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ORIGINAL RESEARCH ARTICLE

ANALYTICAL, NUMERICAL AND COMPUTATIONAL MULTISCALE MODELLING TECHNIQUES FOR HETEROGENOUS MATERIALS: A REVIEW

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ABSTRACT

This paper reviews the analytical, numerical as well as the computational homogenization multiscale modelling schemes for determining the effective material properties for heterogeneous medium at the macroscopic level. It also looked at the limitations of the analytical homogenization techniques in simulating the effective non linear heterogeneous material behaviours (for example the rapid localization of damage and so on) as well as the advancements of the computational techniques in addressing these limitations. In addition, the possible future trends for the computational technique such as the development of a fully coupled micro-macro computational scheme were also discussed. It was concluded that although, the analytical technique was quite popular and straight forward, its inability to capture rapid localization of damage limited its application and that numerical and computational schemes were able to address these limitations as they relied on the establishment of constitutive relations for the macroscopic problems in a numerical form through which the macroscopic problems were constructed and solved in a nested manner.

1.0 Introduction

Most engineering materials (steel, concrete, polymer-blends, functional materials and so on) are inherently heterogeneous in nature (Figure 1) when viewed at a particular scale and are mostly referred to as composites (Nguyen et al., 2012; Matous et al., 2017).

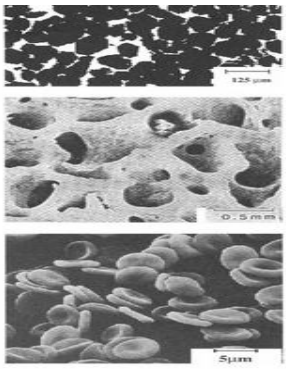

Figure 1: Natural random heterogeneous material adapted from Torquato (2013).

Studies (LLorca et al., 2007; Kouznetsova et al., 2012) have shown that, the macroscopic behaviour of these composite materials are linked to their mechanical behaviour as well as the details of their microstructure (that is volume fraction, spatial distribution of the different phases and inter-phases, their morphological properties, sizes and shapes et cetera). These micro-structural material details tend to evolve by undergoing phase transformations under the application of thermo-mechanical loadings as well as advanced forming operations; thus, making it essential to understand the relationship between the microstructure properties and the macroscopic material behaviour (also known as the micro-macro structure property relation). It is hoped that by taking advantage of this micro-macro structure-property relationship, it should be possible to manipulate the material microstructure so as to influence the macroscopic mechanical behaviour of the composite material to obtain desired results. For example, "improved strength and toughness, high stiffness and high damping, improved thermal conductivity and electrical permittivity, improved permeability" et cetera (Kanoute et al., 2009); consequently, improving the materials performance in special industrial applications from an engineering perspective, provides an economic alternative to the designing of new materials with desirable macroscopic characteristics (Nguyen et al., 2012; LLorca et al., 2007).

Establishing this micro-macro structure-property relation has been a major challenge in computational micromechanics as well as material science as it is not feasible to carry out an upfront experimental measurement where all the micro-structural characteristics are explicitly considered. It is the need to provide an efficient modelling strategy, to better understand the relationship between material micro-structure and macroscopic properties (that is the micro-macro structure property relation) leading to the determination of the general macroscopic homogenised constant value for the heterogeneous material, that has lead to the development of the multiscale models. This is because for the analysis of composite materials, it is the effective or homogenised material property that is used as opposed to the properties of the separate components that make up the material (Kanoute et al., 2009; Nguyen et al., 2012).

Multiscale modelling, is therefore, an area of study which involves resolving problems which have significant characteristics at multiple scales of resolution. It usually entails modelling from the smallest scale of the material to a much larger scale (for example, from nanoscale that is quantum level to the macroscale that is continuum level as shown in figure 2) This is usually achieved through the use of various models at the different scales of resolution which are then coupled either analytically, numerically or computationally (Engquist et al., 2007; Weinan and Jianfeng, 2011).

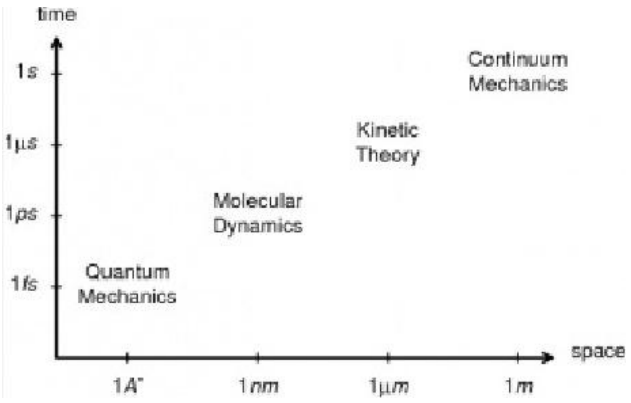

Figure 2: Illustration of the multi-scale modeling hierarchy adapted from Weinan and Jianfeng (2011).

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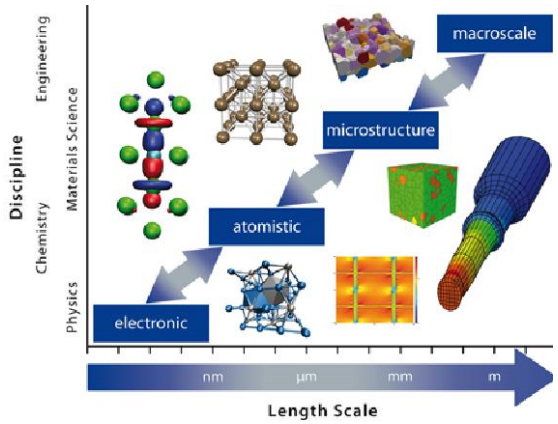

Figure 3: A seamless integration of models of the different length scales into one coherent multiscale modelling frame work. Adapted from ICAMS webpage Ruhr University Germany

Although, most engineering problems are solved at the macroscopic scale, the results obtained from such analysis are not sufficiently precise while the direct micro-scale modelling of engineering problems are not cost effective and offer too much information; hence the need for multiscale modelling (Weinan and Jianfeng, 2011; Kanoute et al., 2009). The driving force behind carrying out multiscale modelling is to achieve a balance between accuracy and efficiency by coupling together both the microscopic and macroscopic models; thus, providing an accurate predictive tool which is considered crucial in engineering and material science (Engquist et al., 2007).

This paper reviews the advancements in multiscale modelling of composite material (such as steel, concrete, polymer-blends, and so on) which are used for various industrial applications to determine their macroscopic material properties such as stress and stain fields in addition to their macroscopic material behaviour such as their energy absorption at high strain rates, cracking, creep, et cetera by using the various homogenization methods (Nguyen et al., 2012; Aliyu, 2019).

2. Homogenisation techniques

As previously mentioned, the significance of modelling across multiple-scales is that the predictions obtained from such modelling techniques are more precise and accurate (Weinan and Jianfeng, 2011). The conventional multi-scale modelling of composites is either carried out within the framework of homogenisation methods or the concurrent method depending on whether the scales are distinctively separated or coupled (Nguyen et al., 2012).

The fundamental aim of homogenisation techniques is to determine the effective properties for heterogeneous materials from the mechanical behaviour of the materials constituents' microstructure; thus, providing a means for replacing the heterogeneous material with a homogenous one.

For many decades now, quite a number of micromechanical modelling techniques dealing with heterogeneous materials have been developed (Kanoute et al., 2009). The micromechanical modelling technique to be adopted in achieving a homogenised constant material value for a heterogeneous or composite material falls into one of three main categories. In the first category, schemes employed used high resolutions at certain sections of the domain where fine (microscopic) scale detail of the microstructure morphology (i.e. at cracked tips, and interfaces) needs to be determined. For the second category, the schemes rely on the description of the

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macrostructure from the analysis of the underlying fine (microscopic) scale problem while the third category uses schemes which allows for some sections of the domain to be completely resolved at the fine microscopic scale and the other sections resolved by using the effective macroscopic response (Nemat-Nasser and Hori 1999; Sluis et al., 2000; Kouznetsova et al., 2012; Torquatom, 2013; Matous et al., 2017).

Schemes under the above three categories will be discussed in the following sections Analytical/mathematical homogenisation, Numerical homogenisation as well as Computational homogenisation.

2.1 Analytical/mathematical homogenisation

Initial research on homogenization techniques can be attributed to the works of Voigt (1889) and Reuss (1929). They were both able to develop models which gave rough estimates of the upper and lower bound values of the effective moduli of heterogeneous materials. Both models only took into account the volume fraction. This limited its application as the influence of other characteristic properties of the microstructure was not taken into consideration.

2.1.1 General procedure

As the principle objective of homogenization is to describe the effective properties of the composite material from the mechanical behaviour of the materials constituents' microstructure as shown in Figure 4.

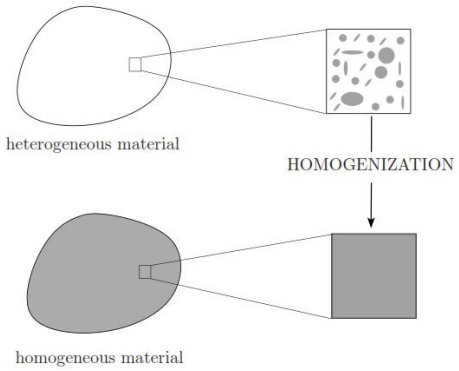

Figure 4: Schematic representation of homogenization of material (Temizer and Zohid 2006; cited in Nyguyen et al. 2012).

The bridging of length scales is necessary and this is carried out by volume averaging and is denominated homogenization (LLorca et al., 2007).

$$\bar{\epsilon} = \frac{1}{\Omega}\int_{\Omega} \epsilon(x)d\Omega \text{ and } \bar{\sigma} = \frac{1}{\Omega}\int_{\Omega} \sigma(x)d\Omega \qquad (1)$$

where: Ω is the microscopic sample; $\boldsymbol{\varepsilon}(\boldsymbol{x})$ microscopic stress; $\boldsymbol{\sigma}(\boldsymbol{x})$ microscopic strain; $(\boldsymbol{x})$ position vector; $(\bar{\boldsymbol{\varepsilon}})$ macroscopic strain and $(\bar{\boldsymbol{\sigma}})$ macroscopic stress.

While the expression which gives the denominated localization is given by:

$$\epsilon(x) = A(x):\bar{\epsilon} \quad \text{and} \quad \sigma(x) = B(x):\bar{\sigma} \qquad (2)$$

where: $\boldsymbol{A}(\boldsymbol{x})$ and $\boldsymbol{B}(\boldsymbol{x})$ are the stain and stress concentration tensors.

The increasing complexity of the microscopic mechanical behaviour and geometries hinders the underlying objective of the above technique. Hence, the simplifications of the above

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assumptions are necessary which leads to a number of homogenization models with the most significant simplification being the "mean-field approach which approximates the strain and stress fields by phase-wise constant fields" $\boldsymbol{\epsilon_i}$ and $\boldsymbol{\sigma_i}$ given in equation 3.

$$\epsilon_i = A_i : \bar{\epsilon} \text{ and } \sigma_i = B_i : \bar{\sigma} \quad (3)$$

where:

$\boldsymbol{A_i}$ − strain concentration tensor for the phase i

$\boldsymbol{B_i}$ - stress concentration tensor for the phase i (LLorca et al., 2007)

In adopting this principle, Eshelby (1957), came up with an effective medium approximation in obtaining the overall effective properties of the heterogeneous medium where the microstructure is composed of a matrix and a spherical or ellipsoidal inclusion. He also noted that the strain field within the inclusion was constant.

So that for a linear constitutive equation:

$$\sigma_i = L_i : \varepsilon_i; \quad (4) \qquad L = \sum_i^N f_i L_i : A_i \quad (5)$$

$$I = \sum_i^N f_i A_i = \sum_i^N f_i B_i \quad (6)$$

$$\epsilon_i = A_i^{dil} : \bar{\epsilon} \quad (7)$$

$$\text{where } A_i^{dil} = \left[I + S_i : L_m^{-1} : (L_i - L_m)\right]^{-1} \quad (8)$$

The elastic stiffness tensor of the effective material (L) can then be evaluated from equations (1), (6) and (8) as:

$$L = L_m + f_i\left[(L_i - L_m) : A_i^{dil}\right] \quad (9)$$

where: $\boldsymbol{L_m}$- Stiffness tensor for the matrix

$\boldsymbol{L_i}$- Elastic stiffness tensor for the inclusion

$\boldsymbol{L}$- Effective elastic stiffness tensor

N- Number of phases

I-Identity tensor

$\boldsymbol{S_i}$- Eshelby's tensor for the inclusion.

$\boldsymbol{A_i}^{dil}$ - Strain concentration tensor for the dilute condition

dil- dilute

f_i - Volume fraction

This Eshelby effective medium approximation was further extended by Hill (1965)

Along the lines of this mean field approximations, Kröner (1958) came up with a self consistent approach for obtaining the effective material property for a matrix and spherical or ellipsoidal inclusions in the elastic regime. The main idea behind this approach is that for a composite composed of scattered particles, it is possible to assume that the composite is composed of a particle of one phase embedded in an effective medium. In his work, the strain concentration tensor A_i^{sc} was obtained from the Eshelby dilute solution in Eqn. (8) above by replacing the matrix elastic constant (L_m) in Eqn. (8) with those of the effective medium (^{L}) to give the resulting expression in equation (10)

$$\boldsymbol{A_i^{sc} = [I + S_i : L^{-1} : (L_i - L)]^{-1}} \quad (10)$$

The effective material property $(\boldsymbol{L})$ was then be evaluated by substituting Eqns. (10) in (5) to obtain Eqn. (11).

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$$L = \sum_{i}^{N} f_i L_i : \left[I + S_i : L^{-1} : (L_i - L) \right]^{-1} \quad (11)$$

This self consistent approach was further extended to non-linear cases in the studies carried out by Hill (1965), Hutchinson (1976) and Bereviller (1979).

The effective properties of the heterogeneous medium in an elastic regime can also be evaluated using the variation principles. Employing this technique gives an upper and a lower bound value for the effective property. The simplest works on this variation principle were those of Voigit and Ruess (Hill, 1963). In their models the strain energy density function $^{\omega}(x,^{\varepsilon})$ and the complementary energy density function $^{u}(x,^{\sigma})$ were expressed in terms of a homogenous phase potential as:

$$\omega(x,\varepsilon) = \sum_{r=1}^{N} \chi^{(r)}(x)\, \omega^{(r)}(\varepsilon) \quad (12)$$

$$u(x,\sigma) = \sum_{r=1}^{N} \chi^{(r)}(x)\, u^{(r)}(\sigma) \quad (13)$$

where:

$\omega^{(r)}(\varepsilon)$ and $u^{(r)}(\sigma)$ – are the homogeneous phase potentials and $\chi^{(r)}(x)=1$ if x $\boldsymbol{\epsilon}$ $\Omega^{(r)}$ or zero.

Firstly, the effective strain and complementary potentials ($\widetilde{W}(\bar{\varepsilon})$ and $\widetilde{U}(\bar{\sigma})$) for the heterogeneous medium is achieved by averaging their minimum potential energies given as:

$$\widetilde{W}(\bar{\varepsilon}) = \min_{\boldsymbol{\varepsilon}(x)\in k} \langle \omega(x,\varepsilon) \rangle \quad (14)$$

$$\widetilde{U}(\bar{\sigma}) = \min_{\boldsymbol{\sigma}(x)\in s} \langle u(x,\sigma) \rangle \quad (15)$$

(Kanoute et al., 2009)

Where:

$\widetilde{\boldsymbol{W}}(\bar{\boldsymbol{\varepsilon}})$ – Average minimum complimentary potential

$(\bar{\boldsymbol{\varepsilon}})$ - Average of the actual strain field $\boldsymbol{\varepsilon}$

$\widetilde{\boldsymbol{U}}(\bar{\boldsymbol{\sigma}})$ -Average minimum complimentary strain

$(\bar{\boldsymbol{\sigma}})$ - Average of the actual strain field $\boldsymbol{\sigma}$

While the strain energy and complementary density functions as given in the McCauley brackets (that is equation (14) and (15)) gives the volume averages in the domain Ω.; $\bar{\boldsymbol{\varepsilon}}$ and $\bar{\boldsymbol{\sigma}}$ are the average strain and stress fields while k is the set of kinematically admissible strains and S is the set of statically admissible stresses. The effective strain and stress potential for the elastic heterogeneous medium at the macroscale is therefore given by the Voigt and Ruess model as shown in Eqns. (18) and (19):

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(a) Voigt model $$\widetilde{W}(\bar{\varepsilon}) = \frac{1}{2}\,\bar{\varepsilon} : \bar{L} :\, \bar{\varepsilon} \qquad (16)$$

$$\bar{L} = \sum_{r=1}^{N} c^{(r)}\, L^{(r)} \qquad (17)$$

To arrive at the above expressions, Voigt assumed that the strain field within the heterogeneous medium was constant.

$$\widetilde{U}(\bar{\sigma}) = \frac{1}{2}\,\bar{\sigma} : \bar{M} :\, \bar{\sigma} \qquad (18)$$

(b) Ruess model $$\left(\bar{L}^{-1}\right)^{-1} = \sum_{r=1}^{N} c^{(r)}\,(L^{(r)})^{-1} \qquad (19)$$

The assumption in Ruess model is that a uniform stress was applied to the polycrystals with resulting comparable stresses in the constituent crystallite.

where:

L- Is the effective elastic tensor

M- Compliance tensor

$c^{(r)}$ - The volume fraction for the phase r

$\boldsymbol{L}^{(r)}$ - The elasticity tensor for the phase r

Hill (1952), noted that because of the assumptions of a constant strain field in Eqn. (14) and a constant stress field in Eqn. (15), Voigt model gives an upper bound estimate as shown in Eqn. (16) while Ruess model gives a lower bound estimate as shown in Eqn. (17)

$$\bar{W}(\bar{\varepsilon}) < \frac{1}{2}\,\bar{\varepsilon} : \bar{L} :\, \bar{\varepsilon} \qquad (20)$$

$$\bar{U}(\bar{\sigma}) \leq \frac{1}{2}\,\bar{\sigma} : \bar{M} :\, \bar{\sigma} \qquad (21)$$

In adopting the variation principle, Voigt and Ruess have only taken into account the volume fraction of each phase (one-point limit) which limited the application of their model as the influence of other characteristic properties of the microstructure on the effective properties of the heterogeneous medium have not been taken into consideration.

Hashin and Shtrikman (1962a, 1962b and 1963), also employed the variation principles but took into account the polarization fields and were able to derive much tighter bounds for the effective properties of heterogeneous materials (two-point bounds) in comparison to that obtained from the Voigt and Ruess model (one-point limit).

$$K_1 + \frac{v_2}{\frac{1}{k_2 - k_1} + \frac{3(1-v_2)}{3k_1 + 4\mu_1}} \leq k^* \leq k_2 + \frac{1 - v_2}{\frac{1}{k_1 - k_2} + \frac{3v_2}{3k_2 + 4\mu_2}} \qquad (22)$$

$$\mu_1 + \frac{v_2}{\frac{1}{\mu_2 - \mu_1} + \frac{6(1-v_2)(k_1 + 2\mu_1)}{5\mu_1(3k_1 + 4\mu_1)}} \leq \mu^* \leq \mu_2 + \frac{1 - v_2}{\frac{1}{\mu_1 - \mu_2} + \frac{6v_2(k_2 + 2\mu_2)}{5\mu_2(3k_2 + 4\mu_2)}} \qquad (23)$$

where:

k_1,μ_1– Bulk moduli in the first phase of the microstructure

k_2,μ_2– Shear moduli in the second phase of the microstructure

v_2 – Volume fraction in the second phase (Konoute et al., 2009)

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This technique was later expanded by Torquato (2001) by including the details of the phase arrangement in his model (three-point bounds).

The variation technique was further extended to non-linear cases in the work carried out by Talbot and Willis 1985 and Willis 1986. Further advancement in variation principles has lead to the Ponte Castaneda (1991, 1992) and Talbot and Willis (1992) variation principles in estimating the effective properties of non-linear composites (such as, the rapid localization of damage, energy absorption at high strain rates that is large plastic deformations and so on) as well as the Suquet variation principles for power law composites. As an improvement on Voigt upper bound estimate of the effective macroscopic properties for rigid plastic material, Olson (1994) came up with his own variation principles for perfectly plastic composites.

Lately, homogenization schemes employed in the analysis of elasto-plastic composite materials has been reviewed by scholars such as: Ponte Castaneda and Suquet (1998) as well as Chaboche et al. (2005). In their opinion the schemes can be categorised into two groups, namely, those based on the use of secant stiffness tensor and those based on the use of tangent stiffness tensor.

Schemes based on the secant formulations dealt with plastic deformations within the frame work of non-linear elasticity, where the effective secant stiffness tensor is used to assess the relationship between the stress and strains at the elasto-plastic stages. This approach is best adopted when the composite material is subjected to monotonic and proportional loading (LLorca et al., 2007). The elasto-plastic tangent modulus approach for evaluating the mechanical response of composites was presented by Hill (1965) where he linearized the local constitutive equation by bringing it back in an incremental form:

$$\boldsymbol{\sigma}(\mathbf{x}) = \boldsymbol{L}(\mathbf{x}):\boldsymbol{\varepsilon}(\mathbf{x}) \qquad (24)$$

where: L is the tangent modulus (Konoute et al., 2009).

The initial models based on this approach gave very stiff predictions of the flow stress. The source of the inaccuracy was attributed to the anisotropic characteristic of the tangent stiffness tensor. More accurate predictions of the flow stress were obtained by adopting an isotropic estimation of the tangent operator (Chaboche et al., 2005).

Another homogenizational approach is the mathematical asymptotic homogenization theory which employs an asymptotic expansion of the displacement and stress fields based on a ratio of the length scales (ς). This technique gives both the effective overall properties such as the effective stiffness as well as the local stress and strain values (Kouznetsova et al., 2012).

2.2 Numerical Homogenization Schemes

In computational micromechanics, the macroscopic or effective behaviour of composites is obtained through the solution of the boundary value problem (BVP) for a representative volume element (RVE) of the microstructure by using numerical techniques. Within this frame work, it is possible to obtain the local values of the field variable which facilitates the accurate simulation of crack nucleation and growth of damage as well as the localization of strains leading to damage which is a major advantage of the technique over analytical homogenizational schemes (LLorca et al., 2007; Zohdi and Wriggers 2005).

2.2.1 Numerical simulation schemes

The current advancements in computing power and simulation tools, facilitating the solution of boundary value problems (BVP) of representative volume element (RVE) of composites or

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heterogeneous materials, of a size statistically sufficient enough to represent the microstructure without introducing undesired or non-existent properties is a welcome development in the computational micromechanics community. These numerical strategies (fast fourier transform algorithms, boundary element method as well as the finite element method FEM) adopted in the solution of BVP are not only computationally efficient but also facilitates the solution of problems involving complex geometries. Although the FEM is the most preferred in the micromechanics community because of its mesh generation capabilities as well as its ability to implement complex constitutive equations; it tends to produce large models when simulating micro fields in regions with large strain gradient (LLorca et al., 2007). The Voronoi cell finite element method (VCFEM) was introduced as an innovation to the FEM in solving non-linear problems in composite materials. This technique is designed to simulate the behaviour of the composite material microstructure having different morphologies. In order to capture the variation in morphology, the finite element discretization was obtained by using Voronoi tessellations where every Voronoi cell contains an inclusion embedded in the matrix representing the basic hybrid finite element (Moorthy and Ghosh 1994; LLorca et al., 2007).

This formulation lowers the cost of computation in determining the micro fields in heterogeneous materials as the hybrid finite element reduces the number of degrees of freedom (d.o.f) in the analysis (Moorthy and Ghosh 1996, 2000). A three-dimensional VCFEM (Figure 5) for analysing composite material with randomly distributed composites was developed by Ghosh and Moorth (2004).

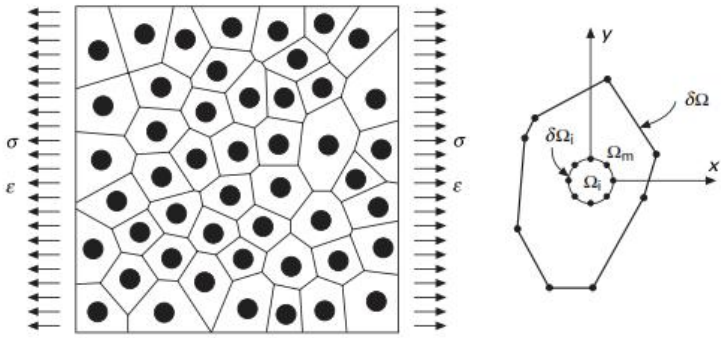

Figure 5: A two-dimensional Voronoi cell finite-element mesh and detail of one Voronoi finite element adapted from Llorca et al. (2007)

This technique was further extended by Li and Ghosh (2006). They came up with the extended Voronoi cell finite element method (X-VCFEM) used to model interfacial debonding in heterogeneous materials. In computational micromechanics, the use of efficient simulation tools (that is the domain decomposition method, iterative solvers such as: the conjugate gradient method) capable of solving BVP for RVE is key as most micromechanics simulations require very large models with complex non-linear behaviour (Zohdi and Wriggers, 2005).

The numerical homogenization discussed, gives emphasis on multiscale techniques based on coupled homogenization techniques and numerical analysis of the RVE for both periodic and non periodic (random) microstructure morphological compositions as shown in Figure 4.

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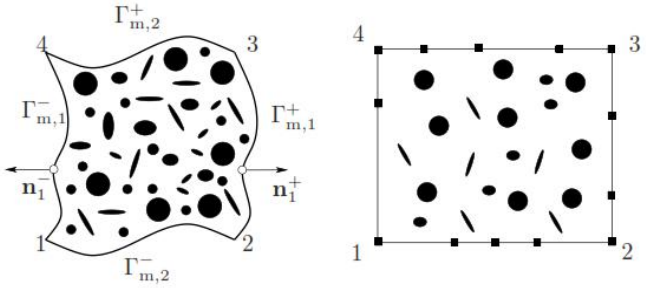

Figure 6: Schematic representation of periodic and non periodic RVE from Nguyen et al. (2012).

2.2.2 Asymptotic homogenization

One such multiscale modelling technique is the coupling of asymptotic homogenization and finite elements. In this method the mathematical asymptotic concept is adopted in solving multiple scale problems by coupling finite element problems across length scales. This homogenization technique adopts an asymptotic expansion of the displacement and stress field on natural scale parameters see Eqn. (25) (Kanoute et al., 2009; Nguyen et al., 2012). As such, it is important to distinguish both length scales, as the ratio of the length scales $\left(\boldsymbol{R}/\boldsymbol{r}\right)$describes the small parameter (ς)

$$that\ is\ \left(\boldsymbol{R}/\boldsymbol{r}\right) = \varsigma \qquad (25)$$

where: R and r are the position vectors on the macro and microscale respectively (Figure 6).

$$\mathrm{u}\left(\mathrm{R,r} = \frac{\mathrm{R}}{\varsigma}\right) = \mathrm{u}^0(\mathrm{R}) + \varsigma \mathrm{u}^1(\mathrm{R,r}) + \mathrm{O}^2 \qquad (26)$$

Eqn. (26) gives the asymptotic expansion of the displacement field

where:

$U^0(R)$ – Macroscopic displacement field

$U^1(R,r)$ – Periodic first order fluctuations or perturbations due to the microstructure referred to as fast and slow variables respectively.

ς - A small positive number linking the length scales at the macro and micro level

u- Displacement field

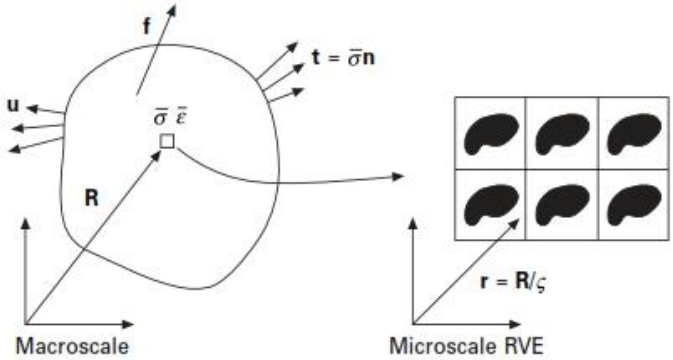

Figure 7: Schematic strategy for the multi-scale simulation based on the finite element method and asymptotic homogenization adapted from LLorca et al. (2007)

This asymptotic expansion is regarded as an approximate solution of the boundary value problem (BVP) especially when ς is reasonably small.

The stress field is given as:

$$\epsilon(\mathrm{R,r}) = \overline{\mathrm{grad}}^{\mathrm{s}}\,\mathrm{u} = \mathrm{Grad}^{\mathrm{s}}\mathrm{u} + \frac{1}{\varsigma}\mathrm{grad}^{\mathrm{s}}\mathrm{u}$$

$$= \mathrm{Grad}^{\mathrm{s}}\mathrm{u}^0 + \mathrm{grad}^{\mathrm{s}}\mathrm{u}^1 + \varsigma\,\mathrm{grad}^{\mathrm{s}}\bar{\mathrm{u}}^1 \qquad (27)$$

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While the asymptotic expansion of the stress field assuming a linear elastic behaviour is given in Eqn. (28) as:

$$\sigma(R,r) = L : \epsilon(R,r) = L : \overline{grad}^{s} u$$

$$= \sigma^{1}(R,r) + \varsigma\sigma^{2}(R,r) + \ldots \qquad (28)$$

The homogenized stiffness tensor $\bar{L}$ according to Llorca et al. (2007) is computed from mean strain value $\overline{\sigma}^{-1}$ as:

$$\overline{\sigma} = \frac{1}{\Omega}\int_{\Omega}\sigma^{1}\,d\Omega = \left[\frac{1}{\Omega}\int_{\Omega} L : \left(I + \frac{\partial\chi(r)}{\partial r}\right)d\Omega\right] : Grad^{s}u^{0} = \bar{L} : Grad^{s}u^{0} \qquad (29)$$

Although, this technique can be used for composites with either a local periodic microstructure (that is microstructure having different morphologies) or global periodicity (that is having repetitive cell units) as shown in Figure 7, it is however, mostly restricted to simple microscopic geometries at very small strains (ς) as well as simple material models (mostly at small strains) where the macroscopic fields are virtually stable at the microscopic length scale.

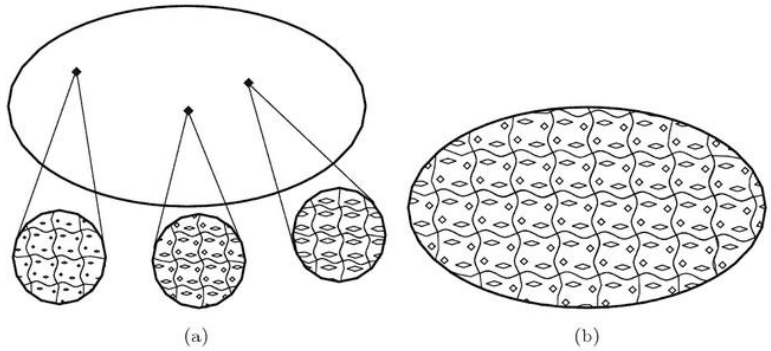

Figure 8: A representation of a microstructure (a) with local periodicity and (b) with global periodicity from Kouznetsova et al. cited in Galvanetto and Aliabadi (2010)

This homogenizational approach offers not only the effective material properties, but also gives information on the local micro fields (LLorca et al., 2007; Kanoute et al., 2009; Kouznetsova et al., 2001).

2.2.3 Mesh Superposition Method

This multiscale technique was introduced by Fish (1992), where he superimposed an additional mesh on the macroscopic (or global) mesh especially in the regions of high stress and strain gradients with the aim of obtaining detailed information on the heterogeneous material microstructure at critical regions (crack tips, interfaces et cetera).The less critical benign regions of the heterogeneous materials, were modelled using coupled finite element method with asymptotic homogenization technique. In summary, numerical homogenization is used in the field having benign deformations while concurrent method is used in the critical regions of high stress and strain gradients where there is a substantial variation in the macroscopic field as shown in Figure 9 (Nguyen et al., 2012).

The grading arrangement of the displacement field (u) in Figure 9 is of a hierarchical nature as the displacement field has been separated into global u^{G} and local u^{L} regions respectively that is

$$\mathbf{u} = u^{G} + u^{L} - displacement\ field \qquad (30)$$

$$\mathbf{u} = u^{G} + u^{L} - displacement\ field \qquad (31)$$

$u^{L} -$ displacement field in the local mesh with respect to the global mesh

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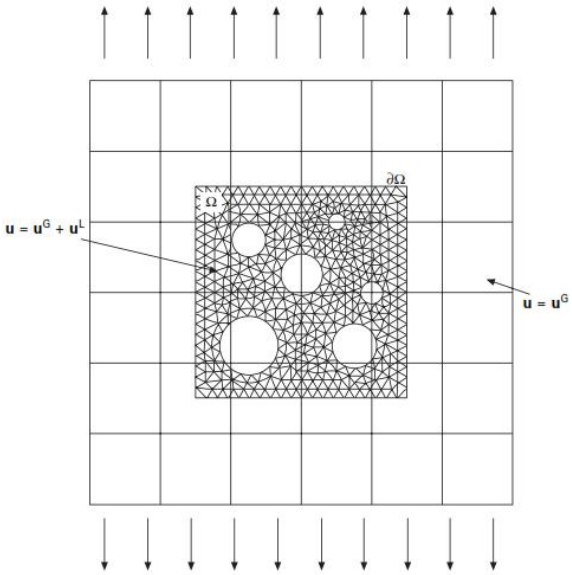

Figure 9: Schematic representation of the mesh superposition method from LLorca et al. (2007).

This hierarchical nature of the displacement field facilitates the modelling of the exact behaviour of the heterogeneous material microstructure in areas of high strain gradient. To ensure homogenous displacement compatibility at the boundary points between the local and global meshes, the local displacement field must equal zero (that is $\mathrm{u}^{\mathrm{L}} = 0 \ \text{at} \ \partial\Omega$) while stiffness matrix ($\mathbf{K}^{\mathrm{GL}}$) that links the displacement degrees of freedom of the global and local meshes are obtained from a system of equilibrium equations as given in Eqn. (32)

$$\begin{bmatrix} \mathrm{K}^{\mathrm{G}} & \mathrm{K}^{\mathrm{GL}} \\ \mathrm{K}^{\mathrm{GL}} & \mathrm{K}^{\mathrm{L}} \end{bmatrix} \begin{pmatrix} \mathrm{u}^{\mathrm{G}} \\ \mathrm{u}^{\mathrm{L}} \end{pmatrix} = \begin{pmatrix} \mathrm{f} \\ 0 \end{pmatrix} \qquad (32)$$

which can be arrived at by deriving the Navier equations from the overall displacement field given in Eqn. (30)

where:

K^{G} and K^{L} – Stiffness matrix obtained from local and global meshes

K^{GL} - Stiffness matrix that combines the displacement d.o.f of the global and local meshes

f - Nodal force vector

2.2.4 Embedded Cell Method

For this technique the model adopted describes the characteristics of the microstructure in detail at critical core regions which are then embedded within a homogenous medium. The finite element mesh of the core region is much finer than the embedding medium hence; it is capable of capturing fast variations in field which ensues as a result of damage. The mesh of the embedding medium is coarse, it is able to relay the macroscopic far field to the core region by implementing displacement continuity which links the core and the embedding region (LLorca et al., 2007; Nguyen et al., 2012). This technique has proven to be quite invaluable in accurately simulating the fracture process in localized regions. The technique as shown in Figure 10 was adopted Gonzalez and LLorca (2006), in simulating fracture behaviour in fibre reinforced composites. They were able to accurately show from the multiscale computational model the main deformation and failure micromechanism.

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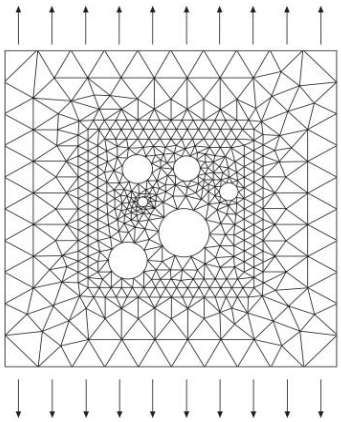

Figure 10: Schematic representation of the embedded cell method from LLorca et al. (2007).

2.3 Modern Multiscale Modelling

As stated earlier the essence of multi-scale modelling is to take advantage of simplicity and efficiency that exists by coupling both microscopic and macroscopic models. It can therefore be stated that the task of multiscale modelling is to devise a coupled macroscopic-microscopic computational method which is not only efficient but also capable of giving the required information with the desired accuracy as opposed to solving the full microscopic model (Weinan and Jianfeng, 2011). While the traditional multiscale solvers as given in Table 1 are general purpose microslovers which give solution of the microscale model (that is it focuses on just on scale), the modern multiscale method also listed in Table 1 gives macroscopic behaviour from data obtained from the microstructure either sequentially or concurrently at a cost much less than the general microsolvers such that:

$$\frac{\text{Cost of multiscale method}}{\text{cost of microscale slover on the full domain}} \ll 1 \qquad (33)$$

Table 1: Classical and modern multiscale technique

Traditional Multiscale Methods	New Multiscale Techniques
Multigrid Method	Car- Parrinello Method
Domain Decomposition Method	Quasi-continuum Method
Wavelet-based Methods	Optimal Prediction
Adaptive Mesh Refinement	Heterogeneous Multiscale Method
Fast Multipole Method	Gap-tooth Scheme
Conjugate Gradient Method	Adaptive Mode Refinement

Adapted from Weinan et al. (2007).

The objective of multiscale modelling, is striking a balance between accuracy and feasibility hence, the focus here will be on the heterogeneous multiscale method (HMM) with a close methodology to the computational homogenization method used in computational mechanics (Matous et al., 2017). The idea behind this technique is to work out the incomplete macroscopic model by obtaining the required data from the microstructural model. There are two major components to the heterogenous multiscale methodology namely:

The overall macroscopic scheme for approximating the macroscopic variable U

$$\mathrm{U} = \mathrm{Qu} \qquad (34)$$

Also known as the compression operator, where:

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U- is the local averages of the microscopic variables (u) over the macro cells

The scheme for evaluating the missing macroscopic data from the microscopic model u

The overall macroscopic scheme for approximating the missing macroscopic data (for example the stiffness matrix, transition rates and so on) from the microscopic model is achieved by solving the micro models locally subject to the following constraint:

$$\tilde{\mathrm{Q}}\mathrm{u} = \mathrm{U} \qquad (35)$$

Where:

$\tilde{Q}$-is an estimate of Q and U in the present state of the macrostructure

The above two processes (1 and 2) as well as the macro state variable U are linked to each other by the compression (U) as well as the reconstruction (R) operators given in Eqns. (36) and (37) in that order; having the property I known as the gradient operator given in equation (38).

$$\mathrm{U} = \mathrm{Qu} \qquad (36)$$
$$\mathrm{RU} = \mathrm{u} \qquad (37)$$
$$I = QR \qquad (38)$$

In summary, The heterogeneous multiscale methodology, essentially entails reconstructing the micro state from U then evolving the micro state using the microscopic model subject to certain constraint ($\tilde{Q}u = U$) to evaluate the missing data from u. This way the coupling between both the macro and micro models is done in such a way that the constraints for setting up the micro models are obtained from the macro models while the micro model in turn, provides the much needed constitutive data for the macro model (Weinan and Jianfeng, 2011;Weinan et al., 2007; Weinan et al., 2003).

2.3.1 Computational Homogenization

The last few decades have seen the development of an alternative multiscale method for micro-macro coupling adopted in the homogenization of complex heterogeneous materials know as the computational homogenizational technique also called global-local analysis or finite element analysis in a more particular form (Kouznetsova et al., 2012). With computational homogenization the details of the macroscale models are computed on-the-fly from the microscale models as simulations are ongoing (Weinan and Jianfeng, 2011). This characteristic nature of the computational homogenizational method makes it suitable in obtaining the effective mechanical behaviour of materials with evolving microstructural geometries, phase transformation as well as nonlinear mechanical problems (large deformations, initiation and propagation of cracks, dislocation mechanics and defects, creep and stress relaxation) (Matous et al., 2017). In this method, materials are generally examined using characteristic volume (that is RVE_s) as shown in Figure 11.

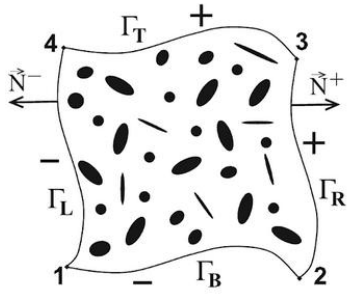

Figure 11: A two dimensional representative volume element from Kouznetsova et al. (2001).

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while the homogenization process relies on the principles of separation of scales where the molecular length scale l_μ is smaller than microscopic length scale of the RVE l_m which in turn is much smaller than the typical size of the macroscopic sample l_M that is $l_\mu < l_m \ll l_M$ as shown in Figure 12 . The information obtained from this length scales are volumetrically averaged in a hierarchical order(that is $l_\mu < l_m \ll l_M$) to obtain the homogenous macroscopic properties such as stiffness tensor, the gradient tensor (F_M) , the stress tensor (P_M) and so on (Kouznetsova et al., 2012); Geers et al., 2010; Matous et al., 2017).

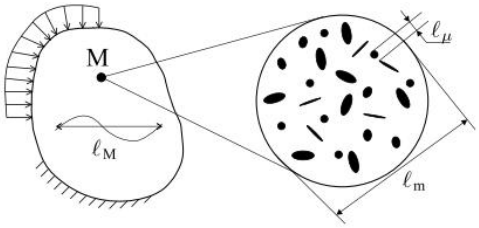

Figure 12: Length scales relevant for the separation of scales principles adapted from Matous et al. (2017).

2.3.2 Basic Theory of Micro-Macro Modelling

In computational homogenization, the macroscopic or effective behaviour of composites is obtained by the following basic procedures listed below and schematically shown in Figure 13.

Firstly, define the RVE and the local constitutive equations to obtain input variables. Next carry out a construction of boundary conditions for the RV E_s from the above input variables as well as the solution of the boundary value problem (BVP) for the (RV E_s) of the composite using numerical techniques. This is also known as down scaling or macro-to-micro transition. The internal fields (output variables) obtained from the solution of the BVP of the RV E_s are then volumetrically averaged (or homogenized) using averaging theorems (i.e. coupling between micro and macro levels) to obtain the regularized or effective material properties used in the macroscopic analysis at component level. This is also known as up scaling or micro-to-macro transition (Kouznetsova et al., 2001; Grytz and Mechke 2007; Nguyen et al., 2012; Petracca et al., 2016).

This regularization process is therefore referred to as "homogenization" (Zohdi and Wriggers 2008). An advantage of this computational homogenization over other homogenizational schemes is that the microscopic constitutive behaviour is defined as the simulations are ongoing thus, making it suitable for predicting the mechanical behaviour of composites with complex microstructure as well as adequately accounting for microstructure evolution under complex loading (Feyel and Chaboche 2000; Kouznetsova et al., 2001; Ozedmir et al., 2008; Weinan and Jianfeng, 2011; Weinan et al., 2007; Nguyen et al., 2012).

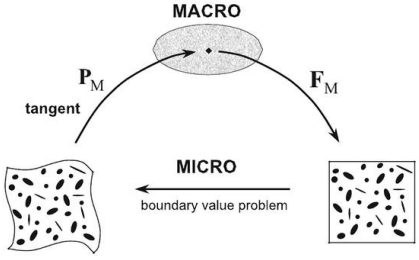

Figure 13: A schematic representation of the computational homogenizational scheme adapted from Kouznetsova et al., cited in Galvanetto and Aliabadi (2010).

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In the computational homogenizational scheme shown, F_M is the gradient tensor for any point on the macro solid which is used to set up the boundary condition imposed on the RVE boundary Γ_m (Figures 11 and 12) with a microscopic domain Ω_m of size l_m. A solution of the BVP for the RVE should give the macroscopic stress tensor P_M which is achieved by the volume averaging of the microstructural stresses over the RVE (Kouznetsova et al., cited in Galvanetto and Aliabadi 2010). Implementing the above process in a finite element frame work gives the finite element method for computational homogenization which has been used in two-dimensional problems. The results from two-dimensional scheme showed the importance of fibre/matrix interface strength on the macroscopic behaviour (damage and failure phases) of the composite materials (Feyel 1999; Kouznetsova et al., 2001). This scheme has been further extended to treat three dimensional problems by facilitating large deformations and rotations making it appropriate for dynamic problems on a finer scale. It can also be used on homogenous materials (on a finer-scale) with various shapes of RVE (Wiechert and Wall 2010).

2.3.3 Averaging theorems

Based on the principles of separation of scales, the RVE is much smaller than the characteristic macroscopic sample that is $l_m \ll l_M$ therefore; the internal body forces at the macroscale are generally overlooked so that the static equilibrium state of the RVE is mathematically expressed as:

$$\nabla_m . \sigma_m = 0 \text{ in } \Omega_m \qquad (39)$$

(Kouznetsova et al., cited in Galvanetto and Aliabadi 2010)

where:

∇_m – Gradient operator

σ_m – Microscopic stresses

2.3.3.1 Deformation averaging theorem

As the actual coupling of the micro-macro kinematic quantities are based on averaging theorems (Kouznetsova et al., cited in Galvanetto and Aliabadi 2010), the deformation gradient tensor F_M at any point on the macroscopic solid (Figure 13) is given by volume averages of the microstructural deformation gradient tensor.

$$F_M = \frac{1}{V_o} \int_{V_o} F_m \, dV_o = \frac{1}{V_o} \int_{\Gamma_o} x \, N \, d\Gamma_o \qquad (40)$$

The above expression for F_M was obtained after transforming the integral of the un-deformed volume of the RVE to a surface integral using the divergent theorem (Kouznetsova et al., cited in Galvanetto and Aliabadi 2010).

where:

F_M- Macroscopic deformation gradient tensor

F_m - Microscopic deformation gradient tensor

V_o– Reference domain

$\forall$ for every δ_x in the domain

X – Un-deformed position

x - Deformed position (Kouznetsova et al., cited in Galvanetto and Aliabadi 2010).

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2.3.3.2 Energy averaging theorem

Generally referred to as the Hill-Mandel macro-homogeneity principle, ascertains that the macroscopic volume averages on the RVE (given by the expression in Eqn. (41) which is expressed in terms of work conjugate set as given in Eqn. (41) can also be stated in terms of RVE surface quantities given in Eqn. (42).

$$\frac{1}{V_o}\int_{V_o} \boldsymbol{P}_m : \delta \boldsymbol{F}_m{}^{C}\, dV_o = \boldsymbol{P}_m : \delta \boldsymbol{F}_m{}^{C} \quad \forall\, \delta_{\mathbf{x}} \qquad (41)$$

$$\delta W_{OM} = \frac{1}{V_o}\int_{V_o} P_m : \delta F_m{}^{C}\, dV_o = \frac{1}{V_o}\int_{\Gamma_o} P.\,\delta_x d\Gamma_o \qquad (42)$$

where: P_m is the first Piola – Kirchhoff stress tensor

(Grytz and Mechke 2007; Kouznetsova et al., cited in Galvanetto and Aliabadi 2010).

2.3.4 Representative Volume Elements (RVE$_s$)

The RVE is the smallest material volume statistically representative of the microstructure of the heterogeneous material or the smallest volume of the heterogeneous material that exactly replicates the macroscopic behaviour (Drugan and Willis 1996; LLorca et al., 2007; Kouznetsova et al., cited in Galvanetto and Aliabadi 2010). Accurate simulations in continuum micromechanics rely on simulating the behaviour of the RVE of the heterogeneous material. With traditional computational homogenizational models, different RV E_s have been used at various points on the microstructure to ensure accuracy (LLorca et al., 2007).

Based on the model introduced by Grytz and Meschike (2007) shown in Figure 14 it is possible to use the same RVE at all points on the microstructure.

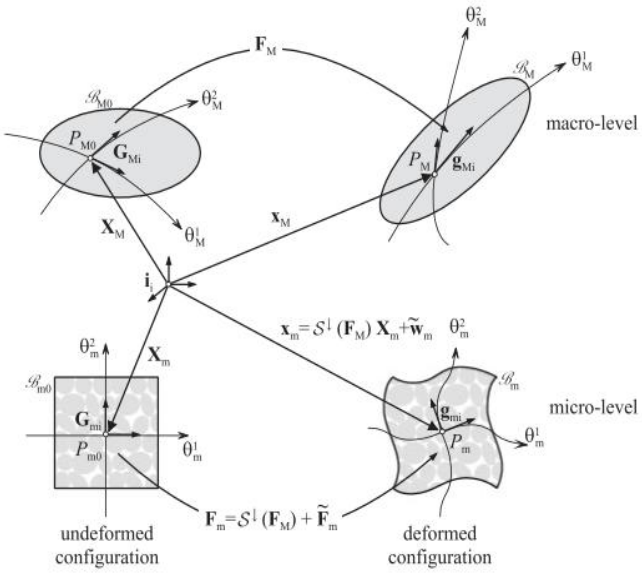

Figure 14 Schematic representation of the micro-macro computational homogenization of finite deformation in curvilinear coordinates adapted from Grytz and Mechke (2007).

Similarly, the computational schemes addressed so far are applicable in the standard Cartesian coordinates (that is one physical space), but with this development, the scheme can be applied to address problems formulated in curvilinear coordinates in the three-dimensional Euclidean space both at the macro and micro levels. Grytz and Mechke 2007, employed this technique in the multiscale analysis of a spherical shell subjected to internal pressure shown in figure 15 where the homogenization of the 3D microstructure was carried out numerically at the macro level. Similarly, only two RVEs were considered all through the shell thickness.

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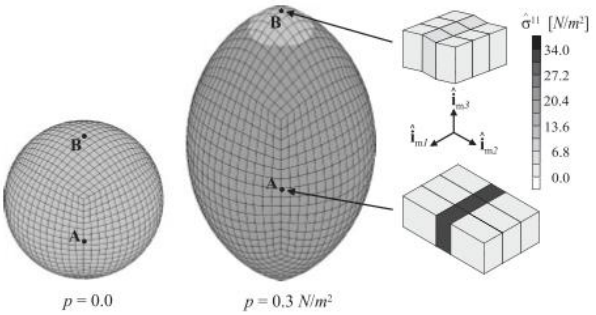

Figure 15: Spherical shell subjected to internal pressure-undeformed and deformed configurations of the macro-structure and the underlying micro-structure with the distribution of the Cauchy stresses $\tilde{\boldsymbol{\sigma}}^{11}$ adapted from Grytz and Mechke (2007).

From their study, they came to the conclusion that simplification of recommended computational scheme for problems formulated in curvilinear coordinates (such as the use of the same RVE and so on), greatly simplified the solution of the multiscale problem when assessed against the traditional approaches using only a single physical space for both micro and macro scales thus demonstrating the efficiency of the proposed scheme over the traditional schemes particularly for problems in 3D Euclidean space.

From this study, the efficient application of computational homogenization in different physical space at different scales was demonstrated (Grytz and Mechke 2007).

3. Conclusion

From the review of the existing mathematical, numerical and computational homogenizational scheme for composite materials, it has been shown that:

Prior to the development of digital computers as well as the corresponding development in simulation tools (that is the fast fourier transform, the boundary element method and more recently the finite element method) as a means of analysing multi-scale models, the Analytical/mathematical homogenization technique was considered the main workhorse to simulate the macroscopic mechanical behaviour of multi-phase heterogeneous material from the behaviour of the representative volume element (RVE) of the microstructure of the material. The straight forwardness of the fundamental assumptions of the technique made it quite popular. Despite its popularity (in computing internal stress in multiphase materials during deformation) the inability of the method to capture rapid localization of damage has limited the application of the method in computing mechanical behaviour of material where progressive damage is involved. Although, the method describes quite accurately the effective macroscopic properties of the heterogeneous material in the elastic system it is not as effective in the nonlinear regime which has been the major drawback for this technique.

With the current technological developments in simulating technologies the above limitation of the mathematical homogenization schemes in simulating the effective non linear heterogeneous material behaviour were addressed by adopting computational homogenizational schemes which rely on established constitutive relations for the macroscopic problems in a numerical form through which the macroscopic problems are constructed and solved in a nested manner.

It can therefore be seen that:

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The homogenization schemes in general, have proven to be an invaluable tool for obtaining heterogeneous macroscopic material properties from the mechanical properties of the material microstructure.

The accuracy of the analytical schemes is limited to elastic systems which are mostly applicable for accurately modelling microstructures with simple geometrical features. A limitation which has largely been attributed to the simplifications adopted in the analytical homogenisation models preventing it from capturing rapid localization of strains, nucleation, growth of damage as well as complex loading paths which causes phase transformation .

Computational homogenization on the other hand,

Has been able to give accurate predictions of the macroscopic material behaviour in non-linear systems.

It allows the pragmatic assumption of local periodicity in the material microstructure which further improves on the accuracy of the results obtained.

The major drawback of this technique is that the completely coupled micro-macro technique is quite expensive to simulate computationally.

This has however been compensated for by adopting numerical strategies where the benign fields are modelled using coupled homogenization and finite elements and then carrying out detailed micro-macro analysis in the core regions (crack tips, interfaces) where it is essential to obtain a detailed information of the stress and strain fields at the core regions since it is the information from these regions that govern failure mechanisms.

4. Future trends

A major hindrance of the computational homogenizational scheme is in the development of a fully coupled micro-macro technique. A development of a fully coupled scheme is highly needed in order to be able to validate computational homogenizational multiscale models against experimental results without have any discrepancies at relatively low cost.

Furthermore, the application of this computational homogenizational scheme in designing as well as enhancing existing engineering materials by manipulating the microstructure is still lacking and needs more study. A significant improvement in this area will be highly invaluable in applications of engineering material for particular industrial applications. For example, the designing of novel lightweight materials such as: magnesium alloys, aluminium alloys, amorphous polymers etcetera which are energy efficient and aid in facilitating the reduction of greenhouse gas emissions from buildings, transportation and industrial sector.

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