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Author(s): A. Ionita, Z# 204587, T-1/T-Division
B. Clements, Z# 104233, T-1/T-Division
E. Mas, Z# 165959, ADWP

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Modeling Aspects of the Dynamic Response of Heterogeneous Materials

A. Ionita^a, B.E. Clements^b and E.M. Mas^c
Los Alamos National Laboratory, Los Alamos, NM, U.S.A.
^aionita@lanl.gov, ^bbcclements@lanl.gov, ^cmas@lanl.gov

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Abstract. In numerical simulations of engineering applications involving heterogeneous materials capturing the local response coming from a distribution of heterogeneities can lead to a very large model thus making simulations difficult. The use of homogenization techniques can reduce the size of the problem but will miss the local effects. Homogenization can also be difficult if the constituents obey different types of constitutive laws. Additional complications arise if inelastic deformation. In such cases a two-scale approach is preferred and this work addresses these issues in the context of a two-scale Finite Element Method (FEM). Examples of using two-scale FEM approaches are presented.

Introduction

Consider a heterogeneous domain H subjected to a dynamic load. With the appropriate boundary and initial conditions, the equations of motion describing the wave propagation in this medium are

$$\operatorname{div} \sigma = \rho \ddot{v}, \quad (1)$$

where σ is the Cauchy stress, ρ is the density, and v and $\dot{v}$ are the velocities and accelerations, respectively. One assumes that the heterogeneous domain is composed of a distribution of inclusions in a viscoelastic matrix having the following constitutive laws

$$\hat{\sigma} = C(\dot{\epsilon} - \dot{\epsilon}^a), \quad (2)$$

for the inclusions, where $\hat{\sigma}$ represents an objective stress rate, C the material tensor, $\dot{\epsilon}$ the strain rate and $\dot{\epsilon}^a$ the total inelastic strains, and

$$\sigma = \int_0^t 2\mu(t-\tau) \dot{\epsilon}(\tau) d\tau + \int_0^t K(t-\tau) \dot{\phi}(\tau) d\tau, \quad (3)$$

for the matrix, where K and μ are the bulk and shear relaxation functions, respectively. In dynamic applications using the Finite Element Method (FEM) capturing the details of the local structure of the heterogeneous material requires a very fine spatial discretization with a very small time step, resulting in excessively large computation times. A practical approach, which can avoid the aforementioned situations is the use of the Representative Volume Element (RVE) concept [1]. Hence the initial heterogeneous domain is replaced by an equivalent homogenized domain having an effective material tensor. This will decrease considerably the size of the problem but it will miss the local effects due to the material heterogeneity at the RVE level.

A step to refine the aforementioned analyses is to use a two-scale FEM approach, a technique which combines the FEM with an RVE model for the local structure. In this formulation one defines two

spatial variables: a global variable x (associated with the first scale) for the homogenized domain and a local variable y (associated with the second scale) for the RVE level related to x by $y = x/\eta$ where η represents the changing in scale parameter. Accordingly two sets of stresses, strains, etc. are defined for each scale. The link between the scales is provided by Hill's relation [1]

$$\langle \sigma d\epsilon \rangle = \langle \sigma \rangle \langle d\epsilon \rangle, \quad (4)$$

where $\langle \rangle$ denotes the RVE volumetric average. Equation (4) represents the basis for the *localization* problem, i.e. finding the stresses, strains etc. at scale y knowing their variations at scale x [1]. In a typical two scale approach ($\eta \rightarrow 0$) the following decomposition can be made [1]

$$v = V + \eta \tilde{v} \quad \Rightarrow \quad \dot{\epsilon} = \dot{E} + \tilde{\epsilon}, \quad (5)$$

where $V, \dot{E}$ are the velocity and strain rate at scale x and $\tilde{v}, \tilde{\epsilon}$ represents the velocity and strain rates define at scale y . Using Eq. (5), the semidiscrete two-scale FEM formulation yields

$$\mathbf{M}\dot{\mathbf{V}} = \mathbf{F}^{ext} - \mathbf{F}^{int}(\langle \sigma \rangle), \quad (6)$$

where $\mathbf{M}$ is the mass matrix, $\dot{\mathbf{V}}$ are the vector of nodal accelerations, $\mathbf{F}^{ext}$ are the external forces and $\mathbf{F}^{int}$ are the internal forces which depends now on the stresses $\langle \sigma \rangle$. Hence the main focus is to determine $\langle \sigma \rangle$ which requires a representation of the RVE local structure. An important simplification in determining $\langle \sigma \rangle$ follows the fact that when $\eta \rightarrow 0$ the dynamics of the problem at the y scale can be neglected and therefore the *localization* can be treated as a quasi-static problem. Under these circumstances the dynamics of the problem is treated at the x scale while the y scale is used to determine the material response. In the next sections examples of two-scale FEM approaches for dynamic analysis of heterogeneous materials are presented.

Two-Scale FEM-MOC

The Method of Cells (MOC) represents a method to determine $\langle \sigma \rangle$ by using a simplified representation of the RVE [2]. In two-scale FEM using MOC, $\langle \sigma \rangle$ is calculated each Gauss integration point of the finite element of the x scale. This approach was applied successfully to study the dynamic response of PBX9501 [3]. PBX9501 is a heterogeneous material consisting of a bimodal distribution of HMX grains ("large" and "small") in a viscoelastic matrix (binder). A micrograph of PBX9501 is shown in Fig. 1 (a). Experiments on PBX9501 have shown a high rate dependency combined with a softening in the stress-strain curve and yielding. In building a model for PBX9501 one can consider that the rate dependency is due to the binder while the yielding is attributed to the HMX particles. Based on experiments one can regard the stress-strain softening as a damage of the material due to the formation of microcracks during the deformation. Due to the complex behavior and structure of PBX9501 simplifications are necessary. One of the current approaches represents PBX9501 as heterogeneous material consisting of a distribution of large HMX grains in a new viscoelastic matrix called the "dirty binder" (DB) obtained from the homogenization of the binder and the small grains [4].

Figure 1: (a) A micrograph of PBX9501. (b) RVE idealization in MOC. (c) RVE represented by a finite element E of the x scale discretization. Note the local y scale discretization of E .

In MOC this model is further simplified by representing an RVE of PBX9501 as in Fig. 1(b). The size of HMX cell relative to the RVE is determined by the volume fraction of the large HMX grains in PBX9501 after the small grains are accounted for in the DB. By imposing the continuity of displacements and equilibrium of tractions along the interfaces between the DB and HMX and employing periodic boundary conditions an average value for the $\langle \sigma \rangle$ can be determined [3]. In this model HMX follows a constitutive law of the type (1) and DB of the type (2). Cracking and plasticity is introduced only for the HMX through a damage and plasticity model [4].

The above formulation was applied to study the dynamic response of PBX9501 in the Split Hopkinson Pressure Bar test (SHPB). For the analysis the entire SHPB test was modeled. In Fig. 2 only the sample region is shown. Figure 3 shows the numerical response using FEM+MOC versus the experimental results. In can be observed that the model predicts the peak stress and the softening due to the cracking in the first part of the stress-strain curve. The differences between the numerical and experimental results in the last part of the curve are due most likely to the large cracks formation.

Figure 2: The FEM model used to simulate the SHPB test.

Two-Scale FEM-FEM

Characteristic of a typical two-scale FEM approach of heterogeneous materials is that $\eta \rightarrow 0$. This implies that the $RVE \ll$ finite element size of the x scale discretization. However there are situations, such as in PBX9501 applications, in which the RVE becomes comparable with the finite element size i.e. $\eta \approx 1$. To account for this aspect a new two-scale FEM approach was proposed [5]. The idea is to relax the decomposition (5) by taking the two-scale representation of $\dot{\epsilon}$ not relative to $\dot{E}$ but to a different value $\dot{E}_\Lambda$ related to $\dot{E}$ through a *deformation scaling tensor* Λ . Thus

$$\dot{\epsilon} = \dot{E}_\Lambda + \tilde{\epsilon}_\Lambda, \quad \dot{E}_\Lambda = \Lambda \dot{E}, \quad \Rightarrow \quad \dot{\epsilon} = \Lambda (\dot{E} + \tilde{\epsilon}). \quad (7)$$

Figure 3: Numerical vs. experimental stress-strain results for PBX9501 in the SPHB test.

For the present article one considers that both the heterogeneities and the matrix follow a constitutive law given by Eq. (1) with $\tilde{\varepsilon}^a = 0$. For simplicity one assumes also that RVE is represented by a finite element E of the x scale discretization as shown in Fig. 1(c). Using the Principle of Virtual Power applied on E and admitting the conservation of momentum relative to E while passing from scale x to y one obtains the following localization equation

$$\operatorname{div}(\Lambda^T C \Lambda \tilde{v}) + \rho \Omega^2 \tilde{v} = -\operatorname{div}(\Lambda^T C \Lambda V), \quad \text{with the constraint} \quad \langle \rho \tilde{v} \rangle = 0. \quad (8)$$

In Eq. (8) $\Omega^2 = K_E / M_E$ where K_E represents an equivalent stiffness of the finite element E and M_E is the mass of E . Λ can be determined by imposing the condition that the elastic response of E , using the present two-scale approach, to be the same as the response of the heterogeneous domain enclosed by E . In the present two-scale FEM-FEM formulation both scales are solved using FEM. Thus each element of the x scale mesh is discretized in finite elements as shown in Fig. 1(c) and applying the standard FEM formulation on Eq. (8) one obtains

$$\begin{bmatrix} \mathbf{k} - \Omega^2 \mathbf{m} & \mathbf{q}^T \\ \mathbf{q} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \tilde{\mathbf{v}} \\ \lambda \end{Bmatrix} = \begin{Bmatrix} \mathbf{L}^T \mathbf{V} \\ \mathbf{0} \end{Bmatrix}, \quad (9)$$

where $\mathbf{k}$ and $\mathbf{m}$ are the stiffness and mass matrix of E , $\mathbf{q}$ introduces the constraint equation $\langle \rho \tilde{v} \rangle = 0$ and $\mathbf{L}$ defines the stiffness coupling matrix between scales. Solving Eq. (9) with $\tilde{v} = 0$ on the boundary of E , one obtains the fluctuating velocity field $\tilde{v}$ and then the total strain rates from the Eq. (7). The stresses are then determined from the constitutive law (1).

To illustrate the new two-scale FEM approach a 3D numerical example was considered. On a coarse mesh (Fig. 4(b)) was mapped an RVE composed of two materials with a random local configuration (Fig. 4(a)) resulting in a heterogeneous domain (Fig. 4(c)).

Figure 4: Construction of heterogeneous domain.

After determination of Λ the heterogeneous domain was subjected in the z direction to a velocity triangular pulse applied on the top surface while the opposite surface was fixed in the same direction. The analysis was performed using three approaches denoted by D,T and H. In the D-analysis the problem was analyzed by a regular FEM using Fig. 4(c) mesh. One refers to this solution as “exact” since heterogeneous domain is discretized up to the heterogeneities level. In the T-analysis the problem was analyzed using the present two-scale FEM approach using the Fig. 4(b) mesh for the x scale combined with the Fig. 4(a) mesh for the y scale. In the H-analysis the problem was analyzed using a regular FEM with constant material tensor equal to $\langle C \rangle$ (the homogenized domain) and the Fig. 4(b) mesh. During the analyses an element E located in the center of the domain (Fig. 4(b)) and the average response of the corresponding region in Fig. 4(c) were monitored. The results are shown in Fig. 5. One remarks that the present two-scale FEM approach offers a closer solution simultaneously in both stress and strains to the “exact” results as compared with the H-solution.

Figure 5: Stress and strains in the z direction vs. time for an applied triangular velocity pulse.

Figure 6(a) shows a typical stress distribution of the present two-scale FEM in the element E . In Figs. 6(b) and 6(c) are presented the distributions of velocity and stress in the z direction in the

section S of the element E (Fig. 6(a)). The distribution of the Von Mises stress in the same section S is shown in Fig. 6(d).

Conclusions

In this article two examples of using two-scale FEM analysis for heterogeneous materials were presented. The two-scale FEM technique allows to model the response of heterogeneous materials when the constituents follow different types of constitutive laws, a case in which homogenization may be difficult. For the cases in which the RVE becomes comparable with finite element size of the first scale discretization, a new approach was proposed. The numerical examples using the new approach have shown good agreement in both the stress and strain with a full-scale solution. Regarding the inelastic deformations it is important to note that since the second scale is used to obtain the material response, any inelastic deformation needs to be treated at that level.

Figure 6: Stress and velocity distributions for an element E in the present two-scale FEM approach.

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