Estimation of modeling error in two-scale homogenization of heterogeneous materials

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Abstract

Two-scale homogenization technique is used to model periodic metal matrix composites in elastic-plastic range and the hp-adaptive FEM is used to improve efficiency of numerical analysis in micro and macro scales. Since in some parts of the domain homogenization may result in large modeling error, the estimation of this error is crucial for reliability of the results. Thus, we present in this paper certain possibilities of modeling error estimation.

Keywords: multiscale modeling, homogenization, error estimation, adaptive finite element method

1. Introduction

In this research we consider metal matrix composites reinforced by another metallic material, that is distributed periodically. For both materials elastic-plastic model with kinematic hardening was assumed. In order to reduce time of computation two-scale homogenization technique is used to replace heterogeneous structure by homogeneous body with effective material parameters. We use RVE (*representative volume element*) approach at micro-level to compute effective parameters for macro-level [2, 3, 4]. The hp-adaptive finite element method [1] is used in both scales.

2. Algorithm of computational homogenization

The algorithm of computational homogenization for inelastic problems may be briefly presented in the following form:

1. Discretization (initial mesh generation, selection of RVEs, initial homogenized problem solution)
2. Iterative computation of macro-scale $\Delta\boldsymbol{\varepsilon}_0$
   - error estimation; possible repetition of the RVE solution in the case of mesh refinement
   - $\boldsymbol{C}_{\text{eff}}^{\text{ep}}$ or $\langle\Delta\boldsymbol{\varepsilon}^*\rangle$ computation
   - Transfer of effective parameters to Gauss points
   - Solution of macro-scale problem with effective material parameters or effective plastic strains $\langle\Delta\boldsymbol{\varepsilon}^*\rangle$
   - Error estimation for $\Delta\boldsymbol{\varepsilon}_0$ (return to micro-scale possible)
3. Macro-scale error analysis, in the case of mesh refinement GO TO 2
4. If load increment necessary GO TO 2
5. STOP

3. Formulations

3.1. Macro-scale problem

At the macro-scale the weak formulation of the problem may be stated as follows:
Find averaged displacement field $\boldsymbol{u}_0(\boldsymbol{x},t) \in \boldsymbol{V}_0 + \hat{\boldsymbol{u}}_0$, inelastic strains $\boldsymbol{\varepsilon}_0^*$, and stresses $\boldsymbol{\sigma}_0$, such that at every time instant $t \in [0,T]$

$$\int_\Omega \boldsymbol{\varepsilon}_0(\boldsymbol{v}) : \boldsymbol{C}_{\text{eff}}\, \dot{\boldsymbol{\varepsilon}}_0(\dot{\boldsymbol{u}}_0)\,\mathrm{d}\Omega = \int_{\partial\Omega_N} \hat{\dot{\boldsymbol{t}}}_0\, \boldsymbol{v}\,\mathrm{d}s + \int_\Omega \boldsymbol{\varepsilon}_0(\boldsymbol{v}) : \boldsymbol{C}_{\text{eff}}\, \dot{\boldsymbol{\varepsilon}}_0^*\,\mathrm{d}\Omega$$

$$\text{or} \quad \int_\Omega \boldsymbol{\varepsilon}_0(\boldsymbol{v}) : \boldsymbol{C}_{\text{eff}}^{\text{ep}}(t)\, \dot{\boldsymbol{\varepsilon}}_0(\dot{\boldsymbol{u}}_0)\,\mathrm{d}\Omega = \int_{\partial\Omega_N} \hat{\dot{\boldsymbol{t}}}_0\, \boldsymbol{v}\,\mathrm{d}s \tag{1}$$

$\forall \boldsymbol{v} \in \boldsymbol{V}_0 = \{\boldsymbol{v} \in [H^1(\Omega)]^n,\ \boldsymbol{v} = 0 \text{ na } \partial\Omega_D\}$

where $\boldsymbol{C}_{\text{eff}}$ stands for tensor of elastic effective material parameters and $\boldsymbol{C}_{\text{eff}}^{\text{ep}}$ is effective elastic-plastic tensor. $\partial\Omega_D$ i $\partial\Omega_N$ are the parts of Dirichlet and Neumann boundary conditions, respectively, $\partial\Omega_D \cup \partial\Omega_N = \partial\Omega$ and $\partial\Omega_D \cap \partial\Omega_N = \emptyset$ (in each direction), $\hat{\dot{\boldsymbol{t}}}_0,\ \hat{\dot{\boldsymbol{u}}}_0$ are the known traction and displacements.

3.2. Micro-scale problem

The problem in micro-scale is defined in RVEs, which are associated to selected points of the macro-body. Each RVE represents detailed information about the microstructure and for each RVE appropriate initial–boundary value problem is defined. These micro-scale problems may be stated in the following form after assuming boundary conditions on the basis of macro-scale strains:
Find displacements $\boldsymbol{u}(\boldsymbol{x},t)$, inelastic strains $\boldsymbol{\epsilon}^*(\boldsymbol{x},t)$ and stresses $\dot{\boldsymbol{\sigma}}(\boldsymbol{x},t)$, such that for every $t \in [0,T]$

$$\int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{v}) : \boldsymbol{C}\, \dot{\boldsymbol{\varepsilon}}(\dot{\boldsymbol{u}})\,\mathrm{d}\Omega = \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{v}) : \boldsymbol{C}\, \dot{\boldsymbol{\varepsilon}}^*\,\mathrm{d}\Omega + \int_{\partial\Omega_N} \hat{\dot{\boldsymbol{t}}}\, \boldsymbol{v}\,\mathrm{d}s \tag{2}$$

$\forall \boldsymbol{v} \in \boldsymbol{V}_0$

where $\boldsymbol{C}$ is the tensor of elastic material parameters. We assumed classical associative, rate-independent, J_2 flow plasticity rule with linear kinematic hardening, where the stresses are bounded by the Mises yield surface.

4. Homogenization error estimation

Replacement of heterogeneous domain by a homogenized body with effective material parameters, will introduce error resulted from incomplete information about the microstructure. Thus, sometimes the homogenization cannot be used at least for certain part of the domain [5].

The algorithm of homogenization error estimation for an elastic body may be stated in the following way:

1. Compute effective material parameters.
2. Solve homogenized problem with effective properties $\rightarrow \boldsymbol{u}^0$.
3. Compute residuum for heterogeneous body that corresponds to homogenized solution $\boldsymbol{u}^0$

$$r_i = 2\mu(u^0_{i,jj} + u^0_{j,ij}) + \lambda u^0_{k,kj}\delta_{ij} - f_i \quad \text{in } \omega_k \tag{3}$$

$$J_i = t_i^+ - t_i^- \quad \text{on } \partial\omega_k \qquad i,j = 1,2,3$$

where ω_k i $\partial\omega_k$ are finite element domains and element interfaces, respectively.

Wherever $h||\boldsymbol{r}|| + ||\boldsymbol{J}||$ is large homogenization should not be used.

5. Preliminary numerical results for elastic problems

We considered L-shape 3D domain, where the metal matrix is reinforced by another metallic material, that is distributed uniformly (Fig.1).

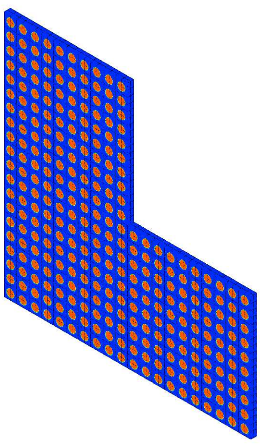

Figure 1: Material distribution of heterogeneous domain in section.

After solution of homogenized problem the residuum, as well as traction jumps (3) are computed for each finite element and used as the modeling error indicator. Wherever they are large, the material is not homogenized (Fig.2) and the solution is computed once more for such only partially homogenized domain.

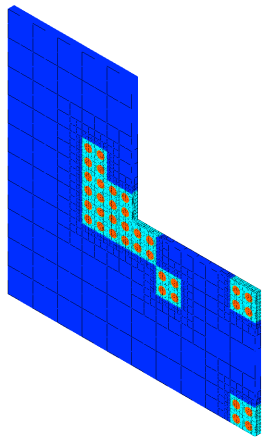

Figure 2: Partially homogenized domain.

We also consider in this work assessment of the homogenization error by the following upper bound proposed in [5]

$$||\boldsymbol{u} - \boldsymbol{u}_0||_E \leq \zeta_{\text{upp}} \stackrel{\text{def}}{=} \left\{ \int_\Omega \mathscr{I}_0 \nabla \boldsymbol{u}^0 : \boldsymbol{C} \mathscr{I}_0 \nabla \boldsymbol{u}^0 \,\mathrm{d}\boldsymbol{x} \right\}^{1/2} \tag{4}$$

where $\mathscr{I}_0 = \boldsymbol{I} - \boldsymbol{C}^{-1}\boldsymbol{C}_{\text{eff}}$.

Another possibility of modeling error estimation is based on solution of heterogeneous problem in selected subdomains with boundary conditions assumed on the basis of homogenized solution.

6. Concluding remarks

The hp-adaptive FEM was used at both macro and micro scales for inelastic problems. Preliminary results show that the proposed approach allows to indicate the parts of the body where homogenization cannot be used. In our further work this approach will be extended for inelastic problems, tested for effectiveness and compared with the other possible error assessments.

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