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Variational eigenstrain multiscale finite element method

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Abstract

A new subgrid (subscale) finite element method is proposed, which is termed as *the variational eigenstrain multiscale method*. It combines the essential ideas of Hughes' variational multiscale formulation [Comput. Methods Appl. Mech. Engrg. 127 (1995) 387] with Eshelby's inclusion theory [Proc. R. Soc. Lond. A 252 (1957) 561] and Mura's equivalent eigenstrain principle [Micromechanics of Defects in Solids, Martinus Nijhoff Publisher, 1987] to homogenize numerical error due to finite element discretization.

By synthesizing variational multiscale method with the equivalent eigenstrain principle, we have developed a new finite element formulation that can automatically homogenize its own discretization errors so that it may attain better accuracy in a coarse scale finite element computation than that of the original coarse scale finite element computation. The paper provides the theoretical foundation of the method as well as two numerical examples that illustrate and validate the proposed method.

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1. Introduction

The so-called variational multiscale method invented by Hughes et al. [7–9] is a computational paradigm that is capable of dealing with multiscale phenomena. On the other hand, the so-called equivalent eigenstrain principle, which was established by Eshelby [3,4] and was later perfected by Mura [11], is a homogenization method in micromechanics that has been used in many engineering applications.

The proposed variational multiscale method is a new subscale method that combines the essential ideas of both methods and synthesizes them to formulate a "genetically adaptive" finite element formulation that is capable of correcting its own discretization errors. The basic idea of the new method is:

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The residue strains of the coarse scale solution are viewed as a form of eigenstrains due to numerical discretization, which will generate a disturbance field or correction displacement field that is viewed as the fine scale solution. By homogenizing the displacement fields at the two different scales, one may derive an self-adjusting, or "smart" weak formulation that is capable of minimizing discretization error for a given mesh.

In this approach, one finds the fine scale solution by utilizing Eshelby's eigenstrain formulation or single inclusion solution. By substituting the fine scale solution into the coarse scale weak formulation, one can form a new homogenized coarse scale weak form, subsequently solves the homogenized coarse scale problem, and obtains a numerical solution with better accuracy.

It should be noted that the multiscale homogenization method proposed in this paper is different from the widely spread *asymptotic multiscale homogenization methods* (e.g. Sanchez-Palencia [13], Guedes and Kikuchi [5], Tong and Mei [17] and many others). There is no physical inhomogeneities involved in the problems discussed here. The fictitious inhomogeneities, or eigenstrains, are numerical errors due to mesh discretization. By homogenizing the discretization error, we hope to achieve better accuracy with minimum computations.

This article is organized as follows. In Section 2, we first formulate the variational multiscale eigenstrain theory for two-dimensional linear elasticity problems. Section 3 describes the corresponding discrete finite element formulation and implementation. Two numerical examples are presented in Section 4 and a few remarks are made in Section 5.

2. Variational eigenstrain multiscale formulation

In this paper, we formulate a variational eigenstrain multiscale formulation in the context of linear elasticity theory.

Consider a simply connected domain, $\Omega \in \mathbb{R}^d$ (*d* is the dimension of the physical space and in the rest of the paper d = 2 unless otherwise is indicated). Displacement boundary conditions and traction boundary conditions are prescribed on the boundary of $\Gamma_u \cup \Gamma_t = \partial \Omega$ and $\Gamma_u \cap \Gamma_t = \emptyset$. We are interested in the following boundary-value problem of elastostatics:

$$\sigma_{ji,j} + b_i = 0, \quad \forall \mathbf{x} \in \Omega, \tag{2.1}$$

$$u_i = u_i^0, \quad \forall \mathbf{x} \in \Gamma_u, \tag{2.2}$$

$$\sigma_{ij}n_j = t_i^0, \quad \forall \mathbf{x} \in \Gamma_t, \tag{2.3}$$

where σ_{ij} is the Cauchy stress components that are linked with infinitesimal strain components by the generalized Hooke's law,

$$\sigma_{ij} = C_{ijk\ell} \epsilon_{k\ell},$$

and $C_{ijk\ell}$ is the elastic tensor. The infinitesimal strain is defined as the symmetric part of displacement gradient,

$$\epsilon_{ij} = u_{(i,j)} = \frac{1}{2} (u_{i,j} + u_{j,i}).$$

Define the trial function and test function spaces

$$\mathscr{S} = \Big\{ \mathbf{u}(\mathbf{x}) | \mathbf{u}(\mathbf{x}) \in [H^1(\Omega)]^d, \ \mathbf{u} = \mathbf{u}^0, \ \forall \mathbf{x} \in \Gamma_u \Big\},$$
(2.4)

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$$\mathscr{V} = \left\{ \mathbf{w}(\mathbf{x}) | \mathbf{w}(\mathbf{x}) \in [H^1(\Omega)]^d, \ \mathbf{w} = \mathbf{0}, \ \forall \mathbf{x} \in \Gamma_u \right\}.$$
(2.5)

Note that standard notations in functional analysis (e.g. Adams [1] or Brenner and Scott [2]) are used here without elaboration.

The variational statement of the above boundary-value problem is:

Find $\mathbf{u} \in \mathscr{S}$ such that

$$\int_{\Omega} w_{(i,j)} C_{ijk\ell} u_{(k,\ell)} \, \mathrm{d}\Omega = \int_{\Omega} w_i b_i \, \mathrm{d}\Omega + \int_{\Gamma_t} w_i t_i^0 \, \mathrm{d}S, \quad \forall \mathbf{w} = w_i \mathbf{e}_i \in \mathscr{V},$$
(2.6)

where \mathbf{e}_i is the basis vector for the Cartesian coordinate.

Define three bi-linear forms

$$a(\mathbf{w},\mathbf{u}): \mathscr{V} \times \mathscr{S} \to \mathbb{R}, \quad a(\mathbf{w},\mathbf{u}):= \int_{\Omega} (\nabla \otimes \mathbf{w}): \mathbf{C}: (\nabla \otimes \mathbf{u}) \,\mathrm{d}\Omega,$$
(2.7)

$$(\mathbf{w}, \mathbf{b})_{\Omega} : \mathscr{V} \times [H^{-1}(\Omega)]^d \to \mathbb{R}, \quad (\mathbf{w}, \mathbf{b}) := \int_{\Omega} \mathbf{w} \cdot \mathbf{b} \, \mathrm{d}\Omega,$$
 (2.8)

$$(\mathbf{w},\mathbf{t})_{\Gamma_t}: [H^{1/2}(\Omega)]^d \times [H^{1/2}(\Omega)]^d \to \mathbb{R}, \quad (\mathbf{w},\mathbf{t})_{\Gamma_t}:=\int_{\Gamma_t} \mathbf{w} \cdot \mathbf{t} \, \mathrm{d}S.$$
(2.9)

We can then rewrite the weak form (2.6) as

$$a(\mathbf{w}, \mathbf{u}) = (\mathbf{w}, \mathbf{b})_{\Omega} + (\mathbf{w}, \mathbf{t}^0)_{\Gamma_t}, \quad \forall \mathbf{w} \in \mathscr{V}.$$
(2.10)

2.1. Two-scale formulation

Following Hughes et al. [9], we assume that the solution of the weak form (2.10) can be decomposed into two solutions with different spatial resolutions, i.e.

$$\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}',\tag{2.11}$$

$$\mathbf{w} = \overline{\mathbf{w}} + \mathbf{w}',\tag{2.12}$$

where $\overline{\mathbf{u}}$ and $\overline{\mathbf{w}}$ may be viewed as the coarse scale weak trial and test solutions; whereas \mathbf{u}' and \mathbf{w}' may be viewed the fine scale trial and test solutions.

Accordingly, we can decompose the trial function space and test function space into the direct sum of coarse scale space and fine scale space, i.e. $\mathscr{S} = \overline{\mathscr{S}} \oplus \mathscr{S}'$ and $\mathscr{V} = \overline{\mathscr{V}} \oplus \mathscr{V}'$.

We adopt the assumptions made by Hughes et al. [9] that on the boundary

$$\overline{\mathbf{u}}(\mathbf{x}) = \mathbf{u}_0, \quad \forall \mathbf{x} \in \Gamma_u, \text{ and } \overline{\mathbf{u}} \in \overline{\mathscr{S}}, \tag{2.13}$$

$$\mathbf{u}'(\mathbf{x}) = 0, \quad \forall \mathbf{x} \in \Gamma_u, \text{ and } \mathbf{u}' \in \mathscr{S}',$$
(2.14)

$$\overline{\mathbf{w}}(\mathbf{x}) = 0, \quad \forall \mathbf{x} \in \Gamma_u, \text{ and } \overline{\mathbf{w}} \in \overline{\mathscr{V}},$$
(2.15)

$$\mathbf{w}'(\mathbf{x}) = 0, \quad \forall \mathbf{x} \in \Gamma_u, \text{ and } \mathbf{w}' \in \mathscr{V}'.$$
 (2.16)

The weak form (2.10) then becomes

$$a(\overline{\mathbf{w}} + \mathbf{w}', \overline{\mathbf{u}} + \mathbf{u}') = (\overline{\mathbf{w}} + \mathbf{w}', \mathbf{b})_{\Omega} + (\overline{\mathbf{w}} + \mathbf{w}', \mathbf{t}^0)_{\Gamma_{\ell}}.$$

Since \overline{w} and w' are independent, one can obtain the weak formulations at different scales, i.e.

$$a(\overline{\mathbf{w}},\overline{\mathbf{u}}) + a(\overline{\mathbf{w}},\mathbf{u}') = (\overline{\mathbf{w}},\mathbf{b})_{\Omega} + (\overline{\mathbf{w}},\mathbf{t}^0)_{\Gamma_L}, \qquad (2.17)$$

$$a(\mathbf{w}', \overline{\mathbf{u}}) + a(\mathbf{w}', \mathbf{u}') = (\mathbf{w}', \mathbf{b})_{\Omega} + (\mathbf{w}', \mathbf{t}^0)_{\Gamma_t}.$$
(2.18)

Assume that the bi-linear form between the fine scale test function and the prescribed traction vector is negligible, i.e.

$$(\mathbf{w}',\mathbf{t}^0)_{\Gamma_t}=0$$

It is not difficult to show that the solution of weak form (2.18) is the weak solution of the following boundary value problem (e.g. Renardy and Rogers [12]):

$$C_{ijk\ell}u'_{k,\ell i} + C_{ijk\ell}\overline{u}_{k,\ell j} + b_i = 0, \quad \forall \mathbf{x} \in \Omega,$$

$$(2.19)$$

$$u_i' = 0, \quad \forall \mathbf{x} \in \Gamma_u, \tag{2.20}$$

$$\sigma'_{ij}n_j \approx 0, \quad \forall \mathbf{x} \in \Gamma_t.$$

In Eq. (2.19), the term $\overline{R}_i = C_{ijk\ell}\overline{u}_{k,\ell} + b_i \neq 0$ is the residual of the coarse scale solution, or the residual of the resolved scale, which will not be zero since coarse scale numerical solution is not the exact solution. Moreover, the distribution of this residual is not homogeneous over the whole domain. We may replace this term by an equivalent term with equivalent eigenstrains

$$\overline{R}_i = C_{ijk\ell} \overline{u}_{k,\ell j} + b_i =: -C_{ijk\ell} \epsilon^*_{k\ell,j}.$$

We can then solve the fine scale displacement field as the disturbance field driven by the residual of the coarse scale displacement field, or the equivalent eigenstrain. In other words, by solving the BVP (2.19)–(2.21), we may be able to express the fine scale solution in terms of the residual of the coarse scale solution. Using the terminology of micromechanics (e.g. Mura [11]), we are utilizing Eshelby's inclusion solution to express a subgrid fine scale correction due to the numerical error of coarse scale discretization. In principle, the fine scale solution of Eqs. (2.19)–(2.21) may be solved and can be expressed in the following form:

$$u'_{(i,j)}(\mathbf{x}) = T_{ijk\ell} \epsilon^*_{k\ell}(\overline{\mathbf{u}}, \mathbf{b}, \mathbf{x}).$$
(2.22)

Here $T_{ijk\ell}$ is an abstract transformation operator and the eigenstrains are functions of coarse scale solution, $\mathbf{\bar{u}}$, body force **b**, and spatial coordinates.

Substituting (2.22) into the equilibrium equation, we may obtain the following equilibrium equation:

$$\left[C_{ijk\ell}(\overline{u}_{(k,\ell)} + T_{k\ell mn}\epsilon^*_{mn})\right]_{,i} + b_i = 0.$$
(2.23)

Because ϵ_{ij}^* are related with $\overline{u}_{(i,j)}$, we may eventually find a homogenized elastic tensor, $C_{ijk\ell}^{\rm H}$, and a homogenized body force, $b_i^{\rm H}$, so it allows us to derive a homogenized equilibrium equation at coarse scale

$$\left[C_{ijk\ell}^{\mathrm{H}}\overline{u}_{(k,\ell)}\right]_{,j} + b_{i}^{\mathrm{H}} = 0, \qquad (2.24)$$

together with the homogenized boundary conditions

$$\overline{u}_i = u_i^{\mathrm{H}}, \quad \forall \mathbf{x} \in \Gamma_u, \tag{2.25}$$

$$\overline{\sigma}_{ji}n_j = t_i^{\mathrm{H}}, \quad \forall \mathbf{x} \in \Gamma_t, \tag{2.26}$$

and the corresponding coarse scale weak formulation:

Find $\overline{\mathbf{u}} \in \mathscr{S}$ such that

$$\int_{\Omega} \overline{w}_{(i,j)} C^{\mathrm{H}}_{ijk\ell} \overline{u}_{(k,\ell)} \,\mathrm{d}\Omega = \int_{\Omega} \overline{w}_i b^{\mathrm{H}}_i \,\mathrm{d}\Omega + \int_{\Gamma_l} \overline{w}_i t^{\mathrm{H}}_i \,\mathrm{d}S, \quad \forall \overline{\mathbf{w}} = \overline{w}_i \mathbf{e}_i \in \mathscr{V}.$$
(2.27)

The objective of the new method is to find the homogenized elastic stiffness tensor or the corresponding finite element stiffness matrix, and to replace the initial coarse scale weak formulation with the homogenized weak formulation (2.27), which has the ability to adjust discretization error automatically. By doing so, it is believed that the coarse scale solution of homogenized weak formulation (2.27) could be more accurate than the naive coarse scale solution of (2.6) with virtually the same computational cost.

In contrast to the early version of variational multiscale method, the proposed variational eigenstrain multiscale method solves the fine scale solution analytically, or analytically in approximation. There are different ways to obtain the fine scale solution. In what follows, we discuss the three approaches that we have explored so far.

2.2. Fine scale solution: (I) global G-Galerkin solution

In the first approach, we consider the following global Galerkin weak form associated with the Green's function of the original Euler–Lagrange equation (G-Galerkin weak form), i.e.

$$\int_{\Omega} G_{mi}^{\infty}(\mathbf{y} - \mathbf{x}) \Big\{ C_{ijk\ell} u'_{k,\ell j}(\mathbf{x}) + C_{ijk\ell} \overline{u}_{k,\ell j}(\mathbf{x}) + b_i(\mathbf{x}) \Big\} d\Omega = 0, \quad \forall \mathbf{y} \in \Omega,$$
(2.28)

where the symbol, $G_{mi}^{\infty}(\mathbf{x}, \mathbf{y})$, denotes the Green's function of the Navier's equation in an infinite domain, which is the solution of the following BVP:

$$C_{ijk\ell}G_{mk,\ell j}^{\infty}(\mathbf{y}-\mathbf{x}) + \delta_{mi}\delta(\mathbf{y}-\mathbf{x}) = 0, \quad \forall \mathbf{x}, \ \mathbf{y} \in \mathbb{R}^d,$$
(2.29)

$$G_{mk}^{\infty}(\mathbf{y} - \mathbf{x}) \to 0, \ \mathbf{x}, \ \text{or} \ \mathbf{y} \to \infty.$$
 (2.30)

Using Somigliana's identity [14], one may write that

$$u_{i}^{\prime}(\mathbf{y}) = \int_{\Omega} (C_{mnk\ell} \overline{u}_{k,\ell n} + b_{m}) G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\partial\Omega} \sigma_{mn}^{\prime}(\mathbf{x}) n_{n} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}S_{x} + \int_{\partial\Omega} \sigma_{k\ell}^{G_{i}^{\infty}}(\mathbf{y} - \mathbf{x}) n_{\ell} u_{k}^{\prime}(\mathbf{x}) \, \mathrm{d}S_{x},$$
(2.31)

where

$$\sigma_{k\ell}^{G_k^{\infty}}(\mathbf{y} - \mathbf{x}) := C_{mnk\ell} G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}),$$
(2.32)

$$\sigma'_{mn}(\mathbf{x}) := C_{mnk\ell} u'_{(k,\ell)}(\mathbf{x}).$$
(2.33)

Integration by parts of (2.31) yields

$$u_{i}'(\mathbf{y}) = \int_{\Omega} (C_{mnk\ell} \overline{u}_{k,\ell}) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) d\Omega_{x} + \int_{\Omega} b_{m} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) d\Omega_{x} + \int_{\partial\Omega} (\sigma_{mn}'(\mathbf{x}) + \overline{\sigma}_{mn}(\mathbf{x})) n_{n} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) dS_{x} + \int_{\partial\Omega} \sigma_{k\ell}^{G_{i}^{\infty}}(\mathbf{y} - \mathbf{x}) n_{\ell} u_{k}'(\mathbf{x}) dS_{x},$$
(2.34)

where

r

$$\overline{\sigma}_{mn}(\mathbf{x}) := C_{mnk\ell} \overline{u}_{(k,\ell)}(\mathbf{x}). \tag{2.35}$$

Based on the boundary conditions (2.20) and (2.21), we have

$$\int_{\partial Q} \sigma_{k\ell}^{G_m^{\infty}}(\mathbf{y} - \mathbf{x}) n_\ell u_k'(\mathbf{x}) \, \mathrm{d}S_x = 0, \tag{2.36}$$

$$\int_{\partial\Omega} \sigma'_{ij} n_j G^{\infty}_{im} \,\mathrm{d}S_x = 0. \tag{2.37}$$

To this end, we obtain an estimate for the fine scale solution

$$u_{i}'(\mathbf{y}) \approx \int_{\Omega} \left(C_{mnk\ell} \overline{u}_{k,\ell} \right) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\Omega} b_{m} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\partial\Omega} \overline{\sigma}_{mn}(\mathbf{x}) n_{n} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}S_{x}.$$
(2.38)

As a first step approximation, we neglect the contribution from the boundary term in Eq. (2.38). Subsequently

$$u_i'(\mathbf{y}) \approx \int_{\Omega} \left(C_{mnk\ell} \overline{u}_{k,\ell} \right) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_x + \int_{\Omega} b_m G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_x.$$
(2.39)

We consider the following assumptions on discretization error:

1. The discretization error of an individual element, e, is uniformly distributed on a hypersphere, Ω_e^c (a sphere in 3D and a circle in 2D), which is the minimum size hypersphere that can encompass the element, e, as shown in Fig. 1. Precisely speaking

$$\langle \overline{u}_{(i,j)} \rangle_{\Omega_{\alpha}^{c}} = \langle \overline{u}_{(i,j)}^{e} \rangle_{\Omega_{\alpha}}.$$
(2.40)

- 2. The fine scale solution is mainly affected by the local residual of the coarse scale solution and the long range interaction within the residual field can be neglected. When $\mathbf{y} \in \Omega_e$, the fine scale solution can only "*feel*" the discretization error of the coarse mesh due to the element, Ω_e , and discretization errors due to other elements may be neglected;
- 3. The coarse scale residual may be approximated by its volume average.

Let $\mathbf{y} \in \Omega_e$. Based on the approximation 3, we can first express the fine scale displacement field as

$$u_{i}'(\mathbf{y}) \approx \int_{\Omega} (C_{mnk\ell} \overline{u}_{k,\ell}) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\Omega} b_{m} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x}$$
$$\approx \int_{\Omega} (C_{mnk\ell} \langle \overline{u}_{k,\ell} \rangle_{\Omega}) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\Omega} \langle b_{m} \rangle_{\Omega} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x}.$$
(2.41)



Fig. 1. Equivalent circular domain for representative element, Ω_e .

Consider $\Omega = M \cup \Omega_{\rho}^{c}$

$$\langle \overline{u}_{(k,\ell)} \rangle_{\Omega} = \frac{1}{\Omega} \int_{\Omega} \overline{u}_{(k,\ell)} \, \mathrm{d}\Omega_{x} = \frac{1}{\Omega} \left(\frac{M}{M} \int_{M} \overline{u}_{(k,\ell)} \, \mathrm{d}\Omega_{x} + \frac{\Omega_{e}^{c}}{\Omega_{e}^{c}} \int_{\Omega_{e}^{c}} \overline{u}_{(k,\ell)} \, \mathrm{d}\Omega_{x} \right)$$

$$= (1 - f_{e}^{c}) \langle \overline{u}_{(k,\ell)} \rangle_{M} + f_{e}^{c} \langle \overline{u}_{(k,\ell)} \rangle_{\Omega_{e}^{c}},$$

$$(2.42)$$

and

$$\langle b_m \rangle_{\Omega} = (1 - f_e^{\rm c}) \langle b_m \rangle_M + f_e^{\rm c} \langle b_m \rangle_{\Omega_e^{\rm c}},\tag{2.43}$$

where $f_e^c = |\Omega_e^c|/|\Omega|$.

Then based on the approximation 2, when $\mathbf{y} \in \Omega_e$, we neglect the contribution from the rest of the elements ("matrix"), ¹

$$\langle \overline{u}_{(k,\ell)} \rangle_{\Omega} = f_e^{\mathsf{c}} \langle \overline{u}_{(k,\ell)} \rangle_{\Omega_e^{\mathsf{c}}}, \tag{2.44}$$

$$\langle b_m \rangle_{\Omega} = f_e^{\rm c} \langle b_m \rangle_{\Omega_e^{\rm c}} \tag{2.45}$$

and

$$\int_{\Omega} C_{mnk\ell} G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \,\mathrm{d}\Omega_x \approx \int_{\Omega_e^c} C_{mnk\ell} G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \,\mathrm{d}\Omega_x, \tag{2.46}$$

$$\int_{\Omega} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \,\mathrm{d}\Omega_x \approx \int_{\Omega_e^{\infty}} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \,\mathrm{d}\Omega_x.$$
(2.47)

Based on approximation 1, the coarse scale residual due to element, e, is uniform or quasi-uniform on Ω_{e}^{c} . This means that

$$\langle \overline{u}_{(k,\ell)} \rangle_{\Omega_e^c} = \overline{u}_{k,\ell}^e, \tag{2.48}$$

$$\langle b_m \rangle_{O^c} = b_m$$
, if b_m is constant. (2.49)

Eq. (2.48) is the generalization of the assumption that the average strain in the hypersphere Ω_e^c equals the "average strain" in the element, *e*, i.e. Eq. (2.40).

In real computation, for an arbitrary point, $\mathbf{y} \in \Omega$, we have the following approximation:

$$u_{i}^{\prime}(\mathbf{y}) \approx \mathbf{A}_{e=1}^{n_{\mathrm{el}}} \left\{ \left(f_{e}^{\mathrm{c}} \int_{\Omega_{e}^{\mathrm{c}}} C_{mnk\ell} G_{im,n}^{\infty}(\mathbf{y}-\mathbf{x}) \,\mathrm{d}\Omega_{x} \right) \overline{u}_{(k,\ell)}^{e} H(\Omega_{e}) + f_{e}^{\mathrm{c}} \left(\int_{\Omega_{e}^{\mathrm{c}}} G_{im}^{\infty}(\mathbf{y}-\mathbf{x}) \,\mathrm{d}\Omega_{x} \right) b_{m} \right\},$$
(2.50)

where n_{el} is the total number of elements in the coarse discretization, and the assembly operator $\mathbf{A}_{e=1}$ is defined in [6].

Furthermore, one can find the fine scale strain field by taking spatial derivative

$$\epsilon_{ij}' = u_{(i,j)}' \approx \bigwedge_{e=1}^{n_{\rm el}} \left\{ \left(\frac{f_e^{\rm c}}{2} \int_{\Omega_e^{\rm c}} C_{mnk\ell} (G_{im,nj}^{\infty} + G_{jm,ni}^{\infty}) \mathrm{d}\Omega_x \right) \overline{u}_{(k,\ell)}^e H(\Omega_e) + \frac{f_e^{\rm c}}{2} \left(\int_{\Omega_e^{\rm c}} (G_{im,j}^{\infty} + G_{jm,i}^{\infty}) \mathrm{d}\Omega_x \right) b_m \right\}.$$

$$(2.51)$$

¹ We neglect the interaction of coarse scale residual among different elements.

Define

$$S_{ijk\ell} := -\frac{1}{2} \int_{\Omega_e^{\circ}} C_{mnk\ell} (G_{im,nj}^{\infty}(\mathbf{y} - \mathbf{x}) + G_{jm,ni}^{\infty}(\mathbf{y} - \mathbf{x})) d\Omega_x, \qquad (2.52)$$

$$F_{ijm}(\mathbf{y}) := \frac{1}{2} \int_{\Omega_e^c} (G_{im,j}^{\infty}(\mathbf{y} - \mathbf{x}) + G_{jm,i}^{\infty}(\mathbf{y} - \mathbf{x})) \mathrm{d}\Omega_x.$$
(2.53)

The global fine scale solution may be written as

$$\epsilon'_{ij}(\mathbf{y}) = - \bigwedge_{e=1}^{e_{el}} \{ f_e^c S_{ijkl} \overline{u}_{k,\ell}^e H(\Omega_e) - f_e^c F_{ijm}(\mathbf{y}) b_m \}, \quad \forall \mathbf{y} \in \Omega$$
(2.54)

where $S_{ijk\ell}$ is the celebrated Eshelby tensor.

2.3. Fine scale solution: (II) local Galerkin formulation

In the second method, instead of forming a global Green function residual form, we consider the following local G-residual form in a local domain, Ω_E , which corresponds to the representative element, $e = 1, 2, ..., n_{el}$

$$\int_{\Omega_E} G_{mi}^{\infty}(\mathbf{y} - \mathbf{x}) \{ C_{ijk\ell} u'_{k,\ell j}(\mathbf{x}) + C_{ijk\ell} \overline{u}_{k,\ell j}(\mathbf{x}) + b_i(\mathbf{x}) \} d\Omega = 0.$$
(2.55)

The representative element, e, is at the center of the local region Ω_E (see Figs. 2 and 3).



Fig. 2. Local fine scale solution.



Fig. 3. Local domain, Ω_E , effective domain, Ω_e^c , and the representative individual element, Ω_e .

Again we choose Ω_E as a hypersphere in \mathbb{R}^d . It is a sphere in three-dimensional space and it is a circle in two-dimensional space.

Again by Somigliana's identity, one can obtain that

$$u_{i}'(\mathbf{y}) = \int_{\Omega_{E}} (C_{mnk\ell} \overline{u}_{k,\ell n} + b_{m}) G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\partial\Omega_{E}} \sigma_{mn}'(\mathbf{x}) n_{n} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}S + \int_{\partial\Omega_{E}} \sigma_{k\ell}^{G_{i}^{\infty}}(\mathbf{y} - \mathbf{x}) n_{\ell} u_{k}'(\mathbf{x}) \, \mathrm{d}S_{x}.$$
(2.56)

Remark 2.1

1. When y is close to the boundary, $\partial \Omega$, the local domain, Ω_E , is no longer a full sphere or a full circle (see Fig. 2). Moreover, the boundary of the local domain, Ω_E , may consist of three parts

$$\partial \Omega_E = \partial_E^{\circ} \cup \Gamma_{Eu} \cup \Gamma_{Et}$$

and $\partial \Omega_E^{\circ} = \partial \Omega_E \cap \Omega$ as shown in Fig. 2.

2. One may choose $\Omega_E = \Omega_e^c$, but it is not necessary.

Integration by parts of (2.56) yields

$$u_{i}'(\mathbf{y}) = \int_{\Omega_{E}} (C_{mnk\ell} \overline{u}_{k,\ell}) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\Omega_{E}} b_{m} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\partial\Omega_{E}} (\sigma_{mn}'(\mathbf{x}) + \overline{\sigma}_{mn}(\mathbf{x})) n_{n} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}S_{x} + \int_{\partial\Omega_{E}} \sigma_{k\ell}^{G_{i}^{\infty}}(\mathbf{y} - \mathbf{x}) n_{\ell} u_{k}'(\mathbf{x}) \, \mathrm{d}S_{x},$$
(2.57)

where

$$\overline{\sigma}_{mn} := C_{mnk\ell} \overline{u}_{(k,\ell)}. \tag{2.58}$$

Again, we neglect fine scale solution on the boundary of the local domain, Ω_E

$$\int_{\partial\Omega_E} \sigma'_{ij} n_j G^{\infty}_{im} \,\mathrm{d}S_x \approx 0, \tag{2.59}$$

$$\int_{\partial\Omega_E} \sigma_{k\ell}^{G_m^{\infty}}(\mathbf{y} - \mathbf{x}) n_\ell u_k'(\mathbf{x}) \, \mathrm{d}S_x = \int_{\partial\Omega_E} C_{ijk\ell} u_k' n_\ell G_{im,j}^{\infty} \, \mathrm{d}S_x \approx 0.$$
(2.60)

These two approximations are being made on the ground that the long range interaction in fine scale field is negligible.

We then obtain an estimate for the fine scale solution

$$u_i'(\mathbf{y}) \approx \int_{\Omega_E} \left(C_{mnk\ell} \overline{u}_{k,\ell} \right) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_x + \int_{\Omega_E} b_m G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_x + \int_{\partial\Omega_E} \overline{\sigma}_{mn}(\mathbf{x}) n_n G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}S_x.$$
(2.61)

There are several ways to further approximate Eq. (2.61). The simplest way is to drop the contribution from the boundary term, i.e.

$$u_i'(\mathbf{y}) \approx \int_{\Omega_E} \left(C_{mnk\ell} \overline{u}_{k,\ell} \right) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_x + \int_{\Omega_E} b_m G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_x.$$
(2.62)

Assume that the coarse scale strain field is a piecewise constant tensor field. This is certainly true for triangle elements and tetrahedral elements, i.e.

$$\overline{u}_{(k,\ell)}(\mathbf{x}) = \sum_{s=1}^{n_{\text{elE}}} \overline{u}_{(k,\ell)}^s H(\Omega_s \cap \Omega_E), \quad \forall \mathbf{x} \in \Omega_E,$$
(2.63)

where n_{elE} is the total number of elements inside Ω_E .

Assume that the fine scale contribution only comes from discretization error of the element Ω_e , if $\mathbf{y} \in \Omega_e$. We may introduce the following approximation:

$$\int_{\Omega_{E}} \left(C_{mnk\ell} \overline{u}_{(k,\ell)}(\mathbf{x}) \right) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} \approx \int_{\Omega_{E}} C_{mnk\ell} \langle \overline{u}_{(k,\ell)} \rangle_{\Omega_{E}} G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x}$$
$$\approx \left(\int_{\Omega_{E}} C_{mnk\ell} G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} \right) \left(f_{E} \overline{u}_{(k,\ell)} H(\Omega_{e}) \right) \tag{2.64}$$

and

$$\int_{\Omega_E} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) b_m \, \mathrm{d}\Omega_x \approx \int_{\Omega_E} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \langle b_m \rangle_{\Omega_E} \, \mathrm{d}\Omega_x \approx \left(\int_{\Omega_E} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_x \right) (f_E b_m H(\Omega_e)), \tag{2.65}$$

where $f_E := |\Omega_e|/|\Omega_E|$.

When $\mathbf{y} \in \Omega_e$, we have the following estimate for the fine scale solution:

$$u_{i}'(\mathbf{y}) = \int_{\Omega_{E}} \left(C_{mnk\ell} G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \,\mathrm{d}\Omega_{x} \right) \left(f_{E} \overline{u}_{(k,\ell)}^{e} H(\Omega_{e}) \right) + \int_{\Omega_{E}} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \,\mathrm{d}\Omega_{x} \left(f_{E} b_{m} H(\Omega_{e}) \right)$$
(2.66)

and

$$u_{i,j}'(\mathbf{y}) = \int_{\Omega_E} \left(C_{mnk\ell} G_{im,nj}^{\infty}(\mathbf{y} - \mathbf{x}) \,\mathrm{d}\Omega_x \right) \left(f_E \overline{u}_{(k,\ell)}^e H(\Omega_e) \right) + \int_{\Omega_E} G_{im,j}^{\infty}(\mathbf{y} - \mathbf{x}) \,\mathrm{d}\Omega_x (f_E b_m H(\Omega_e)).$$
(2.67)

Finally, one can express the fine scale strains in terms of coarse scale strains and the body force, i.e.

$$\epsilon_{ij}'(\mathbf{y}) = -f_E S_{ijk\ell} \overline{u}_{(k,\ell)}^e H(\Omega_e) + f_E F_{ijm}(\mathbf{y}) b_m H(\Omega_e), \quad \forall \mathbf{y} \in \Omega_e.$$
(2.68)

The global fine scale solution may be written as

$$\epsilon_{ij}'(\mathbf{y}) = - \sum_{e=1}^{n_{\text{el}}} f_E \{ S_{ijkl} \overline{u}_{(k,\ell)}^e - F_{ijm}(\mathbf{y}) b_m \} H(\Omega_e) \quad \forall \mathbf{y} \in \Omega.$$
(2.69)

Note that when a mesh is refined, $f_e^c \rightarrow 0$, but $f_E \not\rightarrow 0$. Therefore, the second method does not converge.

We call both methods I and II as the simplest approximations, in which the coarse scale residual contribution due to the boundary term is neglected. Nevertheless, the contribution from the boundary integral may be significant. Without taking into account the contribution from the boundary terms, the improvement on original FEM coarse scale solution is limited.

2.4. Fine scale solution: (III) mean field approach

In the third approach, we still adopt the local Green function based Galerkin weak formulation (see Fig. 3), but the coarse scale residual source term on the boundary of the local domain, $\partial \Omega_E$, is considered. Consider the identity

$$\frac{\partial}{\partial x_n} \langle \overline{\sigma}_{mn} \rangle_{\Omega_E} = 0 \Rightarrow \int_{\Omega_E} \frac{\partial}{\partial x_n} \langle \overline{\sigma}_{mn} \rangle_{\Omega_E} G^{\infty}_{im}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_x = 0.$$

Integration by parts yields

$$\int_{\partial\Omega_E} \langle \overline{\sigma}_{mn} \rangle_{\Omega_E} n_n G_{im}^{\infty} (\mathbf{y} - \mathbf{x}) \, \mathrm{d}S_x - \int_{\Omega_E} \frac{\partial}{\partial x_n} G_{im}^{\infty} (\mathbf{y} - \mathbf{x}) \langle \overline{\sigma}_{mn} \rangle_{\Omega_E} \, \mathrm{d}\Omega_x = 0$$

or

$$\int_{\partial \Omega_E} \langle \overline{\sigma}_{mn} \rangle_{\Omega_E} n_n G_{im}^{\infty} (\mathbf{y} - \mathbf{x}) \, \mathrm{d}S_x + \int_{\Omega_E} G_{im,n}^{\infty} (\mathbf{y} - \mathbf{x}) \langle \overline{\sigma}_{mn} \rangle_{\Omega_E} \, \mathrm{d}\Omega_x = 0.$$
(2.70)

Subtracting (2.70) from (2.61), we have

$$u_{i}'(\mathbf{y}) \approx \int_{\Omega_{E}} (\overline{\sigma}_{mn} - \langle \overline{\sigma}_{mn} \rangle_{\Omega_{E}}) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\Omega_{E}} b_{m} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\partial\Omega_{E}} (\overline{\sigma}_{mn}(\mathbf{x}) - \langle \overline{\sigma}_{mn} \rangle_{\Omega_{E}}) n_{n} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}S_{x}.$$
(2.71)

One may argue that in the integrand the term $(\overline{\sigma}_{mn}(\mathbf{x}) - \langle \overline{\sigma}_{mn} \rangle_{\Omega_E})$ oscillates around zero along the boundary, because its mean $\langle \overline{\sigma}_{mn} - \langle \overline{\sigma}_{mn} \rangle_{\Omega_E} \rangle_{\Omega_E} = 0$. The boundary term in (2.71) can be then neglected. This is in fact a very accurate and a popular approximation used in micromechanics homogenization theory, and it has been widely used in many applications of composite materials (e.g. Willis [18]). We obtain the following estimate on the fine scale solution

$$u_{i}'(\mathbf{y}) \approx \int_{\Omega_{E}} (\overline{\sigma}_{mn} - \langle \overline{\sigma}_{mn} \rangle_{\Omega_{E}}) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\Omega_{E}} b_{m} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x}$$
$$= \int_{\Omega_{E}} C_{mnk\ell} (\overline{u}_{(k,\ell)} - \langle \overline{u}_{(k,\ell)} \rangle_{\Omega_{E}}) G_{im,n}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x} + \int_{\Omega_{E}} b_{m} G_{im}^{\infty}(\mathbf{y} - \mathbf{x}) \, \mathrm{d}\Omega_{x}, \qquad (2.72)$$

which is termed as the mean-field approach.

Now we can express the fine scale strains in terms of coarse scale strain and body force, i.e.

$$\epsilon_{ij}'(\mathbf{y}) = \frac{1}{4} \int_{\Omega_E} C_{mnk\ell} (G_{im,nj}^{\infty} + G_{jm,ni}^{\infty} + G_{in,mj}^{\infty} + G_{jn,mi}^{\infty}) (\overline{u}_{(k,\ell)} - \langle \overline{u}_{k,\ell} \rangle_{\Omega_E}) d\Omega_x + \frac{1}{2} \int_{\Omega_E} (G_{im,j}^{\infty} + G_{jm,i}^{\infty}) b_m d\Omega_x.$$
(2.73)

Suppose that $\mathbf{y} \in \Omega_e$. Then

$$\begin{split} \frac{1}{4} \int_{\Omega_E} C_{mnk\ell} (G_{im,nj}^{\infty} + G_{jm,ni}^{\infty} + G_{in,mj}^{\infty} + G_{jn,mi}^{\infty}) (\overline{u}_{(k,\ell)} - \langle \overline{u}_{k,\ell} \rangle_{\Omega_E}) \, \mathrm{d}\Omega_x \\ &= \frac{1}{4} \int_{\Omega_e^c} C_{mnk\ell} (G_{im,nj}^{\infty} + G_{jm,ni}^{\infty} + G_{in,mj}^{\infty} + G_{jn,mi}^{\infty}) (\overline{u}_{(k,\ell)} - \langle \overline{u}_{k,\ell} \rangle_{\Omega_E}) \, \mathrm{d}\Omega_x \\ &\quad + \frac{1}{4} \int_{\Omega_E - \Omega_e^c} C_{mnk\ell} (G_{im,nj}^{\infty} + G_{jm,ni}^{\infty} + G_{in,mj}^{\infty} + G_{jn,mi}^{\infty}) (\overline{u}_{(k,\ell)} - \langle \overline{u}_{k,\ell} \rangle_{\Omega_E}) \, \mathrm{d}\Omega_x. \end{split}$$

Based on Tanaka-Mori lemma [15]

$$\frac{1}{4} \int_{\Omega_E - \Omega_e^{\rm c}} C_{mnk\ell} (G_{im,nj}^{\infty} + G_{jm,ni}^{\infty} + G_{jn,mj}^{\infty} + G_{jn,mi}^{\infty}) \,\mathrm{d}\Omega_x = 0,$$
(2.74)

we may approximate

$$\frac{1}{4} \int_{\Omega_E - \Omega_e^{\mathbb{C}}} C_{mnk\ell} (G_{im,nj}^{\infty} + G_{jm,ni}^{\infty} + G_{in,mj}^{\infty} + G_{jn,mi}^{\infty}) (\overline{u}_{(k,\ell)} - \langle \overline{u}_{k,\ell} \rangle_{\Omega_E}) \, \mathrm{d}\Omega_x \approx 0, \tag{2.75}$$

if Ω_E is small enough. Thereby for the case of constant body force

$$\epsilon_{ij}'(\mathbf{y}) = -S_{ijk\ell}(\overline{u}_{(k,\ell)}^e H(\Omega_e) - \langle \overline{u}_{(k,\ell)} \rangle_{\Omega_E}) + F_{ijm}(\mathbf{y}) b_m H(\Omega_e), \quad \forall \mathbf{y} \in \Omega_e.$$
(2.76)

In general for $\mathbf{y} \in \Omega$ we may have

$$\epsilon_{ij}'(\mathbf{y}) = - \bigwedge_{e,E=1}^{n_{\rm el}} \{ S_{ijkl}(\overline{u}_{(k,\ell)}^e) H(\Omega_e) - \langle \overline{u}_{(k,\ell)} \rangle_{\Omega_E}) - F_{ijm}(\mathbf{y}) b_m H(\Omega_e) \}.$$
(2.77)

2.5. Two-dimensional elastostatics

For two-dimensional elastostatic problems, the Green's function for an infinite domain is

$$G_{ij}^{\infty}(\mathbf{z}) = \frac{1}{8\pi\mu(1-\nu)} \left(g \frac{z_i z_j}{z^2} - (3-4\nu)\delta_{ij} \ln z \right), \quad \mathbf{z} = \mathbf{y} - \mathbf{x}, \ z = |\mathbf{z}|.$$
(2.78)

Evaluating integrals (2.52) and (2.53), we obtain the following explicit expressions:

$$F_{ijm}(\mathbf{y}) = \frac{1}{16\mu(1-\nu)} [\delta_{ij}y_m - (3-4\nu)(\delta_{im}y_j + \delta_{jm}y_i)], \qquad (2.79)$$

$$S_{ijk\ell} = \frac{1}{8(1-\nu)} \left((4\nu - 1)\delta_{ij}\delta_{k\ell} + (3-4\nu)(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}) \right).$$
(2.80)

3. Finite element implementation

We now return to the coarse scale weak formulation

$$a(\overline{\mathbf{w}},\overline{\mathbf{u}}) + a(\overline{\mathbf{w}},\mathbf{u}') = (\overline{\mathbf{w}},\mathbf{b})_{\Omega} + (\overline{\mathbf{w}},\mathbf{t}^0)_{\Gamma_t}.$$
(3.81)

Consider the simplest approximations, i.e. methods I and II. Substituting

$$\epsilon_{ij}'(\mathbf{y}) = - \bigwedge_{e=1}^{n_{\rm cl}} f_e S_{ijk\ell} \overline{u}_{(k,\ell)}^e H(\Omega_e) + f_e F_{ijm}(\mathbf{y}) b_m H(\Omega_e)$$
(3.82)

into (3.81), we have

$$a(\overline{\mathbf{w}},\overline{\mathbf{u}}) + a(\overline{\mathbf{w}},\mathbf{u}') = \int_{\Omega} \overline{w}_{(i,j)} C_{ijk\ell} \left(\overline{u}_{(k,\ell)} - S_{k\ell m n} \bigwedge_{e=1}^{n_{el}} f_e \overline{u}_{(m,n)}^e H(\Omega_e) \right) d\Omega_x + \int_{\Omega} \overline{w}_{(i,j)} C_{ijk\ell} F_{k\ell m} b_m d\Omega_x$$
$$= (\overline{\mathbf{w}}, \mathbf{b})_{\Omega} + (\overline{\mathbf{w}}, \mathbf{t}^0)_{\Gamma_i} = \int_{\Omega} \overline{w}_i b_i d\Omega_x + \int_{\Gamma_t} \overline{w}_i t_i^0 dS_x, \qquad (3.83)$$

where $f_e = f_e^c$, or f_E .

Eq. (3.83) can then be rewritten as

$$\begin{split} & \bigwedge_{e=1}^{n_{\text{cl}}} \int_{\Omega_{e}} \left(\overline{w}_{(i,j)}^{e} C_{ijmn} (1_{mnk\ell} - f_{e} S_{mnk\ell}) \overline{u}_{(k,\ell)}^{e} \right) \mathrm{d}\Omega_{x} \\ &= \bigwedge_{e=1}^{n_{\text{cl}}} \left\{ \int_{\Omega_{e}} \overline{w}_{i}^{e} (b_{i} + f_{e} C_{ijk\ell} F_{k\ell m,j} b_{m}) \mathrm{d}\Omega + \int_{\Gamma_{i} \cap \partial\Omega_{e}} \overline{w}_{i}^{e} (t_{i}^{0} - f_{e} C_{ijk\ell} F_{k\ell m} b_{m}) \mathrm{d}S_{x} \right\}. \end{split}$$

Denote the homogenized elastic tensor as

$$C_{ijk\ell}^{\rm H} = C_{ijk\ell} + f_e \widehat{C}_{ijk\ell}$$
(3.84)

and

$$\widehat{C}_{ijk\ell} = -2K \frac{1}{2(1-\nu)} \mathbf{E}^1 - 2\mu \frac{(3-4\nu)}{4(1-\nu)} \mathbf{E}^{(2)},$$
(3.85)

where the ${\bf E}$ tensors have the form

$$E_{ijk\ell}^{(1)} = \frac{1}{2} \delta_{ij} \delta_{k\ell}, \quad E_{ijk\ell}^{(2)} = \frac{1}{2} (\delta_{ik} \delta_{j\ell} + \delta_{i\ell} \delta_{kj} - \delta_{ij} \delta_{k\ell}), \quad i, jk, \ell = 1, 2.$$
(3.86)

The homogenized body force has the following expression:

$$b_i^{\rm H} = b_i + f_e C_{ijk\ell} F_{k\ell m,j} b_m, \tag{3.87}$$

where

$$F_{k\ell m,j} = \frac{1}{16\mu(1-\nu)} \left[\delta_{k\ell} \delta_{mj} - (3-4\nu)(\delta_{km} \delta_{\ell j} + \delta_{\ell m} \delta_{kj}) \right].$$
(3.88)

Accordingly, the homogenized traction vector is

$$t^{\rm H} = t_i^0 - f_e C_{ijk\ell} F_{k\ell m} b_m, \tag{3.89}$$

where

$$F_{k\ell m} = \frac{1}{16\mu(1-\nu)} \left[\delta_{ij} y_m - (3-4\nu)(\delta_{im} y_j + \delta_{jm} y_i) \right].$$
(3.90)

Remark 3.1

- 1. One may observe that the homogenized elastic tensor or modified elastic tensor depends on the ratio of effective element size and the size of whole domain. Obviously, when one refines the mesh, $f_e^c = \Omega_e^c / \Omega \rightarrow 0$, the homogenized coarse scale weak form approaches to the original FEM coarse scale weak form. If under h-refinement the original FEM solution converges to the exact solution, the solution of the homogenized coarse scale weak form will converge to the exact solution as well.
- 2. As mesh is refined, it is not necessary, $f_E \rightarrow 0$. Hence the second method may not converge. On the other hand, the essence of the proposed method is intended to increase accuracy without mesh refinement.

4. Numerical computations

Two numerical examples have been carried out to illustrate and to validate the proposed variational multiscale eigenstrain method.

4.1. Cantilever beam

We use both conventional FEM method and variational multiscale eigenstrain method to solve the bending of cantilever beam as a plane stress problem.

The exact solution of this problem is given by Timoshenko and Goodier [16]

$$u_{x} = -\frac{Py}{6\overline{E}I} \left(y - \frac{D}{2} \right) [3x(2L - x) + (2 + \overline{v})y(y - D)],$$
(4.91)

$$u_{y} = \frac{P}{6\overline{E}I} \left[x^{2}(3L-x) + 3\overline{v}(L-x) \left(y - \frac{D}{2} \right)^{2} + \frac{4+5\overline{v}}{4} D^{2}x \right],$$
(4.92)

where

$$I = \frac{D^3}{12},$$
 (4.93)

$$\overline{E} = \begin{cases} E & \text{for plane stress,} \\ E/(1-v^2) & \text{for plane strain,} \end{cases}$$
(4.94)

$$\overline{\nu} = \begin{cases} \nu & \text{for plane stress,} \\ \nu/(1-\nu) & \text{for plane strain.} \end{cases}$$
(4.95)

The corresponding stresses are

$$\sigma_{xx}(x,y) = \frac{P}{I}(L-x)\left(y-\frac{D}{2}\right),\tag{4.96}$$

$$\sigma_{yy}(x,y) = 0, \tag{4.97}$$

$$\sigma_{xy}(x,y) = \frac{Py}{2I}(y-D).$$
(4.98)

The problem has been solved for the plane stress case with Young's modulus E = 1000, Poisson's ratio v = 0.25, and zero body force, i.e. $b_m = 0.0$. The dimensions of the beam are: L = 8.0 and D = 1.0. The prescribed traction and prescribed displacement boundary conditions are illustrated in Fig. 4. Displacement boundary conditions are imposed along the boundary x = 0 by using the exact solution (4.91) and (4.92). The traction boundary condition is imposed on the boundary x = L. The rest of the boundary is traction free.

Two meshes having quadrilateral and triangular elements respectively, with each node having two degrees of freedom, have been used in finite element discretizations. We have used the methods I and III in numerical computations. The domain, Ω_e^c is chosen as the smallest circle that circumscribing an individual element, and the volume fraction, f_e^c , is calculated via dividing the area of the circle, Ω_e^c by the total area of the beam.

The numerical results obtained via variational eigenstrain multiscale method are compared with both exact solution and the conventional finite element solution. The comparisons are depicted in Fig. 5. The numerical solution obtained by using variational eigenstrain multiscale method shows some improvement over the conventional FEM coarse solution based on the comparison in L_2 error norm (see Fig. 6). Also one can observe that the solutions obtained by variational eigenstrain multiscale method are convergent.

In Fig. 6, one can find that for this particular problem the method III provides at least 10% improvement in computations with both meshes. In the computations with quadrilateral mesh, the improvement is over 25%.



Fig. 4. A cantilever beam problem: (a) quadrilateral mesh, and (b) triangle mesh.



Fig. 5. Comparison with the exact solution, the conventional FEM solution, and the solution of the variational eigenstrain multiscale method (III): (a) 32 element mesh, (b) 128 element mesh.

4.2. A plate with a hole

We solve the problem of a plate with a hole, subjected to an unit uniaxial stress along the horizontal direction. The exact solution of this problem is given as

$$u_1(r,\theta) = \frac{a}{8\mu} \left[\frac{r}{a} (\kappa+1) \cos\theta + 2\frac{a}{r} ((1+\kappa) \cos\theta + \cos 3\theta) - 2\frac{a^3}{r^3} \cos 3\theta \right], \tag{4.99}$$

$$u_2(r,\theta) = \frac{a}{8\mu} \left[\frac{r}{a} (\kappa - 3) \sin \theta + 2\frac{a}{r} ((1 - \kappa) \sin \theta + \sin 3\theta) - 2\frac{a^3}{r^3} \sin 3\theta \right],$$
(4.100)

where μ is the shear modulus and κ (Kolosov constant) is defined as



Fig. 6. Comparison of convergence results for the cantilever problem between regular FEM solution and the solution via variational eigenstrain multiscale methods: (a) quadrilateral element (method I), (b) quadrilateral element (method III), (c) triangle element (method I), and (d) triangle element (method III).

$$\kappa = \begin{cases} \frac{3-4v}{3-v} & \text{for plane strain,} \\ \frac{3-v}{1+v} & \text{for plane stress.} \end{cases}$$
(4.101)

The corresponding stresses are

$$\sigma_{11}(r,\theta) = 1 - \frac{a^2}{r^2} \left(\frac{3}{2}\cos 2\theta + \cos 4\theta\right) + \frac{3}{2}\frac{a^4}{r^4}\cos 4\theta,$$
(4.102)

$$\sigma_{22}(r,\theta) = -\frac{a^2}{r^2} \left(\frac{1}{2}\cos 2\theta - \cos 4\theta\right) - \frac{3}{2}\frac{a^4}{r^4}\cos 4\theta,$$
(4.103)

$$\sigma_{12}(r,\theta) = -\frac{a^2}{r^2} \left(\frac{1}{2}\sin 2\theta + \sin 4\theta\right) + \frac{3}{2}\frac{a^4}{r^4}\sin 4\theta.$$
(4.104)

The problem has been solved for the plane strain case with Young's modulus E = 1, Poisson's ratio v = 0.25, and zero body force, i.e. $b_m = 0.0$. Due to symmetry only one quadrant of the plate is considered



Fig. 7. A plate with hole subjected to uniaxial remote stress: (a) problem statement (a = 1; D = 3); (b) discretization error distribution.

for the analysis. The dimensions of one quarter of the plate and prescribed traction/displacement boundary conditions are illustrated in Fig. 7(a). The traction boundary conditions are imposed along x = (a + D) and y = (a + D) using the exact solution (4.102)–(4.104). The rest of the boundary is traction free.

We also note for this particular problem that the discretization error is concentrated near the hole region (see Fig. 7(b)). We therefore use methods I and III only for selective adaptivity of elements around the hole. Meshes of quadrilateral and triangular elements have been used for discretization purposes with each node having two degrees of freedom. Fig. 8 shows above mentioned meshes with elements selected for adaptivity marked around the hole.



Fig. 8. Meshes used for finite element discretization: (a) triangular element, (b) quadrilateral element.



Fig. 9. Comparison of convergence results for the hole problem between regular FEM solution and the solution via variational eigenstrain multiscale methods: (a) quadrilateral element (method I), (b) quadrilateral element (method III), (c) triangle element (method I), and (d) triangle element (method III).

Results are shown in Fig. 9 by comparing L_2 error norm of solutions obtained using variational eigenstrain multiscale method and conventional FEM. Significant improvement in performance can be noticed from the plots. It can also be seen that the proposed method is most useful while dealing with a coarse mesh.

From Fig. 9, one may find that for both meshes there is almost a consistent 25% improvement in accuracy for the solutions obtained by the method III.

5. Concluding remarks

In this work, a new variational eigenstrain multiscale formulation is proposed to construct a homogenized two-scale variational weak formulation for elastostatics. The newly proposed weak formulation has the ability to adjust discretization error automatically, and hence render a better computational performance in a coarse scale numerical computation than conventional finite element coarse scale computations. Preliminary numerical results show that the method provides better accuracy than regular finite element computations without homogenization of discretization error. The adaptive method proposed in this paper is neither *h-adaptivity* nor *p-adaptivity*. Since the fine scale solution is obtained based on Green's function method, we prefer to call it as *the G-adaptivity method*. We are currently working on extending the variational eigenstrain multiscale formulation to three-dimensional problems, developing new eigenstrain multiscale homogenization schemes, and establishing related convergence criterion.

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Appendix A. Tensors $S_{ijk\ell}$ and F_{ijm} of 2D elastostatics

A.1. Derivation of $S_{ijk\ell}$

The Green's function for 2D Navier equations is given as

$$G_{ij}^{\infty}(\mathbf{y} - \mathbf{x}) = \frac{1}{8\pi\mu(1 - \nu)} \left\{ \frac{(y_i - x_i)(y_j - x_j)}{R^2} - (3 - 4\nu)\delta_{ij}\ln R \right\}, \quad i, j = 1, 2,$$
(A.1)

where $R = \sqrt{(y_1 - x_1)(y_2 - x_2)}$.

It can be readily shown that

$$G_{ij,\ell}^{\infty}(\mathbf{y}-\mathbf{x}) = \frac{1}{8\pi\mu(1-\nu)} \left\{ -2\frac{z_i z_j z_\ell}{R^4} + \frac{1}{R^2} (z_j \delta_{i\ell} + z_i \delta_{j\ell}) - (3-4\nu) \delta_{ij} \frac{z_\ell}{R^2} \right\}$$

where $\mathbf{z} = \mathbf{y} - \mathbf{x}$.

For isotropic materials

$$C_{ijkl} = \lambda \delta_{ij} \delta_{k\ell} + \mu (\delta_{ik} \delta_{j\ell} + \delta_{jk} \delta_{i\ell}).$$

Then, one can show that

$$C_{mnk\ell}G_{im,n}^{\infty}(\mathbf{z}) = -\frac{1}{4\pi(1-\nu)} \left\{ 2\frac{z_i z_k z_\ell}{R^4} + \frac{(1-2\nu)}{R^2} (z_k \delta_{i\ell} + z_\ell \delta_{ik} - z_i \delta_{k\ell}) \right\}.$$

Let

$$\ell = -\frac{\mathbf{z}}{|\mathbf{z}|} = \frac{\mathbf{x} - \mathbf{y}}{|\mathbf{z}|}.$$
(A.2)

We may write

$$C_{mnk\ell}G_{im,n}^{\infty}(\mathbf{z}) = \frac{g_{ik\ell}(\ell)}{4\pi(1-\nu)|\mathbf{z}|},\tag{A.3}$$

where

$$g_{ik\ell}(\ell) = 2\ell_i\ell_k\ell_\ell + (1-2\nu)(\ell_k\delta_{i\ell} + \ell_\ell\delta_{ik} - \ell_i\delta_{k\ell}).$$
(A.4)

Let $|\mathbf{z}| = R$ then for $\mathbf{y} \in \Omega_e$ the integration

$$\int_{\Omega_E} C_{mnk\ell} G_{im,n}^{\infty}(\mathbf{z}) \,\mathrm{d}\Omega = \frac{1}{4\pi(1-\nu)} \int_0^r \left(\int_0^{2\pi} \frac{g_{ik\ell}(\ell)}{R} \,\mathrm{d}\omega \right) R \,\mathrm{d}R \tag{A.5}$$

is carried out in the circle, Ω_E (Fig. 10).



Fig. 10. Integration over Ω_E .

Here $x_1 = y_1 + r\ell_1$ and $x_2 = y_2 + r\ell_2$. Since

$$x_1^2 + x_2^2 = a^2 \Rightarrow (y_1 + r\ell_1)^2 + (y_2 + r\ell_2)^2 = a^2$$

where r is the root of the following quadratic equation:

$$r^{2} + 2r(y_{1}\ell_{1} + y_{2}\ell_{2}) + [a^{2} - (y_{1}^{2} + y_{2}^{2})] = 0 \to r^{2} + 2rf - e = 0,$$
(A.6)

where $f = \ell_i y_i$ and $e = a^2 - (y_1^2 + y_2^2)$. The roots of Eq. (A.6) are

$$r(\ell) = -f \pm \sqrt{f^2 + e}.$$

Considering $\sqrt{f^2 + e}$ is an even function of ℓ . We have

$$\int_{\Omega_E} C_{mnk\ell} G_{im,n}^{\infty}(\mathbf{z}) \,\mathrm{d}\Omega = \frac{-y_s}{4\pi(1-\nu)} \int_0^{2\pi} \ell_s g_{ik\ell}(\ell) \,\mathrm{d}\theta. \tag{A.7}$$

Therefore

$$S_{ijk\ell} = -\frac{1}{2} \int_{\Omega_E} C_{mnk\ell} (G_{im,nj}^{\infty}(\mathbf{z}) + G_{jm,ni}^{\infty}(\mathbf{z})) \, \mathrm{d}\Omega_x = \frac{1}{8\pi(1-\nu)} \int_0^{2\pi} (\ell_j g_{ik\ell}(\ell) + \ell_i g_{jk\ell}(\ell)) \, \mathrm{d}\theta.$$
(A.8)

Using the identities (e.g. Krajcinovi [10])

$$\int_0^{2\pi} \ell_i \ell_j \,\mathrm{d}\theta = \pi \delta_{ij},\tag{A.9}$$

$$\int_{0}^{2\pi} \ell_i \ell_j \ell_k \ell_\ell \,\mathrm{d}\theta = \frac{\pi}{4} \left(\delta_{ij} \delta_{k\ell} + \delta_{ik} \delta_{j\ell} + \delta_{i\ell} \delta_{jk} \right). \tag{A.10}$$

One can obtain

$$S_{ijk\ell} = \frac{1}{8(1-\nu)} ((4\nu - 1)\delta_{ij}\delta_{k\ell} + (3-4\nu)(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}))$$
(A.11)

$$= \frac{1}{2(1-\nu)} E_{ijk\ell}^{(1)} + \frac{(3-4\nu)}{4(1-\nu)} E_{ijk\ell}^{(2)}.$$
(A.12)

A.2. Derivation of F_{ijm}

By definition

$$F_{ijm} = \frac{1}{2} \int_{\Omega_E} \left(G_{im,j}^{\infty}(\mathbf{z}) + G_{jm,i}^{\infty}(\mathbf{z}) \right) \mathrm{d}\Omega_x, \tag{A.13}$$

where $\mathbf{z} = \mathbf{y} - \mathbf{x}$.

Considering the fact that

$$\frac{1}{2}(G_{im,j}^{\infty}(\mathbf{z}) + G_{jm,i}^{\infty}(\mathbf{z})) = \frac{-1}{8\pi\mu(1-\nu)} \left\{ \frac{2z_i z_j z_m}{R^4} + \frac{(1-2\nu)(z_i \delta_{jm} + z_j \delta_{im}) - z_m \delta_{ij}}{R^2} \right\}$$

where $R = |\mathbf{z}|$.

Let

$$\ell_i = -\frac{z_i}{R} = \frac{x_i - y_i}{|\mathbf{z}|}.$$

We have

$$F_{ijm} = \frac{1}{8\pi\mu(1-\nu)} \int_0^r \int_0^{2\pi} \left\{ \frac{2\ell_i \ell_j \ell_m}{R} + \frac{(1-2\nu)(\ell_i \delta_{jm} + \ell_j \delta_{im}) - \ell_m \delta_{ij}}{R} \right\} R \, \mathrm{d}R \, \mathrm{d}\theta. \tag{A.14}$$

Again, r is the root of Eq. (A.6), i.e.

$$r(\ell) = -f \pm \sqrt{f^2 + e},$$
(A.15)
re $f = \ell_1 v_1$ and $e = q^2 - (v_2^2 + v_2^2)$

where $f = \ell_i y_i$ and $e = a^2 - (y_1^2 + y_2^2)$.

Substituting (A.15) into (A.14) and using (A.9) and (A.10), one may find that

$$F_{ijm}(\mathbf{y}) = \frac{1}{8\pi\mu(1-\nu)} \int_{0}^{2\pi} (-f)(2\ell_{i}\ell_{j}\ell_{m} + (1-2\nu)(\ell_{i}\delta_{jm} + \ell_{j}\delta_{im}) - \ell_{m}\delta_{ij}) d\theta$$

$$= \frac{-y_{n}}{8\pi\mu(1-\nu)} \int_{0}^{2\pi} \ell_{n}(2\ell_{i}\ell_{j}\ell_{m} + (1-2\nu)(\ell_{i}\delta_{jm} + \ell_{j}\delta_{im}) - \ell_{m}\delta_{ij}) d\theta$$

$$= -\frac{y_{n}}{16\mu(1-\nu)} [-\delta_{ij}\delta_{mn} + (3-4\nu)(\delta_{im}\delta_{jn} + \delta_{in}\delta_{jm})].$$

Finally, we obtain

$$F_{ijm}(\mathbf{y}) = \frac{1}{16\mu(1-\nu)} [\delta_{ij}y_m - (3-4\nu)(\delta_{im}y_j + \delta_{jm}y_i)].$$
(A.16)

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