Modelling steady moisture diffusion in functionally graded materials with the numerical manifold method

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Abstract. Due to the use of bi-cover systems, the numerical manifold method (NMM) is able to solve physical problems with non-conforming mathematical covers. In this work, the NMM is further extended to study steady-state moisture diffusion in 2D functionally graded materials (FGMs). Based on the governing equations, the NMM approximation and the weighted residual method, the NMM discrete equations are derived and the present method is verified through a typical example. Besides, the effect of the graded parameter of the FGMs on the moisture concentration is also investigated.

1. Introduction

Recent years, the numerical manifold method [1] has been drawing extensive attention due to its powerful capability in both continuous and discontinuous modeling, attributing to its dual cover systems, i.e., the mathematical cover (MC) and the physical cover (PC). The main features of the NMM can be summarized as: (1) the MC can be inconsistent with all the domain boundaries, which may reduce the discretization cost to some extent; (2) local physical properties can be represented naturally or through the use of special terms in the approximation; (3) higher-order approximation can be achieved through the use of higher-order local functions on a fixed MC.

Since its advent, the NMM has been applied to solve a variety of problems, e.g., see [2-18]. At present, the NMM is further developed to perform 2D steady moisture diffusion simulation in the functionally graded materials (FGMs), which are a new generation of composites with the volume fraction of the constituents changes gradually, producing a nonhomogeneous microstructure with continuously graded macro-properties. To this end, the remaining paper is organized as follows. The governing equation and associated boundary conditions are listed in Section 2; then, the NMM discrete equations for the concerned problems are provided in Section 3; following in Section 4, a typical numerical example is tested to verify the proposed method; finally, the concluding remarks are drawn in Section 5.

2. Statement of the problem

As shown in figure 1, steady moisture diffusion in a 2D isotropic FGM body Ω is considered. Ignoring any moisture source, the governing differential equation is expressed as [19]

$$\nabla(D(\mathbf{x})\nabla C) = 0 \tag{1}$$

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where ∇ is the gradient operator. D is the moisture diffusion coefficient, which varies with the domain point $\mathbf{x}=(x_1,x_2)$ for the FGMs, and C is the moisture concentration.

The associated boundary conditions are

$$C=\overline{C} \quad (\mathbf{x}\in\Gamma_C) \tag{2}$$

$$-D(\mathbf{x})\frac{\partial C}{\partial x_1}n_1-D(\mathbf{x})\frac{\partial C}{\partial x_2}n_2=\overline{f} \quad (\mathbf{x}\in\Gamma_f) \tag{3}$$

where ∂ denotes the partial derivative. $\overline{C}$ and $\overline{f}$ are, respectively, the applied moisture concentration on the essential boundary Γ_C and the enforced moisture flux on the natural boundary Γ_f. $(n_1,n_2)=\mathbf{n}$ is the outward unit normal to the domain as illustrated in figure 1.

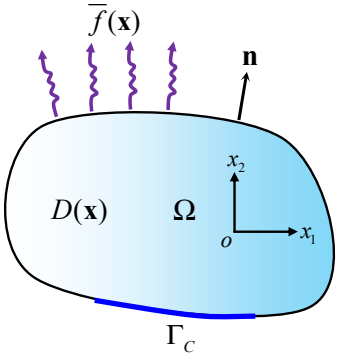


Figure 1. Steady-state moisture diffusion in an isotropic FGM body.

3. The NMM for steady-state moisture diffusion in FGMs

In the NMM, to simulate a given problem, we firstly built an MC, which is composed of a series of mathematical patches (MPs) and should be large enough to cover the whole physical domain. Generally, an MP is formed by arbitrarily-shaped mathematical elements and may be inconsistent with all domain boundaries. Next, the physical patches (PPs) are produced through the intersection of the MPs and the physical domain, and the collection of all PPs gives the PC. Following, the manifold elements (MEs) are generated through the common parts of as many as possible PPs.

Accordingly, the moisture concentration in an ME E is approximated as

$$C^h(\mathbf{x})=\sum_{i=1}^{n}w_i(\mathbf{x})C_i(\mathbf{x}) \tag{4}$$

where n is the number of total PPs shared by E. $w_i(\mathbf{x})$ is the partition of unity weight function defined on the MP containing the ith PP and frequently taken from the finite element shape functions for convenience. $C_i(\mathbf{x})$ is the local function defined on the ith PP. In continuous modeling, $C_i(\mathbf{x})$ is often given by

$$C_i(\mathbf{x})=\mathbf{P}(\mathbf{x})\mathbf{a}_i \tag{5}$$

where $\mathbf{a}_i$ is the vector of unknowns defined on the ith PP and $\mathbf{P}(\mathbf{x})$ is the polynomial basis being

$$\mathbf{P}(\mathbf{x}) = [1, x_1, x_2, ...] \tag{6}$$

Based on the governing equations (equations (1)-(3)), the NMM approximation (equation (4)) and the weighted residual method, the NMM discrete formulations for the present problem are derived as

$$\mathbf{KC} = \mathbf{F} \tag{7}$$

where $\mathbf{C}$ is the vector of all unknowns; $\mathbf{K}$ and $\mathbf{F}$ are, respectively, the global moisture diffusion matrix and the equivalent moisture load vector, both of which are computed ME by ME. The contributions of the ME E are

$$\mathbf{K}^E = \int_{\Omega^E} \mathbf{B}^{\mathbf{T}} D(\mathbf{x}) \mathbf{B} d\Omega + k \int_{\Gamma_C^E} (w_i \mathbf{P})^{\mathbf{T}} (w_i \mathbf{P}) d\Gamma \tag{8}$$

$$\mathbf{F}^E = k \int_{\Gamma_C^E} (w_i \mathbf{P})^{\mathbf{T}} \overline{C} d\Gamma - \int_{\Gamma_f^E} (w_i \mathbf{P})^{\mathbf{T}} \overline{f} d\Gamma \tag{9}$$

where the superscript $\mathbf{T}$ is the matrix transpose. Ω^E, Γ_C^E and Γ_f^E are, respectively, the domain, the essential boundary and the natural boundary associated with E. k is the penalty value for the enforcement of essential boundary condition in equation (2) because of the mismatch of the MC and the physical boundary. The matrix $\mathbf{B}$ is given in block form as

$$\mathbf{B} = [\mathbf{B}_1 \quad \mathbf{B}_2 \quad \cdots \quad \mathbf{B}_i \quad \cdots \quad \mathbf{B}_n] \tag{10}$$

with

$$\mathbf{B}_i = \begin{bmatrix} (w_i \mathbf{P})_{,1} \\ (w_i \mathbf{P})_{,2} \end{bmatrix} \tag{11}$$

where the subscript "$,i$ $(i = 1, 2)$" symbolizes the partial differential with respect to x_i.

4. Numerical example

Consider the steady-state moisture diffusion in a square FGM plate shown in figure 2. The width of the plate is W. The moisture concentrations on the left and right side are, respectively, $\overline{C_1}$ and $\overline{C_2}$, while other edges are insulated. The moisture diffusion coefficient is graded along x_1-axis as

$$D(\mathbf{x}) = D_0 e^{\alpha x_1} \tag{12}$$

where D_0 is a constant and α is the graded parameter.

In the NMM modeling, $W = 1.0$, $D_0 = 1.0$, $\overline{C_1} = 0.0$, $\overline{C_2} = 0.1$. Accordingly, the theoretical solution to the moisture concentration is obtained as

$$C = \overline{C}_2 \frac{e^{-\alpha x_1} - 1}{e^{-\alpha W} - 1} \tag{13}$$

When simulating, an MC composed of square mathematical elements is used. The discretized domain when the MC size (i.e., the edge length of the mathematical element) h =0.05 is provided in figure 3, which contains 441 PPs and 400 MEs. Besides, the polynomial basis in equation (6) is chosen to be constant, and the penalty factor k in equation (8) and (9) is taken as $1.0\times10^{10}D_0$.

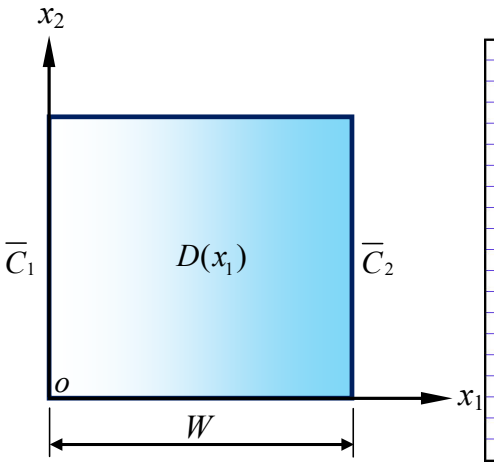


Figure 2. Steady moisture diffusion in an FGM plate.

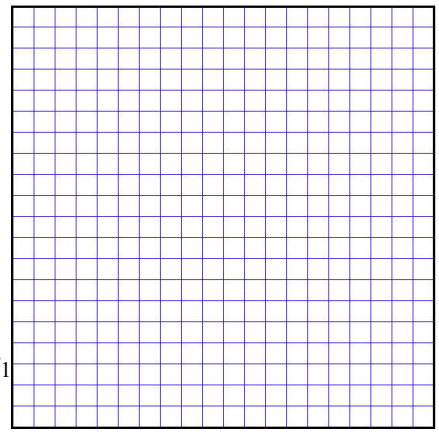
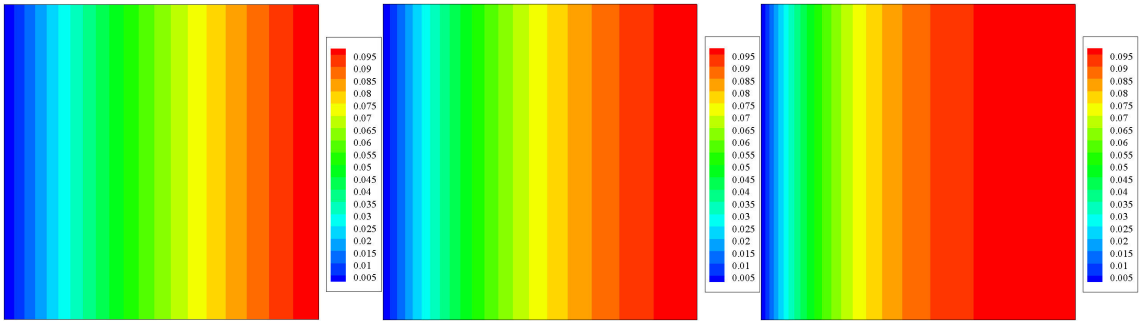


Figure 3. Discretized plate when h=0.05.

In the computations, we mainly investigate the effect of the graded parameter on the moisture concentration field. For this purpose, three cases with $\alpha=1$, 2 and 4 are sequentially tested. The distribution of the moisture concentration in the whole domain at different α is illustrated in figure 4, which suggests that the moisture concentrations change with α and vary only along the horizontal direction, as demonstrated by equation (13).

The calculated moisture concentrations at some sample points, i.e., (0.1, 0.1), (0.2, 0.2) … and (0.9, 0.9) by the NMM are plotted in figure 5, together with the analytical solutions from equation (13). It is easy to find that the present results conform well to the exact ones. Moreover, we can also see that the moisture concentration at a fixed point increases with α.



(a) (b) (c)

Figure 4. Distribution of moisture concentration field: (a) α=1, (b) α=2 and (c) α=4.

5. Concluding remarks

In this paper, the numerical manifold method was further extended to study 2D steady moisture diffusion problems in the FGMs. The corresponding governing equation, boundary conditions and the NMM discrete equations are presented. A typical example is investigated to verify the proposed

method. Regular MC formed by square mathematical elements was adopted to discretize the domain since the MPs may be independent of all physical boundaries. The nice agreement between the NMM results and the analytical ones clearly displays the excellent accuracy of the present approach.

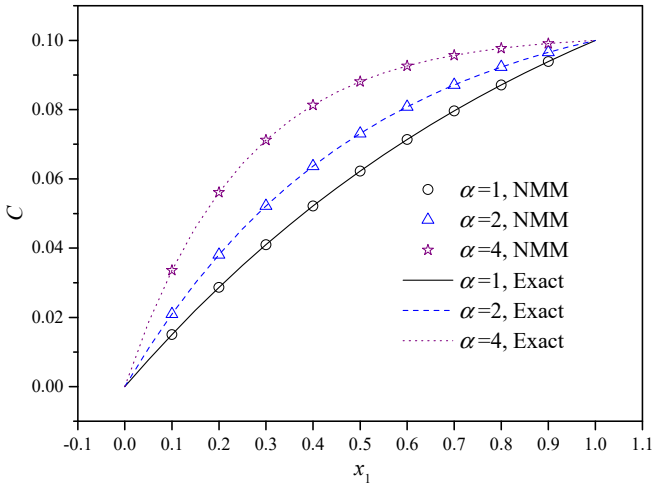


Figure 5. The computed moisture concentrations at different points and graded parameters.

Compared with some other well-known numerical tools (e.g., the finite element method) for continuous diffusion problems, the major advantage of the NMM lies in discretization, where boundary-inconsistent MC is allowed. In addition, as described in Section 1, since the local properties can be captured essentially or by the incorporation of special basis into the NMM approximation, the extension of the present method to other moisture diffusion cases involving discontinuities such as material interfaces or cracks is straightforward.

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