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Review of Computational Homogenization of Materials

Md. Mahabub Hasan Mousum[1], A.M. Rahman[2], Nauman Ehsan Hashmi[3] & Dr. Muhammad Shahid Khan[4]
[1]Department of Mechanical Engineering, Rajshahi University of Engineering & Technology (RUET), Bangladesh
[2]Institute of Solid Mechanics, Karlsruhe Institute of Technology (KIT), Germany
[3,4]School of Chemical and Materials Engineering, NUST, Pakistan
Email: mousum.mahabub@gmail.com; al.rahman@partner.kit.edu, naumaneshanhhashmi@gmail.com, mshahid@scme.nust.edu.pk*

Abstract

Over the recent years, engineering materials have transformed at a rapid pace. The introduction of composite materials and their advantages have led to a revolution in high performance engineering application. The mechanical properties of engineering materials are dependent on their microstructure. Almost all engineering materials in general and composite materials in specific are heterogeneous in nature. The tailoring of microstructure of engineering materials is covered by localization of multiple phases known as homogenization of material. A review of homogenization in computational mechanics of materials is carried out to develop a better understanding of finite element methods applied in materials engineering.

Keywords: Homogenization, computational mechanics of materials, composite materials.

1. Introduction

Mechanical properties of engineering materials are dependent on their microstructure. As per Ortolano et al. [1], the micro-macro mechanics determine the relationship between microstructure and macroscopic response of the material. According to Oller [2], the anisotropic mechanical properties of composite material renders the ineffective utilization of constitutive equations of homogenous materials. Owing to the presence of different phases and heterogeneous nature, a need for development of governing equations for composite materials was felt. As per Michel et al. [3], in homogenization mathematical model is derived from localization of individual constituents.

2. Computational Homogenization: A Brief Introduction

The Basic concept of computational homogenization is derived from numerical breakdown of heterogeneous material into localize homogeneous cell. The localized cell is termed as Representative volume element (RVE). The formation/selection of RVE must take into account all heterogeneity of material. The representative equation for an RVE as per Hill Mandel condition is shown in equation (1).

$$\sigma^M : \varepsilon^M = \frac{1}{V^M} \int_{Vm} \sigma^M : \varepsilon^M \, dV_m \tag{1}$$

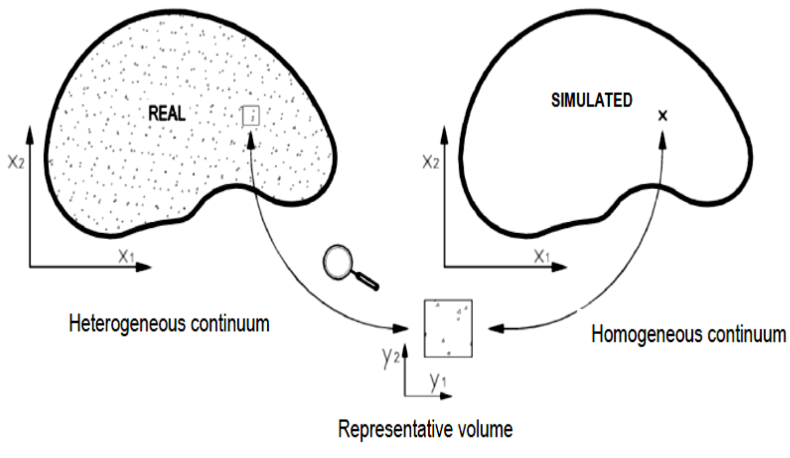

Fig 1. Representation of an RVE in a heterogeneous material

From the point of view of Stavroulakis et al. [4], the states of prescribed linear boundary conditions, prescribed traction and periodic boundary conditions can be applied to RVE. The complete material is divided into numerous RVE for computational purposes. One of the RVE is illustrated in the figure 1.

Different computation models have been developed based on homogenization concept. A brief detail of these models are discussed in subsequent sections.

3. Mathematical Basis of Computational Homogenization

Different computational methods and models were proposed to resolve the problem of heterogeneous materials. The average or heuristic method was proposed by Suquet [5]. As per Hill [6], the characteristic parameters of a material are a result of average distribution of stresses and strains (equation 2).

$$\sigma^x = \langle\sigma\rangle_v \qquad \varepsilon^x = \langle\varepsilon\rangle_v \tag{2}$$

The asymptotic expansion theory splits heterogeneous materials into scales of different magnitudes. The difference in magnitude scale length of microscopic and macroscopic properties divided reference space into two different magnitude spaces. Consequently a global space x_i is used while y_i is used as microscopic scale. The scale of two space is represented by scale relationship ε. A simple representation of mathematical expression is equation (3).

$$y = \frac{x}{\varepsilon} \tag{3}$$

4. Non Linear Problem of Composites Mechanics

The both models discussed deals amicably with the elastic behavior of composite materials. The prediction of inelastic or nonlinear behavior of composite materials is still a challenge. Different mathematical models, extensions, and theories have emerged to resolve the issue. The earlier research on the subject revealed that the macroscopic variables of the problem depend upon the microscopic variables of material. To accurately predict the nonlinear behavior, high computational cost was envisaged. Many mathematical models developed to reduce the computational element. Voronoi finite element method is an innovative approach for solving the nonlinear composite issue. In this method, a medium volume with arbitrary heterogeneity in domain partition is represented by a convex polygon known as Voronoi element. The formulation of Voronoi method is carried out by stress hybrid method. The decomposition of a material domain as per this method is shown the in the figure 2.

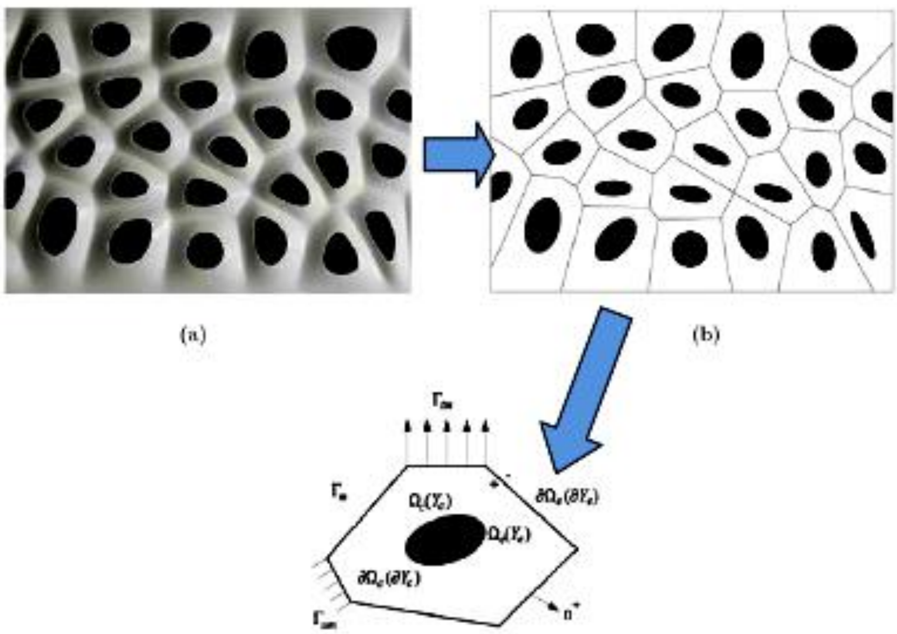

Fig 2. Decomposition of a heterogeneous material into Voronoi elements

The method was further extended by Ghosh et al. [7]. The results obtained by method were good with a lower computational cost. Later on a fracture criteria and adaptive macro-scale method was introduced. The result

obtained by this method for a randomly distributed material are good. However, the precision of the results are lower than the unit cell method.
Unit cell method is a sequential multi-scale procedure. Macroscopic model is induced by using a detailed RVE. Many researcher have used and contributed in development/refinement of this procedure. The main focus of research in this particular technique was on metal matrix composite (MMC). As per Kanouté et al. [8], many extension to unit cell methodology have been proposed and tested till date. Keeping in view the detailed RVE, the method is categorized as precise but computation exhaustive.

5. Transformational Field Analysis (TFA)

TFA analysis was proposed by Dovrak and co-workers. In this method the reduction of internal microscopic variables is carried out by assuming that internal variables are piece wise uniform. The method was developed for elasto-plastic composites. The main basis of TFA is purely elastic distribution of stress and strain and of local eigen stress and eigen strains. In TFA technique, the explicit transitions are based on elastic interaction between sub-volumes of RVE. The plastic strains and thermal strains are considered as eigen strains. The local stress is determined by solving the eigen strain and plastic strains determined by flow rule. The volume 'V' is subdivided in to local sub-domain volume V_r where r = 1, 2, 3…..n such that each contains one phase material. The constitutive equations of the TFA are presented in equation (4).

$$\begin{gathered} \sigma_r(x) = L_r : \epsilon_r(x) + \lambda_x (x) \\ \epsilon_r(x) = \varepsilon_r^{g}(x) + \mu_r(x) \end{gathered} \tag{4}$$

$\mu_r(x)$ is prescribed distribution of local eigen strains and $\lambda_x (x)$ is corresponding eigen stress field. The relation between local and over all field is given by the localization rule, which is presented by the equation (5).

$$\begin{gathered} \varepsilon_r = A_r : E + \sum_s D_{rs} : \mu_s \\ \sigma_r = B_r : \sum - \sum_s F_{rs} : \lambda_s \end{gathered} \tag{5}$$

D_{sr} and F_{sr} are transformation influence tensors. All tensors depend upon local and overall elastic moduli and on the shape and volume fraction of the phases and can be derived independently from inelastic process. In cases where two phases are considered with one sub-volume only for each phase, A_{rs} and D_{rs} (respectively B_{rs} and F_{rs}) can be expressed in close form by eshelby tensor. The TFA has been further extended by taking into account non-linearities due to change in local behavior by temperature and damage. The mathematical expression can be defined with the given equation (6).

$$\sigma_r = L_r : (\varepsilon_r - \varepsilon_r^{GE}) \tag{6}$$

In order to account for intrinsic plasticity, a corrected TFA approach was also formulated. The approach was based on used of asymptotic stiffness tensor. For a model of elasto-plastic phases, the correct TFA technique can be represented by the expression of equation (7).

$$\varepsilon_r = A_r : E + \sum_s D_{rs} : K_s : \varepsilon_s^{p} \tag{7}$$

Where ε^p_s is the plastic deformation in phase S. Moreover it has been assumed that asymptotic tangent stiffness of the local constituent is known. Practically it is obtained from knowledge of hardening rules in each phase. In case of rate dependent plasticity, its modulus is the kinematic hardening parameter. The corrected tensors are obtained by rate forms of localization rule.
The results obtained by this model have demonstrated good accuracy in comparison with the numerical simulations. However, the application of TFA to two phase system may require decomposition of each phase into several subdomains to obtain a satisfactory result. The domain decomposition results in to an increase in number of internal variables. Increase in number of variable resulted into need for further refinement of constitutive equations.

6. Non Uniform Transformation Field Analysis (NTFA)

With the aim of reducing the number of sub-volumes, NTFA was introduced. The plastic strain is decomposed in finite set of plastic modes which can represent large deviations from uniformity. The mathematical expression used is given in the equation (8).

$$\varepsilon^{an}(x) = \sum_k \epsilon_k^{an} \ \mu^k(x) \tag{8}$$

As per Largenton et al. [9], the modes μ^k depends on spatial variable x. The constitutive models of NTFA involve few choices made to obtain reduced order modes (ROM). Choice of plastic modes and evolution

equation for generalized plastic components are the steps involved. The results of material micro level modelling of a three phase nuclear fuel have shown great promise in accuracy (figure 3). The individual constituents of the material would undergo aging under the effect of irradiation. The NTFA model accounts for the aging effect despite usage of non aged constituents material properties. The global and micro response of the composite under review was well captured by the NTFA model.
As per Michel et al. [10], NTFA has certain limitations like selection of appropriate plastic modes, cyclic or non proportional loading conditions and GSM format. For retention of micro-mechanical law, two models are proposed in NTFA. The coupled model and the uncoupled model.

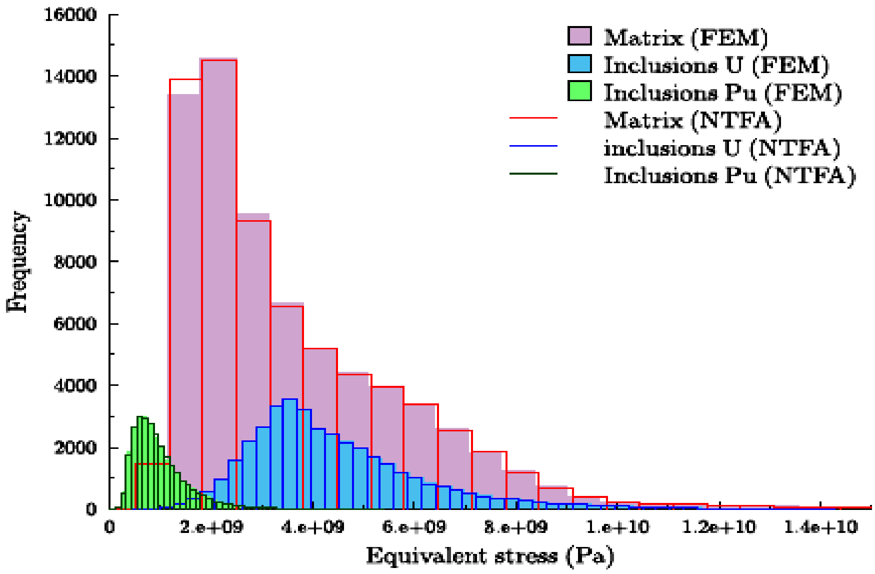

Fig 3. Results of NTFA model application on mixed oxide nuclear fuel

In coupled model, different modes of each phase is supported by a quadratic average. Moreover an internal variable β_r is attached to each phase not to each mode. In uncouple mode, the reduced internal variables are overall strain , the set of all $\varepsilon^{an}{}_k$ and set of tensorial variable β_k associated with each mode. A comparison of results obtained by application of five different loading conditions are shown in the figure 4.

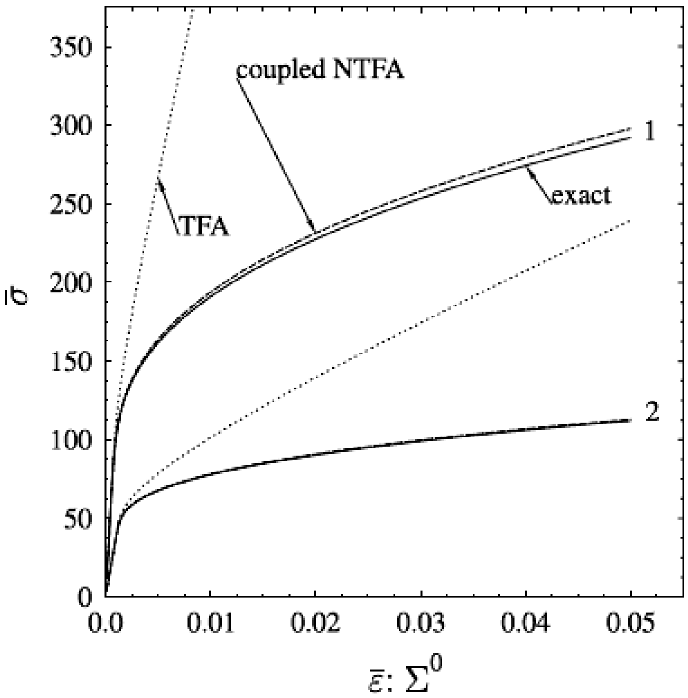

Fig 4. Comparison of results obtained by NTFA, TFA and exact behavior under five loading conditions

Further extension of NTFA was represented by Roussette et al. [11] for elastic visco-plastic composites. The extension of NTFA focused on elastic-visco plastic composites. The constituents of mathematical notation includes free energy (w) and force potential (ψ). The governing mathematical expression of subject extension is equation (9).

$$w(\varepsilon|\varepsilon^{vp}) = \frac{1}{2}\,(\varepsilon - \varepsilon^{vp}) : L : (\varepsilon - \varepsilon^{vp}) \tag{9}$$

The constituents are assumed to be isotropic. The elastic tensor (L) is characterized by bulk modulus (k) and shear modulus (G). Force potential (ψ) depends on second variant of stress. The visco-plastic strain is decomposed in to set of plastic modes. The total number of modes can differ from number of constituents for incompressible visco -plastic. In case of compressible visco-plasticity, the strain is decomposed into traceless tensor fields. The results obtained by this extension are shown in the figure 5.

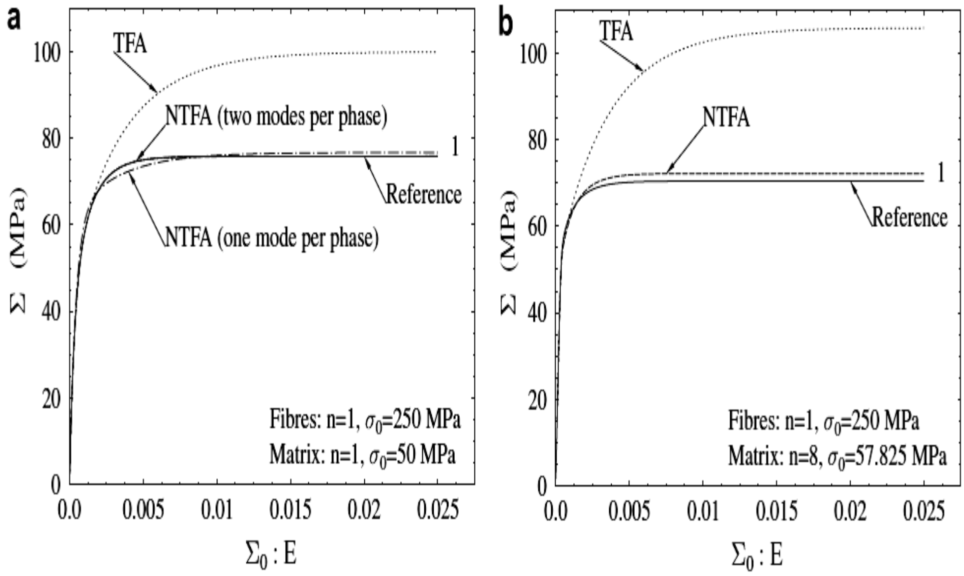

Fig 5. Comparison of result obtained by NTFA for elastic-viscos plastic composite

Different other reduced order models for NTFA are currently under research. Over a passage of time the number of extension to NTFA are expected to increase covering different aspects and classes of composite materials.

7. Conclusion

Composite materials have changed the aspects of computational mechanics of materials. The presence of multiple phase and their specific morphology have posed many issue for prediction of their mechanical behavior by using computational sciences. Over last few decades, many mathematic models of composite materials have surfaced and utilized. Almost every model has its own set of limitations and precision. A comprehensive computational analysis adds to computational cost. Reduced order models (ROM) have emerged to counter this limitation. However, still a lot of aspects and field are left unexplored for the computational scientists.

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