order second moment method. It should be noted that eq.(8) may have multiple solutions in case of using a higher order approximation. In this paper, eq.(8) is solved with a mathemtatical programming method, and when a solution with *i*th order approximation is searched, the obtained optimum solution with assuming *i*-1th order approximatin is used as the initial value for the local optimization.

4. NUMERICAL RESULTS

4.1. Problem settings

In this paper, a square-arranged particle reinforced composite material is assumed as a target material. A schematic view of the particle reinforced composite material is illustrated in Fig,2 and the finite element model of the unit cell is illustrated in Fig.3. The properties of the fiber and the matrix are employed correspond to E-glass and epoxy resin. The expected values of the elastic properties are listed in table 1.

As a microscopic random variation, the case of single random variation independent to other elastic properties is considered. For example, if Young's modulus of resign is randomly varied, other properties are not changing. The volume fraction of particle is 0.3, and the microscopic random variable distributes according to the Gaussian distribution.

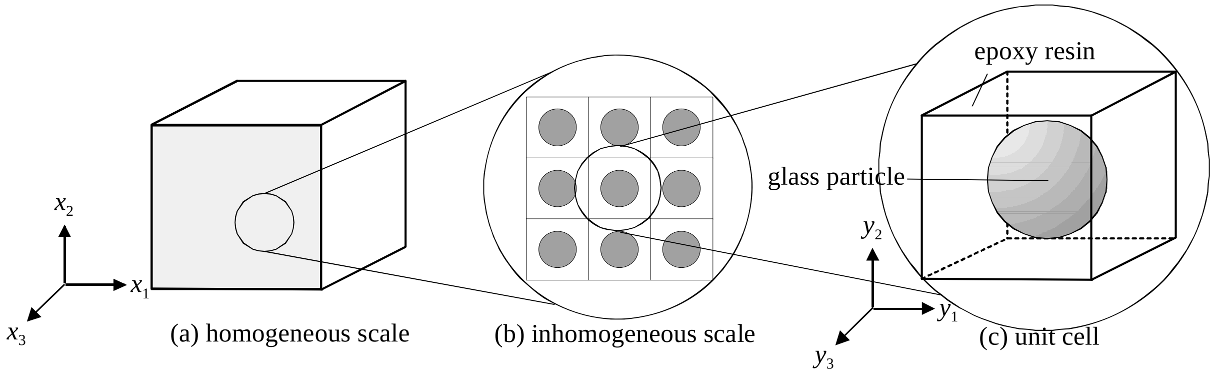

Figure 2. Schematic view of a square-arranged particle reinforced composite material.

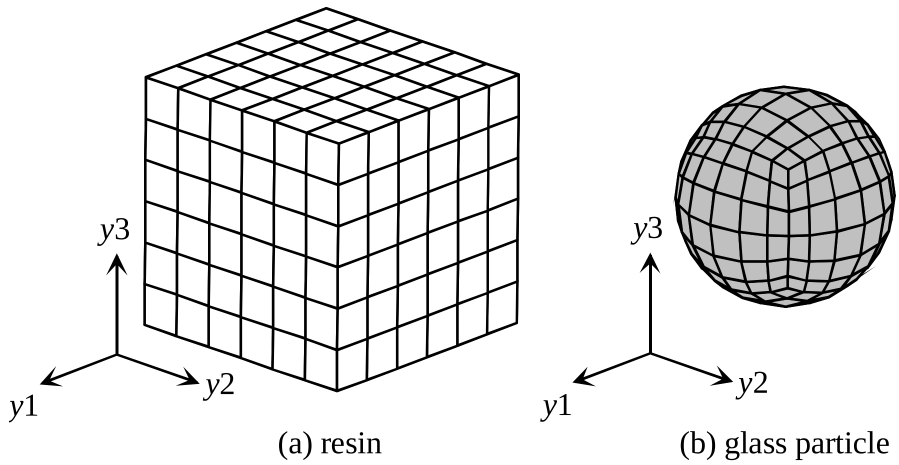

Figure 3. Finite element mesh of the unit cell.

Table 1.Material properties

	Young's modulus (MPa)	Poisson's ratio
Epoxy	4.5	0.39
E-glass	73.0	0.22

In order to construct a surrogate model expressing the random response of the equivalent elastic properties of the particle reinforced composite material with the polynomial response function, 21 sampling points are generated within a certain range of the microscopic random variable in case of the multi-point approximation.

4.2. Results

In this paper, the relative estimation error between the exact CV of the microscopic random variatble and the estimated one with the approximation-based approaches are investigated. The relative error in estimated solution with the perturbation-based approach and the polynomial based approach are compared. In this case, 1st, 2nd and 3rd order approximations are used for the analysis. In case of the multi point approximation, influence of the sampling range is also investigated.

As examples, the relative estimation error for the CV[E_m] estimation from the CV[E^H] and the error for the CV[ν_m] estimation from the CV[ν^H] estimation are iilustrated in Figs. 4 and 5. The legend in the fugres shows the order of the polynomial based approximation. The sampling range shows the normalized range for sampling. For example, 0.1 means $-0.05 \le \alpha \le 0.05$

From Fig.4, it is recognized the proposed approach with both the perturbation-based method and the polynomial approximation approach gives good solutions. The relative estimation error is less than 1%, and each order perturbation-based approach gives better solutions. In case of using the function approximation approach, a better solution can be obtained when an appropreate sampling range and a higher order approximation, but if a low order approximation is employed, the accuracy becomes worse in using a samples within a wide renge.

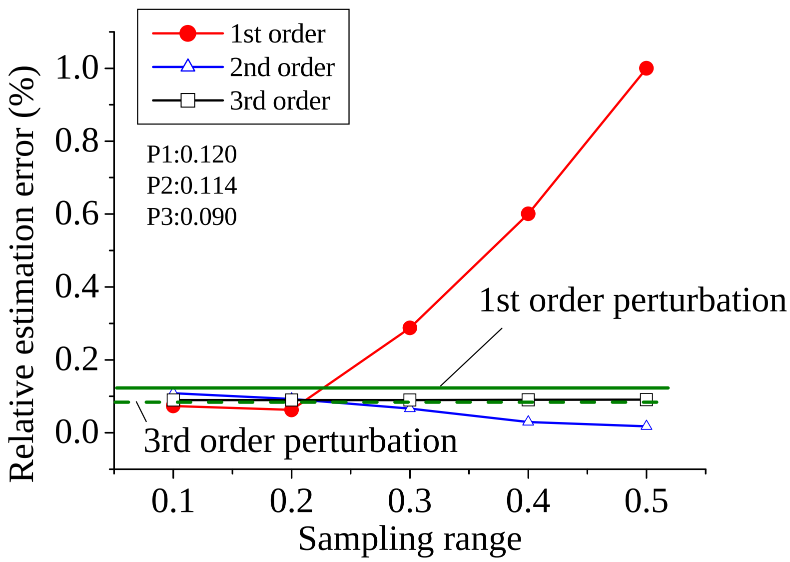

Figure 4. Relative estimation error with the perturbation-based approach and the multipoint approximation for each sampling range. (CV[E_m] estimation from CV[E^H]).

In case of the CV[ν_m] estimation, the estimation errors are larger than the case of the CV[E_m] estimation, which is similar to the case of the direct stochastic homogenization. However, from Fig.5, it can be recognized that a higher order perturbation can give an accurate solution with less than 0.5 % relative estimation error. Also, the multi point approximation based approach also gives better solution especially in case of using the third order approximation, though a low order approximation cannot give an accurate solution. In addition, it should be noted that the multi point approximation with the third order polynomial gives a better solution than the third order perturbation with an appropriate sampling range. Since the perturbation based approach may not always give an accurate estimation in some cases even if a higher order perturbation is used, this result shows possibility of the multi point function approximation based approach for accuracy improvement of the inverse stochastic homogenization analysis.

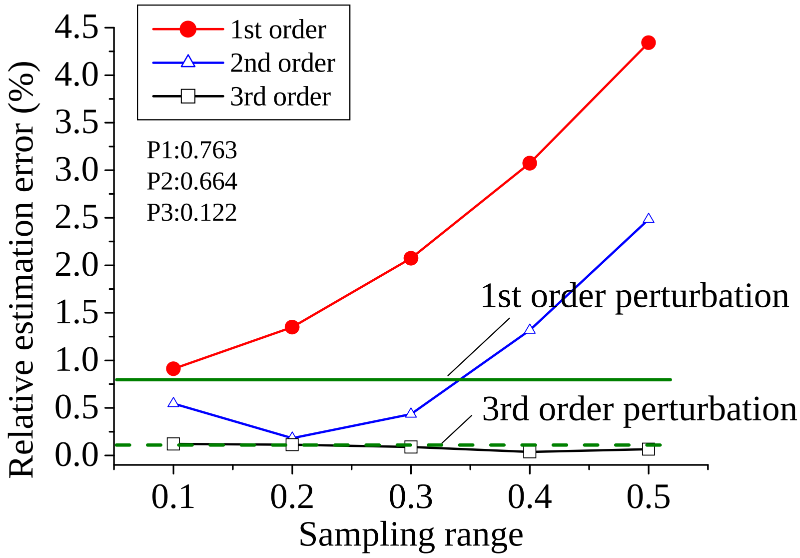

Figure 5. Relative estimation error with the perturbation-based approach and the multipoint approximation for each sampling range. (CV[ν_m] estimation from CV[ν^H]).

5. CONCLUSION

In this paper, the approximatin-based inverse stochastic homogenization analysis methods are proposed. One is the single point approximation approach called the perturbation -based approach, and the other is the multi point approximation approach like the polynoimal based response function approch. The proposed approach is applied for solving the inverse stochatic homogenization problem of a particle reinforced composite material.

From the numerical results, it can be recognized that both the proposed approximation-based approach can be useful for the inverse stochastic homogenization analysis. In the presented case, the third order perturbation method gives an enough accurate solution. Also, the multi-point approximation approach gives good results when an appropreate sampling range can be selected.

In addition, a higher order function approximation-based approach gives a better solution than the 3rd order perturbation approach in some cases, and this result shows possibility of the multi-point approximation based approach for the inverse stochastic homogenization analysis.

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