

# STOCHASTIC FE-BE METHOD FOR HOMOGENIZATION ANALYSIS OF 2-D DIFFUSION PROBLEMS CONSIDERING UNCERTAINTIES OF INCLUSION SHAPE

KAZUHIRO KORO<sup>1</sup>

<sup>1</sup> Niigata University, Department of Civil Engineering  
8050, Ikarashi 2-Nocho, Nishi-ku, Niigata, 950-2181, JAPAN  
kouro@eng.niigata-u.ac.jp and <http://applmech.eng.niigata-u.ac.jp/>

**Key words:** 2-D diffusion problems, homogenization method, spatial variation of inclusion shape, Karhunen-Loève expansion, stochastic FEM, stochastic collocation method.

**Abstract.** The stochastic method for homogenization analysis of diffusion problems considering uncertainties of inclusion shape is developed using a microscopic spectral stochastic BEM and a macroscopic FEM. The spatial variation of inclusion shape is modeled using Karhunen-Loeve expansion with exponential-type covariance kernels. The characteristic function on a 2-D unit cell and the homogenized diffusion tensor are calculated using the spectral stochastic BEM. The macroscale diffusion problems are solved using the stochastic FEM with the polynomial chaos (PC) expansion. Through numerical tests, the expected value and the standard deviation of the concentration in macroscale problems and their distribution are investigated.

## 1 INTRODUCTION

In order to investigate the material diffusion behavior within heterogeneous media, we attempt to estimate the effective diffusion properties and concentration fields through homogenized material diffusion models. The homogenization method is one of powerful tools for predicting the micro- and macroscopic diffusion behaviour. In the formulation, we assume the periodic microstructure represented by a unit cell, and realize scale separation of the material diffusion problems by considering an infinitesimal-size unit cell [1, 2].

In homogenization analysis, a simple geometrical shape and deterministic simulation tend to be adopted because of the simple concepts of infinitesimal periodic microstructure embedded in macroscopic homogenized media. The actual heterogeneous media have several uncertainty on inclusion geometry, arrangement and material properties. The authors [3, 4] has proposed the simulation method in which the homogenized diffusion tensor on the unit cell with spatial variation of inclusion shape is estimated by the spectral stochastic boundary element method (SSBEM) and the macroscopic behavior in homogenized media is simulated using the stochastic finite element method (SFEM). The spatial variation of inclusion shape is modeled by the Karhunen-Loève expansion [5]. The SSBEM analysis is based on the discretization using the

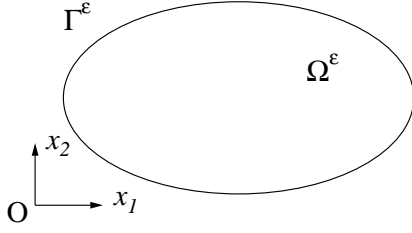


Figure 1: Problem description.

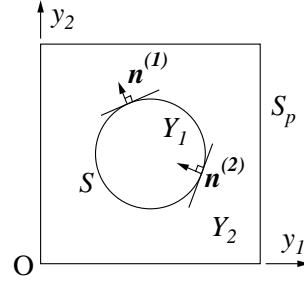


Figure 2: Unit cell.

polynomial chaos (PC) [5], which requires to deal with large degree of freedom of the linear algebraic equations: it is difficult to utilize the higher order function of PC. In [3, 4], we consider only the spatial variation of inclusion shape. The variations of inclusion shape and material parameters have never been considered simultaneously in BE-based homogenization analysis for microscopic heterogeneous media.

In the present paper, we develop the novel simulation method for homogenization analysis of 2-D diffusion problems considering spatial variation of inclusion shape. The deterministic BEM is used for evaluating the homogenized diffusion tensor components corresponding to many patterns of 2-D unit cell. The estimated diffusion tensor is defined as a form of the PC expansion, and is used as the input data of macroscopic diffusion analysis. The PC expansion coefficients of the homogenized diffusion tensor is evaluated by the least squares method in the stochastic collocation method (SCM) [6]. The main advantage of the SCM is to use the conventional deterministic BEM for predicting the homogenized tensor components. The macroscopic concentration field is simulated using the stochastic FEM. The response of the macroscopic concentration in a probability space is approximated with the polynomial chaos. The statistical characteristic values, e.g. the expected value and the standard deviation, is easily evaluated the PC expansion coefficients of the concentration field. The minor expansion of the present method thus enables us to consider the spatial variation of inclusion shape and variation of material parameters simultaneously. Through the numerical tests on a simple 2-D two-scale diffusion problem, we investigate the performance of the present simulation method for homogenized 2-D diffusion problems.

## 2 HOMOGENIZATION METHOD FOR 2-D DIFFUSION PROBLEMS

We now consider a 2-D diffusion problem with a heterogeneous media  $\Omega^\epsilon$  and a boundary  $\Gamma^\epsilon$ , as shown in Figure 1. The concentration  $C^\epsilon$  in the domain  $\Omega^\epsilon$  is governed by the following equation [1]:

$$\frac{\partial C^\epsilon}{\partial t}(\mathbf{x}, t) - \frac{\partial}{\partial x_i} \left[ K_{ij}^\epsilon \frac{\partial C^\epsilon}{\partial x_j}(\mathbf{x}, t) \right] = f(\mathbf{x}, t), \quad (1)$$

where  $K_{ij}^\epsilon$  is the diffusion tensor.

In the homogenization method [1, 2], we now assume that the heterogeneous media  $\Omega^\varepsilon$  have the periodic microstructure as represented in Figure 2. The scale factor  $\varepsilon$  is the ratio between the size of the unit cell  $Y$  and the size of  $\Omega^\varepsilon$ :  $\mathbf{y} = \mathbf{x}/\varepsilon$ . Introducing the asymptotic expansion of  $C^\varepsilon$  in Eq.(1) on small  $\varepsilon$  and imposing the convergence conditions at each order terms, we can derive the governing equations at micro- and macro-scale. The macroscale problems are then described as follows:

$$\frac{\partial C^0}{\partial t}(\mathbf{x}, t) - \frac{\partial}{\partial x_i} \left[ K_{ij}^* \frac{\partial C^0}{\partial x_j}(\mathbf{x}, t) \right] = f(\mathbf{x}, t), \quad (2)$$

where  $C^0$  is the 0th order term of the asymptotic expansion  $C^\varepsilon$ . The homogenized diffusion tensor  $K_{ij}^*$  is calculated with

$$K_{ij}^* = \frac{1}{|Y|} \int_Y K_{ik} \left( \delta_{kj} + \frac{\partial \omega_j}{\partial y_k}(\mathbf{y}) \right) dY \quad (3)$$

In Eq.(3), the characteristic function  $\omega_j(\mathbf{y})$  ( $j = 1, 2$ ) is governed by the following PDEs and boundary conditions:

$$\kappa^{(1)} \frac{\partial^2 \omega_j}{\partial y_i^2} = 0, \quad (\text{in } Y_1) \quad \kappa^{(2)} \frac{\partial^2 \omega_j}{\partial y_i^2} = 0, \quad (\text{in } Y_2) \quad (4)$$

$$\kappa^{(1)} \frac{\partial \omega_j}{\partial n^{(1)}} + \kappa^{(2)} \frac{\partial \omega_j}{\partial n^{(2)}} = -\kappa^{(1)} n_j^{(1)} - \kappa^{(2)} n_j^{(2)}, \quad (\text{on } S) \quad (5)$$

$$\text{periodic condition,} \quad (\text{on } S_p) \quad (6)$$

where  $Y_1$  and  $Y_2$  are the subdomain on the inclusion and the matrix in the unit cell  $Y$  shown in Figure 2, respectively. The diffusion tensor in  $Y_m$  is homogeneous as  $K_{ij}^{(m)} = \kappa^{(m)} \delta_{ij}$ .  $S$  is the interface between  $Y_1$  and  $Y_2$  and  $S_p$  is the outer boundary of the cell  $Y$ , on which the periodic condition is imposed.

### 3 BE-BASED HOMOGENIZATION ANALYSIS

In the homogenization analysis, we use the boundary element method (BEM) to approximately solve the periodic boundary value problems Eq.(4)-Eq.(6). The boundary integral equation corresponding to Eq.(4) is expressed as

$$\frac{1}{2} \omega_j^{(m)} + \int_{\partial Y_m} q^{*(m)} \omega_j^{(m)} d(\partial Y_m) = \int_{\partial Y_m} u^{*(m)} q_j^{(m)} d(\partial Y_m) \quad (7)$$

where the subscript “(m)” denotes the solution in the inclusion ( $m = 1$ ) and the matrix ( $m = 2$ ). The flux is  $q_j^{(m)} = \kappa^{(m)} \partial \omega_j^{(m)} / \partial n^{(m)}$ . The boundary is defined as  $\partial Y_1 = S$  and  $\partial Y_2 = S \cup S_p$ . Discretizing Eq.(7) using boundary elements and collocation method, we obtain the linear algebraic equations on the inclusion  $Y_1$  and the matrix  $Y_2$ , respectively. The conditions

Eqs. (5) and (6) are imposed into the algebraic equations. Solving the equations, we then obtain the approximations of the characteristic function  $\omega_j$  on  $S$  and  $S_p$  and the flux  $q_j^{(m)}$  on  $S$ .

The homogenized diffusion tensor  $K_{ij}^*$  is evaluated using the following equation which is obtained by integrating Eq.(3) by parts:

$$K_{ij}^* = \frac{1}{|Y|} \left[ \frac{1}{d} \left\{ \int_S \kappa^{(1)} y_m n_m^{(1)} dS + \int_{S \cup S_p} \kappa^{(2)} y_m n_m^{(2)} \right\} \delta_{ij} + \int_S \kappa^{(1)} n_i^{(1)} \omega_j^{(1)} dS + \int_{S \cup S_p} \kappa^{(2)} n_i^{(2)} \omega_j^{(2)} dS \right] \quad (8)$$

where  $d$  denotes the space dimensions of the problem:  $d = 2$ .

#### 4 STOCHASTIC MODELING OF SPATIAL VARIATION OF INCLUSION SHAPE

We next consider the stochastic model on spatial variation of inclusion shape. In the present paper, the spatial variation is described using the Karhunen-Loève expansion [5]. The variation of the simulated homogenized diffusion coefficients is evaluated by the stochastic collocation method[6].

We now define the coordinate  $s$  along the mean shape of the interface boundary  $S$ . The fluctuation of the boundary shape is regarded as a stochastic process on the  $s$  coordinate. The covariance kernel of the fluctuation at two points  $s_1$  and  $s_2$  on  $s$  is denoted by  $C(s_1, s_2)$ . Using the eigenvalues  $\lambda_i$  and the corresponding eigenfunctions  $f_i(s)$  of the covariance kernel, we now represent the uncertain boundary shape by the following truncated Karhunen-Loève expansion with  $N_{KL}$ :

$$S(s) = S_0 + \sum_{i=1}^{N_{KL}} \xi_i \sqrt{\lambda_i} f_i(s), \quad (9)$$

where  $\xi_i$  are the independent normal random variables, and  $S_0$  is the mean boundary shape of the interface boundary  $S$ . The homogenized diffusion tensor is then regarded as the function of the random variables  $\xi_i$  ( $i = 1, 2, \dots, N_{KL}$ ).

In the stochastic collocation method, the fluctuated interface boundaries  $S_\beta$  are generated using Eq.(9) and normal random variables  $\xi_i^{(\beta)}$  ( $\beta = 1, 2, \dots, N_s$ ). We then evaluate the homogenized diffusion tensor  $K_{ij,\beta}^*$  by the deterministic BE analysis on the following boundary  $S_\beta$ :

$$S_\beta(s) = S_0 + \sum_{i=1}^{N_{KL}} \xi_i^{(\beta)} \sqrt{\lambda_i} f_i(s), \quad (10)$$

The response of the homogenized diffusion tensor  $K_{ij}^*(\boldsymbol{\xi})$  in the probability space is approximated by the PC expansion as

$$K_{ij}^*(\boldsymbol{\xi}, \boldsymbol{\zeta}) = \sum_{\gamma=0}^{N_{PC}} K_{ij,\gamma}^* \Psi_\gamma(\boldsymbol{\xi}) \quad (11)$$

where  $K_{ij,\gamma}^*$  is the PC expansion coefficients of the homogenized diffusion tensor. The homogenized diffusion tensor  $K_{ij}^*(\boldsymbol{\xi}^{(\beta)})$  is the simulated results on the  $\beta$ th pseudo-random numbers  $\boldsymbol{\xi}^{(\beta)}$ , and then the following relation holds:

$$K_{ij}^*(\boldsymbol{\xi}^{(\beta)}) = K_{ij}^{*(\beta)} = \sum_{\gamma=0}^{N_{PC}} K_{ij,\gamma}^* \Psi_{\gamma}(\boldsymbol{\xi}^{(\beta)}) \quad (12)$$

In the present method, the expansion coefficients  $K_{ij,\gamma}^*$  is evaluated using the least squares method (LSM).

We now define the residual  $R$  in the LSM as

$$R(K_{ij,\gamma}^*) = \sum_{\beta=1}^{N_s} \left[ K_{ij}^{*(\beta)} - \sum_{\gamma=0}^{N_{PC}} K_{ij,\gamma}^* \Psi_{\gamma}(\boldsymbol{\xi}^{(\beta)}) \right]^2 \quad (13)$$

The expansion coefficients are determined by minimizing the residual  $R$  as

$$\frac{\partial R}{\partial K_{ij,\gamma}^*} = \sum_{\beta=1}^{N_s} \left[ K_{ij}^{*(\beta)} - \sum_{m=0}^{N_{PC}} K_{ij,m}^* \Psi_m(\boldsymbol{\xi}^{(\beta)}) \right] \Psi_{\gamma}(\boldsymbol{\xi}^{(\beta)}) = 0 \quad (14)$$

where  $\gamma = 0, 1, \dots, N_{PC}$ . The expansion coefficients  $K_{ij,m}^*$  ( $m = 0, 1, \dots, N_{PC}$ ) are thus obtained by solving Eq.(14) which is a system of linear algebraic equation.

## 5 STOCHASTIC FE ANALYSIS FOR MACROSCALE DIFFUSION PROBLEMS

We now solve the macroscopic boundary value problem Eq.(2) using the stochastic finite element method (SFEM) with the polynomial chaos (PC) expansion. The PC expansion is used to discretize the macroscale concentration  $C^0$  in the probability space. Applying the weighted residual method to Eq.(2) and substituting Eq.(11) into the resulting equation, we then obtain as follows:

$$\int_{\Omega} \frac{\partial C^0}{\partial t} w_c d\Omega + \int_{\Omega} \left( \sum_{l=0}^{N_{PC}} K_{ik}^{*(l)} \Psi_l(\boldsymbol{\xi}, \boldsymbol{\zeta}) \right) \frac{\partial C^0}{\partial x_k} \frac{\partial w_c}{\partial x_i} d\Omega = \int_{\Gamma_q} (\phi_i n_i) w_c d\Gamma + \int_{\Omega} f w_c d\Omega \quad (15)$$

where  $\phi_i = K_{ik}^* \partial C^0 / \partial x_k$ , and  $w_c$  is the weighting function. The space discretization by the finite element method (FEM) results in the following equation:

$$[\mathbf{M}]\{\dot{\mathbf{C}}^0\} + \sum_{l=0}^{N_{PC}} \Psi_l(\boldsymbol{\xi}) [\mathbf{K}^{(l)}]\{\mathbf{C}^0\} = \{\mathbf{f}\} \quad (16)$$

We next introduce the PC expansion into the nodal value vector  $\{\mathbf{C}^0\}$  of the concentration  $C^0$  as

$$\{\mathbf{C}^0\} = \sum_{m=0}^{\tilde{N}_{PC}} \Psi_m(\boldsymbol{\sigma}) \{\mathbf{C}_m^0\} \quad (17)$$

Substituting Eq.(17) into Eq.(16) and calculating the expected value with the homogeneous chaos  $\Psi_\alpha$  as weights, we have

$$\sum_{m=0}^{\tilde{N}_{PC}} \langle \Psi_m \Psi_\alpha \rangle [\mathbf{M}] \{ \dot{\mathbf{C}}^0 \} + \sum_{m=0}^{\tilde{N}_{PC}} \sum_{l=0}^{N_{PC}} \langle \Psi_m \Psi_l \Psi_\alpha \rangle [\mathbf{K}^{(l)}] \{ \mathbf{C}_m^0 \} = \langle \Psi_\alpha \rangle \{ \mathbf{f} \} \quad (18)$$

where  $\alpha = 0, 1, \dots, \tilde{N}_{pc}$ . The concentration  $C^0(t)$  at every time step can be obtained by applying the time-marching scheme into Eq.(18). The expected value  $\langle \{ \mathbf{C}^0 \} \rangle$  and the standard deviation  $\sigma_C$  are evaluated with

$$\langle \{ \mathbf{C}^0 \} \rangle = \{ \mathbf{C}_0^0 \}, \quad \sigma_C = \left[ \sum_{m=1}^{\tilde{N}_{PC}} (C_m^0)^2 \right]^{1/2} \quad (19)$$

## 6 NUMERICAL RESULTS

We now evaluate the homogenized diffusion tensor of the 2-D unit cell as shown in Figure 3, and simulate the macroscale concentration  $C^0$  using the present method. The unit cell consists of an inclusion and a matrix. The mean shape of the inclusion have the circular shape with the radius  $\bar{R}$ . In the present numerical tests, we prescribe into  $\bar{R} = 0.2$  and the coefficients of variation  $\delta_R = 10\%$ . The covariance kernel  $C$  is given by

$$C(\theta_1, \theta_2) = (\delta_R \bar{R})^2 \exp \left[ -\frac{d(\theta_1, \theta_2)}{b} \right] \quad (20)$$

$$d = \min\{|\theta_1, \theta_2|, 2\pi - |\theta_1, \theta_2|\}, b = 1/2\pi$$

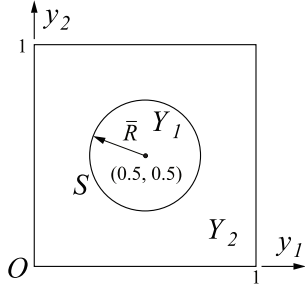
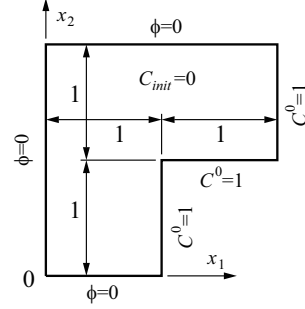
The number of terms on the truncated Karhunen-Loève expansion is  $N_{KL} = 5$ , and the polynomial chaos is given by 1st-order Hermite polynomials. The number of terms on the polynomial chaos is then  $N_{PC} = N_{KL} = 5$ , and  $\tilde{N}_{PC} = 5$ .

The sample macroscale problem is described into the initial- boundary value problem as shown in Figure 4. The macroscopic concentration  $C^0$  is approximated using the 1st-order polynomial chaos:  $\Phi_0 = 1$ ,  $\Psi_i = \xi_i$  ( $i = 1, 2, 3, 4, 5$ ).

In the macroscale analysis, we use 3-node triangular elements for discretizing the weak form Eq.(15), and the 4th-order Runge-Kutta scheme is adopted as the time-marching scheme.

Table 1 indicates the simulated results on the expected values and the standard deviation of the homogenized diffusion tensor  $K_{11}^*$  and  $K_{12}^*$ . The simulated results of the homogenized diffusion tensor components  $K_{11}^*$  and  $K_{12}^*$  can be evaluated with the number of random number pattern  $N_s \leq 500$ . These results are comparable to those of the Monte Carlo Simulation (MCS) simulation.

The simulated PC expansion coefficients of the homogenized diffusion tensor  $K_{ij,\gamma}^*$  for  $N_s = 500$  are tabulated in Table 2. The FE analysis for macroscale diffusion problems shown in Figure 4 is carried out using the present PC expansion coefficients.


**Figure 3:** Sample 2-D unit cell.

**Figure 4:** Sample macroscale problem.

**Table 1:** Expected value and standard deviation of homogenized diffusion tensor components  $K_{11}^*$  and  $K_{12}^*$ . The spatial variation of the inclusion shape is considered.

(a) Expected value.			(b) Standard deviation.		
$N_s$	$\langle K_{11}^* \rangle$	$\langle K_{12}^* \rangle$	$N_s$	$\sigma_{K_{11}^*}$	$\sigma_{K_{12}^*}$
100	0.23726	$6.8108 \times 10^{-6}$	100	$4.3914 \times 10^{-3}$	$1.7186 \times 10^{-3}$
200	0.23725	$2.3157 \times 10^{-6}$	200	$4.4808 \times 10^{-3}$	$1.7135 \times 10^{-3}$
500	0.23727	$5.9626 \times 10^{-6}$	500	$4.4769 \times 10^{-3}$	$1.7019 \times 10^{-3}$
1000	0.23729	$-7.8033 \times 10^{-6}$	1000	$4.4315 \times 10^{-3}$	$1.6962 \times 10^{-3}$
2000	0.23728	$2.8547 \times 10^{-6}$	2000	$4.4352 \times 10^{-3}$	$1.6990 \times 10^{-3}$

Figure 5 depicts the simulated expected value  $\langle C^0 \rangle$  and the standard deviation  $\sigma_{C^0}$  of the macroscale concentration  $C^0$  at  $t = 0.08$ . The initial- and the boundary conditions are prescribed as shown in Figure 4. The influence of the spatial variation of inclusion shape on the simulation results realizes as the standard deviation of the simulated macroscale concentration  $C^0$ . The expected value  $\langle C^0 \rangle$  depends on the distance between an observation point and the sub-boundaries with  $C^0 = 1$ . The standard deviation  $\sigma_{C^0}$  amplifies around the point (1.85, 1.15) with equal distance from the sub-boundaries  $x_1 = 2$  or  $x_2 = 1$ .

## 7 CONSIDERATION OF VARIATION OF DIFFUSION COEFFICIENTS

The expansion of present method enables us to analyze the homogenization problems with not only the spatial variation of inclusion shape but also the variation of the diffusion coefficients of the ingredients. We now assume that the diffusion coefficients of the inclusion and the matrix  $\kappa^{(1)}$  and  $\kappa^{(2)}$  have the variation subjected to the normal distribution. The diffusion coefficients is described using the independent standard normal random variables  $\zeta_1$  and  $\zeta_2$  as

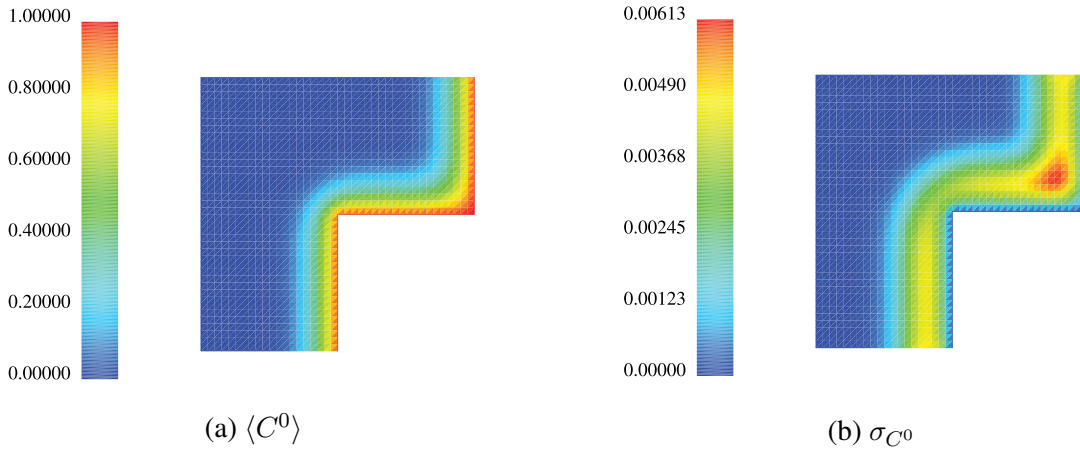
$$\kappa^{(1)} = \bar{\kappa}^{(1)} + \sigma_{\kappa^{(1)}} \zeta_1, \quad \kappa^{(2)} = \bar{\kappa}^{(2)} + \sigma_{\kappa^{(2)}} \zeta_2 \quad (21)$$

where  $\bar{\kappa}^{(m)}$  and  $\sigma_{\kappa^{(m)}}$  ( $m = 1, 2$ ) are the mean value and the standard deviation of  $\kappa^{(m)}$ , respectively. In stochastic collocation method, we have to carry out the deterministic BE-based

**Table 2:** The PC expansion coefficients  $K_{ij,\gamma}^*$  of the homogenized diffusion tensor  $K_{ij}^*$ .  $K_{21,\gamma} = K_{12,\gamma}^*$  and  $K_{22,\gamma}^*$ .

$ij$	$\gamma$	$\Psi_\gamma$	$K_{ij,\gamma}^*$
11	0	1	0.23727
	1	$\xi_1$	$4.0888 \times 10^{-3}$
	2	$\xi_2$	$-3.5637 \times 10^{-5}$
	3	$\xi_3$	$-2.0867 \times 10^{-5}$
	4	$\xi_4$	$-2.3775 \times 10^{-4}$
	5	$\xi_5$	$1.8071 \times 10^{-3}$

$ij$	$\gamma$	$\Psi_\gamma$	$K_{ij,\gamma}^*$
12	0	1	$3.2845 \times 10^{-6}$
	1	$\xi_1$	$5.9626 \times 10^{-6}$
	2	$\xi_2$	$7.9785 \times 10^{-6}$
	3	$\xi_3$	$5.7690 \times 10^{-7}$
	4	$\xi_4$	$-7.2237 \times 10^{-3}$
	5	$\xi_5$	$-1.6864 \times 10^{-3}$



**Figure 5:** The expected value  $\langle C^0 \rangle$  and the standard deviation  $\sigma_{C^0}$  of the macroscopic concentration  $C^0$  at  $t = 0.08$ . The spatial variation of the inclusion shape is considered.

homogenization analysis with the pseudo random numbers  $\xi_i^{(\beta)}$ ,  $\zeta_1^{(\beta)}$  and  $\zeta_2^{(\beta)}$ . The diffusion coefficients  $\kappa_1^{(\beta)}$  and  $\kappa_2^{(\beta)}$  are described by

$$\kappa_\beta^{(1)} = \bar{\kappa}^{(1)} + \sigma_{\kappa^{(1)}} \zeta_1^{(\beta)}, \quad \kappa_\beta^{(2)} = \bar{\kappa}^{(2)} + \sigma_{\kappa^{(2)}} \zeta_2^{(\beta)} \quad (22)$$

The diffusion tensors  $K_{ij}^{(1)}$  and  $K_{ij}^{(2)}$  are then given by  $K_{ij}^{(1)} = \kappa_1^{(\beta)} \delta_{ij}$  and  $K_{ij}^{(2)} = \kappa_2^{(\beta)} \delta_{ij}$ , respectively.

The homogenized diffusion tensor  $K_{ij}^*$  is then regarded as the function of the random variables  $\xi_i$  ( $i = 1, 2, \dots, N_{KL}$ ),  $\zeta_1$  and  $\zeta_2$ .

$$K_{ij}^*(\boldsymbol{\xi}, \boldsymbol{\zeta}) = \sum_{\gamma=0}^{N_{PC}} K_{ij,\gamma}^* \Psi_\gamma(\boldsymbol{\xi}, \boldsymbol{\zeta}) \quad (23)$$

where  $\xi_i$  is defined as Eq.(9).



**Table 3:** Expected value and standard deviation of homogenized diffusion tensor components  $K_{11}^*$  and  $K_{12}^*$ . The spatial variation of the inclusion shape and randomness of the diffusion coefficients are simultaneously considered.

(a) Expected values of $K_{11}^*$ and $K_{12}^*$ .			(b) Standard deviation of $K_{11}^*$ and $K_{12}^*$ .		
$N_s$	$\langle K_{11}^* \rangle$	$\langle K_{12}^* \rangle$	$N_s$	$\sigma_{K_{11}^*}$	$\sigma_{K_{12}^*}$
100	0.23694	$-6.5266 \times 10^{-6}$	100	$2.2447 \times 10^{-2}$	$1.6825 \times 10^{-3}$
200	0.23694	$-1.7873 \times 10^{-5}$	200	$2.2401 \times 10^{-2}$	$1.7109 \times 10^{-3}$
500	0.23698	$3.2845 \times 10^{-6}$	500	$2.2595 \times 10^{-2}$	$1.6687 \times 10^{-3}$
1000	0.23700	$-2.6574 \times 10^{-6}$	1000	$2.2486 \times 10^{-2}$	$1.6839 \times 10^{-3}$
2000	0.23700	$-1.0235 \times 10^{-6}$	2000	$2.2345 \times 10^{-2}$	$1.6973 \times 10^{-3}$

The expansion coefficients  $K_{ij,\gamma}^*$  in Eq.(23) are determined by minimizing the residual  $R$  as

$$R(K_{ij,\gamma}^*) = \sum_{\beta=1}^{N_s} \left[ K_{ij}^{*(\beta)} - \sum_{\gamma=0}^{N_{PC}} K_{ij,\gamma}^* \Psi_{\gamma}(\boldsymbol{\xi}^{(\beta)}, \boldsymbol{\zeta}^{(\beta)}) \right]^2 \quad (24)$$

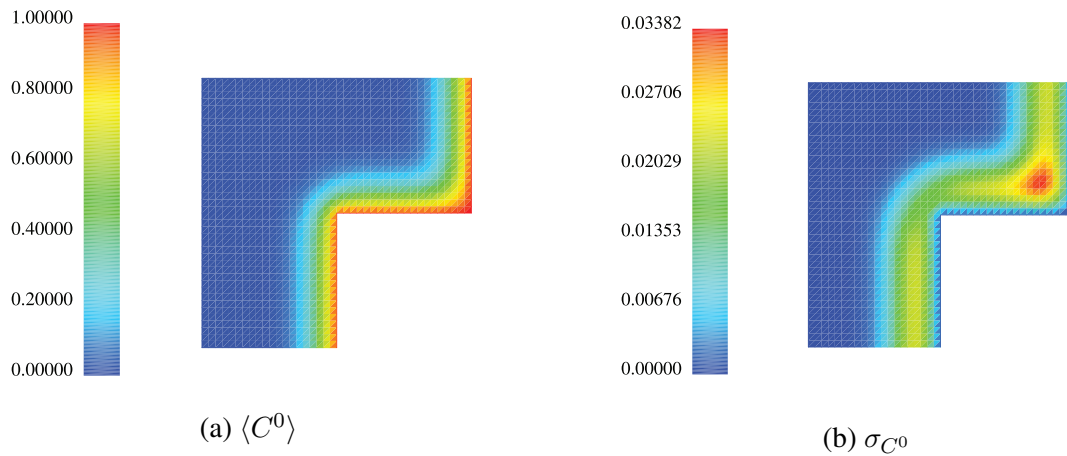
The macroscale problems can be solved with the FE-based method which is presented in the section 5.

Table 3 shows the simulation results of the expected values and the standard deviation of the homogenized diffusion tensor components  $K_{11}^*$  and  $K_{12}^*$  which are evaluated in the unit cell with spatial variation of inclusion shape and randomness of diffusion coefficients. In the present numerical tests, we prescribe  $\langle \kappa_1 \rangle = 1$ ,  $\sigma_{\kappa(1)} = 0.1$ ,  $\langle \kappa_2 \rangle = 0.2$  and  $\sigma_{\kappa(2)} = 0.02$ . The standard deviation of the homogenized diffusion tensor  $K_{ij}^*$  is about 500% of the results for considering only spatial variation of the inclusion shape: the coefficients of variation of the present homogenized tensor  $K_{11}^*$  are approximately 10%.

Figure 6 shows the expected values  $\langle C^0 \rangle$  and the standard deviation  $\sigma_{C^0}$  of the macroscopic concentration  $C^0$  for the initial- baoundary value problems (Figure 4) at  $t = 0.08$ . The distribution of the expected value  $\langle C^0 \rangle$  and the standard deviation  $\sigma_{C^0}$  are similar to the results shown in Figure 5.

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**Figure 6:** The expected value  $\langle C^0 \rangle$  and the standard deviation  $\sigma_{C^0}$  of the macroscopic concentration  $C^0$  at  $t = 0.08$ . The spatial variation of the inclusion shape and the variation of diffusion coefficients are considered.

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