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Computational homogenization of cellular materials capturing micro–buckling, macro–localization and size effects

Thèse présentée par

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Preface

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Van Dung Nguyen

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Abstract

The objective of this thesis is to develop an efficient multi–scale finite element framework to capture the macroscopic localization due to the micro–buckling of cell walls and the size effect phenomena arising in structures made of cellular materials.

Under the compression loading, the buckling phenomenon (so–called micro–buckling) of the slender components (cell walls, cell faces) of cellular solids can occur. Even if the tangent operator of the material of which the micro–structure is made, is still elliptic, the presence of the micro–buckling can lead to the loss of ellipticity of the resulting homogenized tangent operator. In that case, localization bands are formed and propagate in the macroscopic structure. Moreover, when considering a cellular structure whose dimensions are close to the cell size, the size effect phenomenon cannot be neglected since deformations are characterized by a strain gradient.

On the one hand, a classical multi–scale computational homogenization scheme (so–called first–order scheme) looses accuracy with the apparition of the macroscopic localization or the high strain gradient arising in cellular materials because the underlying assumption of the local action principle, in which the stress state on a macroscopic material point depends only on the strain state at that point, is no–longer suitable. On the other hand, the second–order multi–scale computational homogenization scheme proposed by Kouznetsova et al. (2004b) exhibits a good ability to capture such phenomena. Thus this second–order scheme is improved in this thesis with the following novelties so that it can be used for cellular materials.

First, at the microscopic scale, the periodic boundary condition is used because of its efficiency. As the meshes generated from cellular materials exhibit a large void part on the boundaries and are not conforming in general, the classical enforcement based on the matching nodes cannot be applied. A new method based on the polynomial interpolation without the requirement of the matching mesh condition on opposite boundaries of the representative volume element (RVE) is developed.

Next, in order to solve the underlying macroscopic Mindlin strain gradient continuum of this second–order scheme by the displacement–based finite element framework, the presence of high order terms (related to the higher stress and strain) leads to many complications in the numerical treatment. Indeed, the resolution requires the continuities not only of the displacement field but also of its first derivatives. This work uses the discontinuous Galerkin (DG) method to weakly impose these continuities. This proposed second–order DG–based FE^2 scheme appears to be easily integrated into conventional parallel finite element codes.

Finally, the proposed second–order DG–based FE^2 scheme is used to model cellular materials. As the instability phenomena are considered at both scales, the path following technique is adopted to solve both the macroscopic and microscopic problems. The micro–buckling leading to the macroscopic localization and the size effect phenomena can be captured within the proposed framework.

Keywords: *Cellular materials; Computational homogenization; Micro–buckling; Size effect; Finite element; Second order; Periodic boundary condition; Polynomial interpolation; Discontinuous Galerkin; Path following*

Contents

Chapter 1

Motivation

In recent years, there has been a growing interest in artificially micro–structured materials. The behavior of these complex materials not only depends on the materials of which their micro–structure is made, but also on the spatial distribution of their microscopic constituents. For instance, cellular materials can exhibit exceptional properties resulting from their micro–structure arrangement. These materials are used in many engineering applications including aerospace, packaging, shock absorption, *etc*, as discussed by Gibson and Ashby (1997), Banhart (2001), Scheffler and Colombo (2006), Mills (2007), Lefebvre et al. (2008).

Cellular materials exhibit complex deformation mechanisms, as summarized by Gibson and Ashby (1997), Gibson (2000, 2005) for examples. The cellular structures consist of slender members as cell struts and cell faces, which may buckle under compression loading, a phenomenon known as micro–buckling. The micro–buckling of cell walls is the most important deformation mechanism under compression loading. This phenomenon can initiate at the weaker cells and propagate throughout the whole macroscopic structure inside localization bands. The apparition of localization bands due to the micro–buckling of cell walls was observed in experiments by Papka and Kyriakides (1998a,b, 1999a), Chung and Waas (2002), Wilbert et al. (2011), Khan et al. (2012) for honeycombs and by Bart-Smith et al. (1998), Bastawros et al. (2000), Zhou et al. (2004), Dillard et al. (2005), Zhou et al. (2005), Jeon and Asahina (2005), Jang and Kyriakides (2009) for foams. Another important phenomenon in cellular materials is the size effect, which was observed as the dependence of the mechanical behavior on the ratio of specimen and cell sizes. Experiments about the size effect existing in cellular solids were reported by Andrews et al. (2001), Chen and Fleck (2002), Tekoglu et al.

(2011). The size effect can arise from a change in the constraint of the cell walls at the boundary of a specimen as well as from stress–free cut cell edges at the surface of a specimen as noted by Onck et al. (2001).
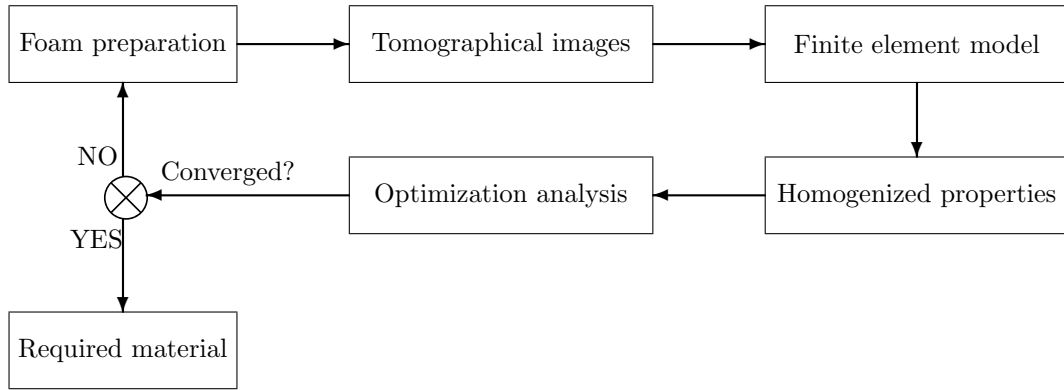

Figure 1.1: "Material tailoring" in order to obtain the required (such as mechanical, electromagnetic, acoustic, etc) material properties for synthesized foams.

Recently, a strong growth in the use of advanced materials in engineering applications motivates "material tailoring", in which the required material properties can be achieved by manipulating the micro–structure, as discussed by Le et al. (2012) for example. Fig. 1.1 depicts a material design procedure based on an optimization analysis for synthesized materials. A high quality finite element model is created from the tomographical images of their micro–structure. The homogenized behavior is then estimated from this finite element model by an appropriate method. After an optimization analysis, the required properties are reached or a correction step is followed. For such a tailoring, in a linear range, it is necessary to provide an efficient method to estimate the homogenized properties from a model of the micro–structure of these materials. When considering non–linear materials and instability (e.g. localization, buckling) phenomena, the homogenized properties are not enough since the structure deformation is not homogeneous at the structural scale, e.g localization bands due to the micro–buckling propagate in the structure made of cellular materials. Therefore, the full structure has to be considered.

The present work is carried out in the context of the "ARC N°09/14−02 BRIDGING" project. In this project, we are interested in studying foamed materials produced by the Chemistry Department. In particular, we are interested in extracting the mechanical properties including micro–buckling to predict their mechanical behavior. These materials are used to shield electromagnetic waves and their electromagnetic properties

depend on their micro–structure. As their micro–structure shape is deformed under mechanical loading, their electromagnetic properties can be modified motivating the study of their deformation. The purpose of this thesis is to model the mechanical properties of structures made of cellular materials in an efficient computational way.

Chapter 2

Finite element modeling of structures made of cellular materials: state of the art

Nowadays, the finite element method is widely used to predict both the elastic and inelastic as well as both the static and dynamic responses of many structures, see the references by Zienkiewicz and Taylor (1977), Crisfield et al. (2012). Because of its ability to model complex structures with complex constitutive behaviors, the finite element method has been widely applied to study the behavior of cellular materials.
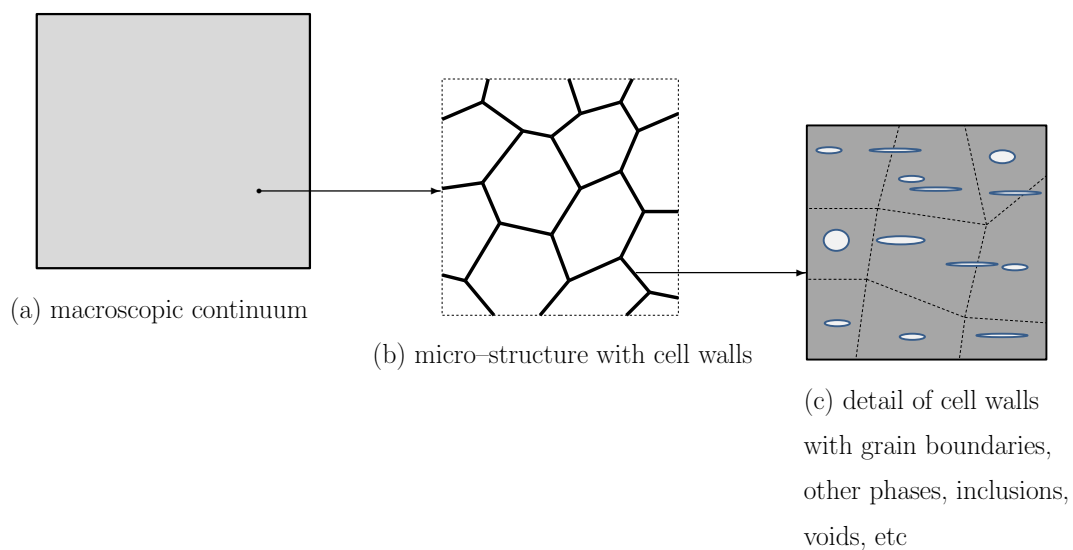

(a) macroscopic continuum

(b) micro–structure with cell walls

(c) detail of cell walls with grain boundaries, other phases, inclusions, voids, etc

Figure 2.1: Multiple scales involved in cellular materials.

In the modeling of structures made of complex micro–structured materials, e.g. cellular materials, the intrinsic mechanical role of the underlying micro–structure in the structural behavior has been widely recognized. Fig. 2.1 shows the multiple scales involved in cellular materials. At the structural scale (so–called macroscopic scale), when the dimensions of a structure are much larger than the cell size, this structure is viewed as a homogeneous medium. The microscopic scale is described by cell walls, cell distribution, cell shape, cell size and thickness of cell walls, *etc.* The cell walls are made of a base–material with the presence of grain boundaries, other phases, inclusions and voids, *etc.* When considering the behavior of structures made of cellular materials, this multi–scale nature must be considered.
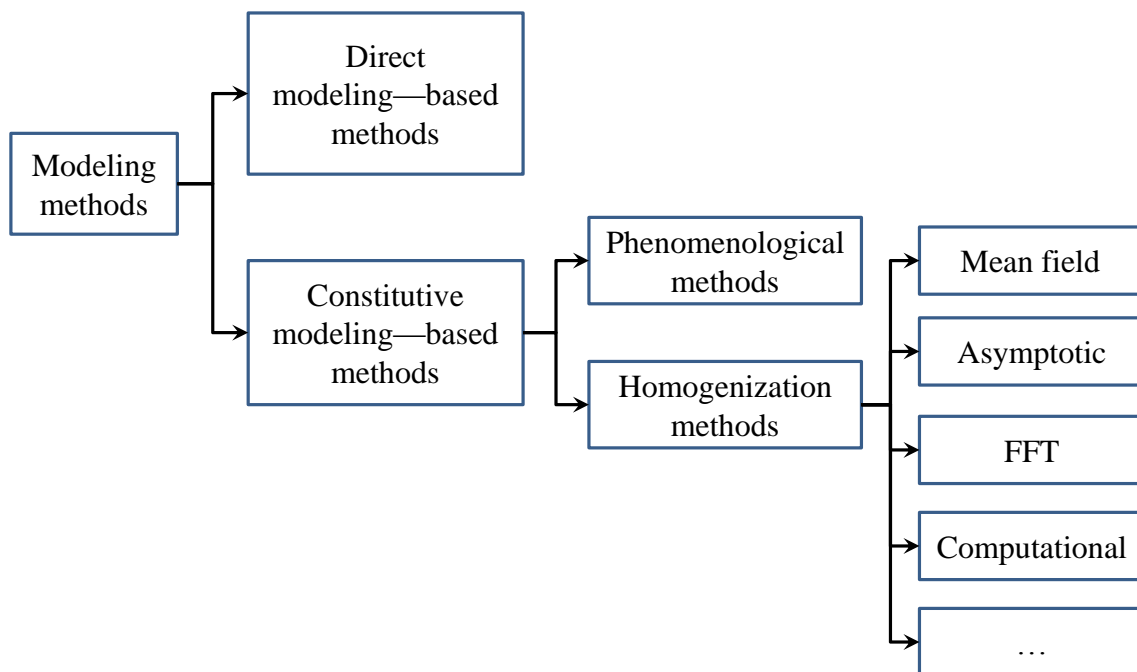
Figure 2.2: Modeling strategy of cellular materials.

From the computational point–of–view, there are basically two approaches used to study the behavior of a structure made of cellular materials: the direct and constitutive modeling–based methods as summarized in Fig. 2.2. A brief review of these methods is given in what follows.

2.1   Direct modeling

In the direct modeling approach, all the discrete cell walls of cellular solids are discretized by standard finite elements, such as beam, shell or bulk ones. Beam elements are a natural choice for cell struts of open–cell foams and cell walls of in–plane arrays of honeycombs in which two dimensional problems are generally adapted. Shell elements are a natural choice for cell faces of closed–cell foams. In general, bulk elements can be used but this leads to an enormous number of unknowns, thus beam and shell elements are usually preferred. With the direct modeling, the whole structure is discretized at once and the mechanical behavior of the cell walls is described by constitutive laws that specify the stress–strain relationship.

As examples, when considering the in–plane behavior of honeycombs, beam elements were used by Papka and Kyriakides (1998a, 1999b) to study the in–plane compression behavior of hexagonal honeycombs, by Mangipudi and Onck (2011) to consider the damage of cell walls of Voronoï honeycombs and by Onck et al. (2001), Chen and Fleck (2002), Tekoglu and Onck (2005, 2008), Tekoglu et al. (2011) to capture the size effect phenomenon. Beam elements were also used to model the crushing of random open–cell foams by Gaitanaros et al. (2012). Li et al. (2014) used shell elements to study the crushing response of three–dimensional random closed–cell foams.

The intrinsic deformation localization and size effect phenomena are directly captured since the deformation state of the cell walls is directly computed. However, the use of direct models to study the behavior of a large structure leads to an enormous number of unknowns. The resolution of the resulting system of equations is still a challenge for modern computers even using parallel computing. Moreover, it is impossible to construct finite element models for large problems with details of cell walls because of the geometrical complexity. Therefore, this approach is strictly limited and suitable for problems with limited sizes.

2.2   Constitutive modeling

While studying the behavior of structures made of cellular materials, when the structure dimensions are much larger than the cell size, the direct modeling–based approach becomes impossible motivating the use of the constitutive modeling–based approach. In this approach, a cellular solid is modeled by a homogeneous medium. The behavior at smaller scales is then taken into account by a suitable material model. This constitutive

law can be modeled by either phenomenological or homogenization methods.

2.2.1   Phenomenological methods

A constitutive law is *a priori* defined and its parameters are identified by curve fitting from numerical tests or experimental results. Some phenomenological models were proposed by Deshpande and Fleck (2000), Miller (2000), Hanssen et al. (2002), Reyes et al. (2003), Forest et al. (2005), Yang et al. (2008). The localization phenomenon can be integrated in the constitutive modeling as proposed by Forest et al. (2005). To deal with the size effect phenomenon, Tekoglu and Onck (2005) used a Cosserat continuum and its parameters were identified from direct modeling results. Dillard et al. (2006) worked with a micro–morphic continuum and its parameters were identified from experiments. Finally, Gibson and Ashby (1997) constructed a micro–mechanical model based on the unit cell of cellular structures.

This approach is more efficient than the direct modeling–based one when considering a large problem because the element size at the macroscopic scale can be much larger than the cell size. However, this approach is still limited by the fact that the details of the micro–structure evolution cannot be observed during the macroscopic loading and by the fact that the material model and its parameters are difficult to be identified.

2.2.2   Homogenization methods

Homogenization methods are applied to determine the apparent or overall properties of heterogeneous materials. Kanoute et al. (2009) gave a survey about homogenization methods for composite materials. The use of homogenization constitutive laws leads to the multi–scale modeling of heterogeneous structures. Fig. 2.3 represents the basic strategy of a general multi–scale approach. At the macroscopic scale, the structure
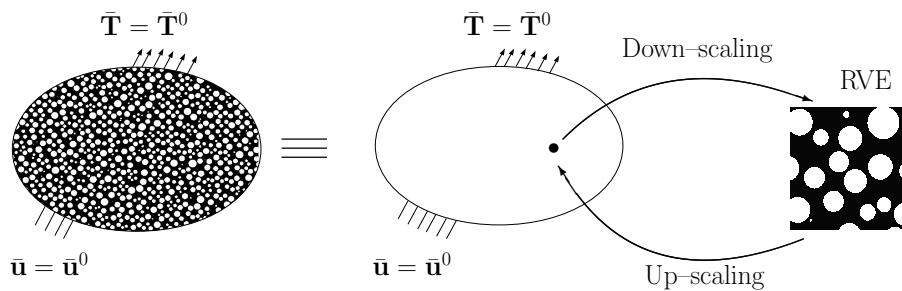

Figure 2.3: Multi–scale homogenization approach for heterogeneous materials.

is considered as a homogeneous medium with prescribed displacement and traction boundary conditions. In order to account for the heterogeneities of the micro–structure, each macroscopic material point is associated with a separate characteristic volume element extracted from the micro–structure at that point. In general for both periodic and random structures, this corresponds to the representative volume element (RVE)[1], see e.g. Kanit et al. (2003). For periodic structures, this characteristic volume can be chosen as the repeated unit cell. Each microscopic boundary value problem (BVP) is then formulated at each macroscopic material point and the stress–strain constitutive relationship at that point is estimated from the resolution of its underlying microscopic BVP. The transition between the different scales is guaranteed by the down–scaling and up–scaling procedures as follows.

- Down–scaling (so–called macro–micro transition): The measures of macroscopic strains (*e.g.* deformation gradient) are computed at each macroscopic point (integration point in the context of the finite element analysis) and used to formulate the microscopic boundary condition of the associated microscopic BVP.

- Up–scaling (so–called micro–macro transition): For given measures of macroscopic strains, the associated microscopic BVP is solved and the macroscopic stress measures (*e.g.* first Piola–Kirchhoff stress) are then computed from its resolution.

This macro–micro separation strategy relies on the principle of separation of scales. Following Zaoui (2002), when considering heterogeneous structures, this principle is formulated as

$$L \gg l_m \gg l_\mu \gg d_0 \text{ and } l_M \gg l_m \,, \tag{2.1}$$

implying that all scales are separated. In Eq. (2.1), L is the size of the macroscopic structure, l_M is the fluctuation length scale of the prescribed mechanical loading, l_m is the RVE size, l_μ is the characteristic length scale of the underlying microscopic heterogeneities and d_0 is lower length bound below which the continuum mechanics is no more valid. In the case of structures made of cellular materials, the condition $l_m \gg l_\mu \gg d_0$ implies that each cell wall is viewed as a homogeneous one. In this case, the continuum mechanics remains valid at the microscopic BVPs. The mechanical behavior of

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[1]A simple definition of RVE following Drugan and Willis (1996): *"It is the smallest material volume element of the composite for which the usual spatially constant (overall modulus) macroscopic constitutive representation is a sufficiently accurate model to represent mean constitutive response"*.

cell walls is usually modeled by certain constitutive laws that specify the stress–strain relationship. The conditions $l_M \gg l_m$ and $L \gg l_m$ lead to consider the macroscopic problem according to the local action principle, in which each macroscopic material point is viewed as the center of its underlying RVE and in which the response of the associated microscopic BVP is homogeneous at the macroscopic point–of–view. Thus two–scale problems can be formulated in terms of classical Cauchy continua.

However, the buckling of cell walls leads to the occurrence of deformation localization bands and the macroscopic length scale l_M tends to become smaller. The condition $l_M \gg l_m$ is no longer fully satisfied. In this case, another enhanced multi–scale scheme must be considered as mentioned by Geers et al. (2010) and as it will be discussed later.

Depending on the method applied to solve the microscopic BVPs, different homogenization methods are available in the literature, *e.g.* mean field, asymptotic, fast Fourier transform, computational, *etc.* In the following, these homogenization methods are briefly recalled.

Mean field homogenization (MFH)

The MFH approach is an efficient (semi–)analytic framework for the modeling of multi–phase materials. Most of MFH methods are based on the extension from the single inclusion results established by Eshelby (1957) to multiple inclusions interacting in an average way. Most common extensions of the Eshelby (1957) solution are the Mori–Tanaka scheme proposed by Mori and Tanaka (1973), Benveniste (1987) and the self–consistent scheme pioneered by Kröner (1958), Hill (1965) for elastic multi–phase materials. The MFH methods were also developed for non–linear behaviors of heterogeneous materials to account for the non–linearity of the constituents such as elastic, visco–elastic, elasto–plastic and elasto–visco–plastic behaviors, as summarized by Pierard (2006) and for damage by Wu et al. (2013a).

The MFH methods are developed for composite materials but they can be extended to porous solids by considering one of their constituents as voids without stiffness. Thus the effective properties depend on the properties of the material of which the solid part is made and on the fraction of the void part. The use of the MFH methods to estimate the elastic properties of cellular solids was studied by Chao et al. (1999), Schjodt-Thomsen and Pyrz (2001), Gong et al. (2011), Miled et al. (2011), Koudelka et al. (2012), Bardella et al. (2012), El Ghezal and Doghri (2013). In the elasto–plastic regime, Kitazono et al. (2003) used this approach to estimate the elastic properties and the yield stress of

closed–cell metal foams but the micro–buckling and size effect phenomena were not dealt with.

The MFH methods are very efficient to estimate the homogenized properties of heterogeneous materials from the computational point–of–view. However, by using semi–analytic formulations, the fluctuations at the micro–structures during the macroscopic loading cannot be accurately observed.

Asymptotic homogenization (AH)

The asymptotic homogenization (AH) approach is an effective tool to model heterogeneous problems with periodic micro–structures. A survey about asymptotic homogenization was given by Kalamkarov et al. (2009). One important assumption of this approach is to distinguish two separate length scales associated to the microscopic and macroscopic problems denoted by l_m and l_M respectively. The scale ratio ε is defined by

$$\varepsilon = \frac{l_m}{l_M} \, . \tag{2.2}$$

In a small neighborhood of each macroscopic point $\bar{\mathbf{x}}$, all physical fields are assumed to depend on both the local coordinates $\bar{\mathbf{x}}$ and microscopic stretched coordinates $\mathbf{x} = \bar{\mathbf{x}}/\varepsilon$. Each physical field, *e.g.* displacement and stress, is expanded into a power series of ε. The equilibrium equation is rewritten for different orders of ε leading to different partial differential equations with periodic boundary conditions. These equations can be numerically solved by the finite element method. The AH approach was mostly applied for linear elastic composite materials, but it can be extended to inelastic behaviors such as elasto–plasticity as achieved by Fish et al. (1997), or such as failure as proposed by Muravleva (2007).

The AH methods are restricted to simple periodic micro–structure geometries and simple material models, mostly at small strains. However, these methods were applied for elastic cellular solids by *e.g.* Fang et al. (2005) and for elasto–plastic ones by *e.g.* Khanoki and Pasini (2013) but the micro–buckling was not computed. Accounting for the non–linear behavior and randomness of cellular materials is still a challenge with this approach.

FFT–based homogenization

The fast Fourier transform (FFT) approach pioneered by Moulinec and Suquet (1994, 1995) is mesh–less and can be used to solve the microscopic BVP with the direct use of digital images of the micro–structure. In order to close the microscopic BVP, the periodic boundary condition is applied. At each Fourier point, which corresponds to a pixel in the case of 2–dimensional images or a voxel in the case of 3–dimensional ones, given mechanical material properties are assigned. The microscopic BVP is then rewritten as an implicit integral equation (so–called Lippmann–Schwinger equation), in which an associated Green operator is introduced. This non–linear equation is iteratively solved in the Fourier space by applying a Fourier transformation. Since the discrete problem of Fourier points is considered, the fast Fourier transform (FFT) is used. The unknown fields (*e.g* displacement and strain) are then obtained at each Fourier point. The basic scheme proposed by Moulinec and Suquet (1994, 1995) for linear elastic behaviors was extended to the non–linear case by Moulinec and Suquet (1998), Idiart et al. (2009), Lebensohn et al. (2012) for examples.

This approach uses digital images instead of detailed meshes of the micro–structure and thus it can be directly coupled with 3–dimensional imaging techniques (*e.g.* tomography). However, the basic scheme proposed by Moulinec and Suquet (1994, 1995) cannot handle problems with the presence of rigid inclusions and voids (like porous solids). Several alternative schemes have been proposed to deal with these problems by Michel et al. (2001), Brisard and Dormieux (2010) for examples, but they are limited to the case of cellular materials with high porosity. However, in the context of cellular materials, this approach can be used to determine the homogenized properties of cell walls as proposed by Němeček et al. (2013).

Computational homogenization (FE^2)

The computational homogenization approach extracts the equivalent properties from the resolution of a finite element analysis on a complex square or cubic representative volume element (RVE), which contains one or several cellular cells of different sizes and shapes. As it models the details of the micro–structure by a finite element analysis, the computational homogenization approach has potentially the ability to capture the micro–buckling of cell walls and the size effect phenomena. As compared with other homogenization methods, the computational homogenization approach is probably the most accurate technique for micro–structured materials with strong non–linear behaviors

and allows assessing the macroscopic influence of the micro–structural parameters with high accuracy. In this thesis, we will investigate the possibility of using this approach to study cellular materials.

Recent reviews about the multi–scale computational homogenization approach were given by Geers et al. (2010), Nguyen et al. (2011). Not only mechanical problems but also thermal problems (Özdemir et al., 2008b), electromagnetic problems (Niyonzima et al., 2012) or multi–physical problems like thermo–mechanical problems (Özdemir et al., 2008a), electro–mechanical problems (Schröder and Keip, 2010) have been addressed with this approach.

As said, while considering computational homogenization methods, each microscopic BVP provides the stress–strain relation at a macroscopic point via the resolution of a finite element problem. Each microscopic BVP is associated with an appropriate boundary condition, *e.g.* periodic boundary condition, related to the macroscopic quantities, *e.g.* macroscopic strains. The micro–structure constituents are modeled with an arbitrary non–linear geometrical framework and with an arbitrary non–linear constitutive laws.

Depending on the scale transition between macroscopic and microscopic BVPs, different computational homogenization schemes were proposed. A comprehensive numerical treatment of a multi–scale computational homogenization procedure in the finite strain framework was given in Kouznetsova (2002). Classical FE^2 (so–called first–order) schemes consider the classical Cauchy continuum at both the macroscopic and microscopic scales. This method is valid when the microscopic and macroscopic length scales are fully separated, as in the works of Miehe and Koch (2002), Kouznetsova (2002) for examples. When the microscopic and macroscopic length scales become comparable (with the presence of localization and failure, *etc*), several enhanced schemes were proposed.

- Second–order FE^2 enhanced schemes: A homogenized generalized continuum is considered at the macroscopic scale. The underlying constitutive law is determined from the resolution of either a microscopic classical Cauchy continuum or a microscopic generalized one. We can refer to the second–order scheme with macroscopic Mindlin strain gradient continuum with the work of Kouznetsova et al. (2004b) and the second–order scheme with macroscopic Cosserat continuum with the works of Onck (2002), Feyel (2003) in which the underlying Cosserat constitutive law is estimated from the resolution of a microscopic classical Cauchy

continuum, as in the work of Feyel (2003) or of a microscopic Cosserat one, as in the work of Onck (2002).

- Continuous–discontinuous FE^2 schemes: The transition from micro–discontinuities to macro–discontinuities was considered by Massart et al. (2007), Belytschko et al. (2008), Souza and Allen (2010), Nguyen et al. (2011) and Coenen et al. (2012).

The FE^2 approach is widely used to estimate the equivalent properties of cellular materials by using the finite element method as reported by Daxner (2010). Sehlhorst et al. (2009) worked with classical FE^2 for in–plane finite strain behaviors of perturbed hexagonal honeycomb. However, the the size effect phenomenon was not considered in this work. Ebinger et al. (2005) used the second–order FE^2 to capture the size effect phenomenon of structures made of elastic honeycombs. The microscopic buckling of cell walls was considered at the microscopic scale with the periodic boundary condition for a specific macroscopic loading (axial, uniaxial, *etc*) for elastic problems by Okumura et al. (2002), Ohno et al. (2002), Jouneid and Sab (2009) for examples and for elasto–plastic problems by Okumura et al. (2004), Takahashi et al. (2010) for examples. The microscopic buckling leading to the macroscopic loss of ellipticity was observed for a given prescribed macroscopic strain by Okumura et al. (2004), Takahashi et al. (2010) for examples. However, the multi–scale study of the interaction between macroscopic instabilities and the microscopic buckling for structures made of cellular materials was not dealt with in these studies.

Other methods

Besides the presented homogenization methods for cellular materials, several other methods were proposed, such as the discrete homogenization method proposed by Reis and Ganghoffer (2012) or such as the numerical homogenization based on the finite cell method with the work of Düster et al. (2012). These works are still limited to the linear elastic regime.

Chapter 3

Contributions

The computational homogenization approach is probably the most accurate technique for micro–structured materials with highly non–linear behaviors and allows assessing the macroscopic influence of the micro–structural parameters in multiple scales. Among all the multi–scale computational homogenization schemes, the second–order FE^2 scheme proposed by Kouznetsova et al. (2004b) exhibits a good capability to capture both the localization and size effect phenomena related to heterogeneous materials. This second–order FE^2 scheme is thus adopted in this thesis to study the behavior of cellular materials. However, this method has never been, to our knowledge, used to predict the localization on structures made of such materials. To this end, we introduce the following three originalities:

- Periodic boundary condition (PBC) enforcement using a polynomial interpolation method: When considering the first–order FE^2 scheme, many numerical studies, as considered by Kanit et al. (2003), Terada et al. (2000), Larsson et al. (2011) for examples, show that the PBC is the most efficient in terms of convergence rate when the size of representative volume element increases. Although rigorous for periodic structures, this conclusion also holds true if the micro-structure does not possess the geometrical periodicity as shown by Kanit et al. (2003), Terada et al. (2000), Larsson et al. (2011). Because of its efficiency, this work takes an interest in applying the PBC in multi–scale problems for arbitrary meshes. Recently, the finite element model of real cellular materials were obtained from micro–tomography, by Youssef et al. (2005), Veyhl et al. (2011), Fiedler et al. (2012) for examples. In these applications, the meshes generated from real materials are non–conforming and therefore, the PBC cannot be enforced by the matching node technique moti-

vating the development of a suitable method for non–conforming meshes based on the polynomial interpolation, see Nguyen et al. (2012). The details of this method are described in chapter 4. In order to apply the PBC within the second–order FE^2 scheme, the polynomial interpolation method is also extended to the second–order FE^2 scheme.

- Second–order discontinuous Galerkin (DG)–based FE^2 scheme: The resolution of the Mindlin (1964, 1965) strain gradient continuum within the second–order FE^2 scheme requires, not only the continuity of the displacement field, but also the continuity of its first derivatives. Since the discontinuous Galerkin (DG) method is known to be an effective tool to weakly constrain the continuity, see the works of Engel et al. (2002), Hansbo and Larson (2002), Noels and Radovitzky (2006, 2008), Bala Chandran (2007) for examples, the DG method is adopted in this thesis to constrain the continuities of the displacement field and of its first derivatives at the macroscopic scale, as developed in Nguyen et al. (2013). The use of DG method to solve the Mindlin strain gradient problem arising on the second–order FE^2 leads to a second–order DG–based FE^2 scheme. This method can be integrated into conventional parallel finite element codes without significant effort. This second–order DG–based FE^2 scheme is detailed in chapter 5.

- Multi–scale computational homogenization of structures made of cellular materials: The proposed second–order DG–based FE^2 scheme is used to consider the macroscopic localization due to the micro–buckling and size effect phenomena in structures made of cellular materials. Because of the presence of instabilities at both scales, the arc–length path following method reported by Wempner (1971), Riks (1979), Bellini and Chulya (1987), Riks (1992), Fafard and Massicotte (1993), Zhou and Murray (1995), is used. The modeling strategy is presented in chapter 6 showing that the micro–buckling leading to the macroscopic localization and the size effect phenomena can be captured within the proposed framework, as shown by Nguyen and Noels (2013).

This thesis is based on the compilation of two published papers by Nguyen et al. (2012, 2013) and on a submitted paper by Nguyen and Noels (2013). These three papers are attached in Appendix A, B and C respectively and summarized in the following three chapters.

Chapter 4

Imposing periodic boundary condition on arbitrary meshes by polynomial interpolation

The related article is given in Appendix A.

In the computational homogenization method, at each macroscopic material point, the stress–strain relation is always available through the resolution of the microscopic boundary value problem (BVP) associated with that point. In order to make the equilibrium state of the RVEs well–posed, the microscopic boundary conditions must be correctly defined. In general, a different choice leads to a different constitutive response. For a general microscopic BVP, three classical boundary conditions –a linear displacement boundary condition (Dirichlet condition), constant traction boundary condition (Neumann condition), or periodic boundary condition– can be used. Numerical studies implemented by Kanit et al. (2003), Terada et al. (2000), Larsson et al. (2011) show that the periodic boundary condition provides a better convergence rate compared to linear and constant traction ones with the increase of the RVE size as shown in Fig. 4.1: for these three kinds of boundary conditions, the increase of the RVE size leads to a better estimation of the effective properties, but for a given RVE size, the periodic boundary condition provides a better estimation than the linear displacement or than the constant traction boundary conditions. Although rigorous for periodic structures, this conclusion also holds if the micro-structure does not possess the geometrical periodicity as shown by Kanit et al. (2003), Terada et al. (2000), Larsson et al. (2011). Because of its efficiency, this work takes an interest in applying the periodic boundary

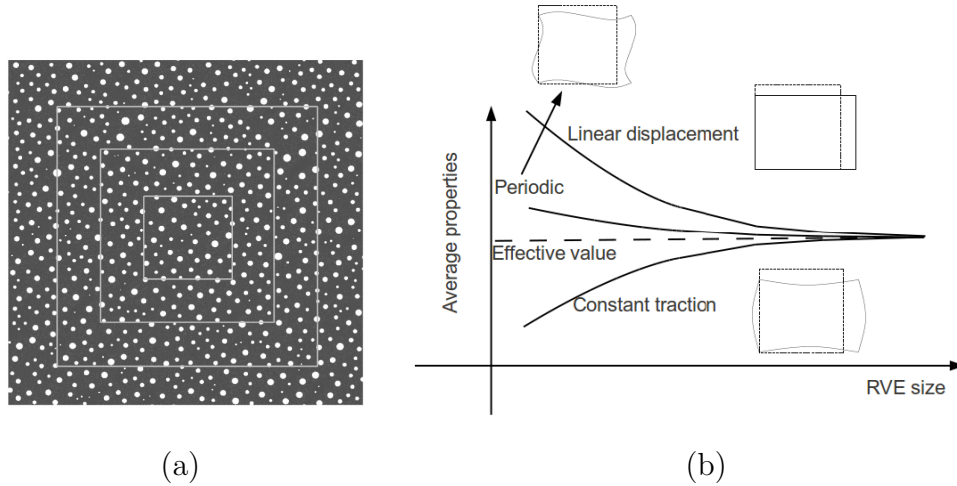(a)   (b)

Figure 4.1: Illustration of the convergence with the RVE size following Terada et al. (2000): (a) Representative volume element (RVE) with different sizes and (b) Convergence of average properties with increasing RVE sizes for different boundary condition types: linear displacement, constant traction and periodic boundary conditions.

condition to arbitrary meshes.

To enforce the periodic boundary condition, the classical method consists in enforcing linear constraints for degrees of freedom of matching nodes on two opposite RVE sides, see Fig. 4.2. This method requires a conforming mesh (so–called periodic mesh) which

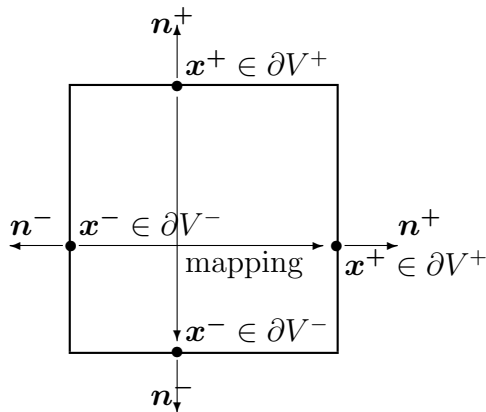Figure 4.2: Matching nodes to apply the periodic boundary condition.

has the same mesh distribution on two opposite parts of the RVE boundary. The enforcement of linear constraints for the degrees of freedom of matching nodes can then be done by the use of the Lagrange multiplier method as achieved by Michel et al. (1999), Miehe and Koch (2002), Kaczmarczyk et al. (2008) or directly by constraint eliminations

as done by Michel et al. (1999), Perić et al. (2010). Recently, the finite element models of cellular materials were obtained from micro–tomography by Youssef et al. (2005), Veyhl et al. (2011), Fiedler et al. (2012) for examples. The meshes generated from real cellular materials are non–conforming and therefore, the periodic boundary condition cannot be enforced using the matching node technique, motivating the development of a suitable method for general settings.

In order to apply the periodic boundary condition without the requirement of conforming meshes, Yuan and Fish (2008) proposed a master/slave approach to impose the periodic boundary condition for non-matching meshes. Larsson et al. (2011) developed a weak enforcement of the periodic boundary condition by introducing independently the finite element discretization of the traction boundary and by allowing the transition from the strongest form (periodic boundary condition) to the weakest form (Neumann condition). Tyrus et al. (2007) implemented the periodic boundary condition for periodic composite materials and for an arbitrary non-periodic mesh by enforcing a linear displacement field at the intersections of fiber and RVE side and a cubic displacement field at the intersection of matrix and RVE side. Although efficient, this method requires *a priori* knowledge of the deformation shape of the RVE and is thus only applicable to a periodic 2D unit-cell (composite fibers located solely at the corners of the 2D-RVE).

This work proposes to enhance the method proposed by Tyrus et al. (2007) by considering new general functions describing the boundary deformation, without requiring *a priori* knowledge of the deformed shape, of the material structure or of the mesh distribution (periodic or non-periodic). In this new method, the displacement field of two opposite RVE sides is interpolated by linear combinations of some shape functions. The degrees of freedom of the two opposite RVE sides are then substituted by the coefficients of these shape functions. This method is general in the 2-dimensional and 3-dimensional cases for periodic or random materials.

For simplicity and efficiency, the two polynomial interpolations chosen in the case of two dimensional problems are: the Lagrange interpolation using the Lagrange shape functions and the cubic spline interpolation using the Hermite shape functions. This method allows the periodic boundary condition to be enforced without the requirement of a periodic mesh, from the "weakest constraint" (linear displacement boundary condition) corresponding to the polynomial order 1 to the "strongest constraint" (periodic boundary condition) corresponding to the infinite polynomial order. Although this last case is theoretical, it can be approximated by an interpolated function of degree high

enough. In the case of three–dimensional problems, the simple Coons patch interpolation formulation based on Lagrange or cubic spline interpolations on the edges of the RVE is developed but other three–dimensional interpolation types can be directly applied. The proposed method is easy to be implemented, and allows extracting effective material properties of a heterogeneous materials using a RVE of reduced size, for periodic and non-periodic structures.

All the mathematical developments and numerical demonstrations are presented in the related article by Nguyen et al. (2012) and given in Appendix A. In this paper, the methodology is formulated in case of small strains but can be directly extended to the non–linear case for both the first– and second–order multi–scale computational homogenization framework. This extension is detailed in chapter 6.

Chapter 5

Second–order multi–scale computational homogenization scheme based on the discontinuous Galerkin method

The related article is given in Appendix B.

The second–order multi–scale computational homogenization scheme proposed by Kouznetsova et al. (2004b), which is an extension from the classical one, is a full gradient geometrically non–linear approach. This scheme considers a macroscopic Mindlin strain gradient continuum combined with the microscopic classical continuum. In this scheme, both the deformation gradient and its gradient are used at each macroscopic material point to define the microscopic boundary condition. The macroscopic first Piola–Kirchhoff and higher–order stresses are computed from the microscopic BVP resolution by the generalized version of the Hill–Mandel macro–homogeneity condition.

In order to solve the macroscopic Mindlin strain gradient continuum, the addition of higher–order terms, which are related to the higher–order stress and higher–order strain, leads to many complications in the numerical treatment of the finite element framework. With the conventional displacement–based finite element formulations, the solution of this second–order continuum requires not only the continuity of the displacement field but also the continuity of its derivatives. In other words, at least the $\mathcal{C}^1$ continuity of interpolation shape functions must be used. In order to resolve these problems, the $\mathcal{C}^1$ finite elements were developed by *e.g.* Papanicolopulos et al. (2009), Papanicolopulos and

Zervos (2012). Alternative approaches consider a mixed formulation as in the works of Amanatidou and Aravas (2002), Shu et al. (1999), or the micromorphic formulation with the work of Hirschberger et al. (2007) from which the strain gradient formulation can be recovered. In these works, the strategy of introducing another unknown field besides the unknown displacement field raises the number of degrees of freedom. Therefore, the use of $\mathcal{C}^0$ conventional continuous elements is preferred. Another effective approach is the continuous– discontinuous Galerkin ($\mathcal{C}^0$/DG) method proposed by Engel et al. (2002), Bala Chandran (2007). This approach, which uses conventional $\mathcal{C}^0$ continuous interpolation shape functions, is formulated in terms of the displacement unknowns only and weakly enforces the continuity of the higher–order derivatives at the inter–element boundaries by the DG formulation. However, in the mentioned works, no multi–scale approach was considered and the material model at the macroscopic scale was linear elastic.

As a generalization of weak formulations, DG methods allow the discontinuities of the problem unknowns in the interior of the domain, see for elliptic problems the works of Ten Eyck and Lew (2006), Noels and Radovitzky (2006) and their references. The domain is divided into sub–domains on which the integration by parts is applied, leading to boundary integral terms on the sub–domain interfaces involving the discontinuities. The role of these terms is to weakly enforce the consistency and the continuity of the problem unknowns. When considering problems involving higher–order derivatives, the DG method can also be seen as a way of weakly imposing the high–order continuity. This advantage has been exploited in the mechanics of beams and plates by Engel et al. (2002), Hansbo and Larson (2002), of shells by Noels and Radovitzky (2008), and of Mindlin's theory by Engel et al. (2002), Bala Chandran (2007). The jump discontinuities in the DG method can be related to the unknown fields and their derivatives or to their derivatives only. The DG methods have also been developed for strain–gradient damage by Wells et al. (2004) and for gradient plasticity by Djoko et al. (2007), McBride and Reddy (2009), where the discontinuity of the equivalent strain across inter–element interfaces is weakly enforced. In mathematical analyzes, the DG methods were also used to weakly impose the $\mathcal{C}^0$ continuity of the displacement field in the works of Abdulle (2008, 2012) when solving multi–scale elliptic problems at the macro–scale.

The purpose of this chapter is to establish a second–order multi–scale computational homogenization for finite deformations based on the DG formulation at the macro–scale, while the micro–problem is formulated in terms of the standard equilibrium and

boundary conditions. The DG method is used to weakly constrain the $\mathcal{C}^1$ continuity by inter–element integrals. The $\mathcal{C}^0$ continuity can be either weakly imposed by the DG formulation or strongly constrained using the conventional $\mathcal{C}^0$ displacement–based finite element. Thus two formulations can be considered:

- The full DG (FDG) formulation, which constrains weakly the $\mathcal{C}^0$ and $\mathcal{C}^1$ continuities, and

- The enriched DG (EDG) formulation with high–order term enrichments into the conventional $\mathcal{C}^0$ finite element framework to weakly constrain the $\mathcal{C}^1$ continuity.

Considering a DG formulation allows traditional finite element to be considered although the strain–gradient continuum is used. Furthermore, as the shape functions remain continuous with the EDG formulation, the number of degrees of freedom in this case is the same as for conventional $\mathcal{C}^0$ finite elements. On the contrary, the FDG method suffers from an explosion in the number of degrees of freedom as the shape functions are now discontinuous. Nevertheless, the FDG formulation is advantageous in the case of parallel implementations using face–based ghost elements as developed by Becker et al. (2011), Wu et al. (2013b).

All the mathematical developments and numerical benchmarks are detailed in the paper by Nguyen et al. (2013) and given in Appendix B. First, a DG method for Mindlin strain gradient problems in finite deformations is developed. Three–dimensional implementations of both the EDG and FDG methods are presented in this paper showing that they can be integrated into conventional parallel finite element codes without significant effort. Then, a non–linear second–order FE^2 scheme based on the DG method is established. The numerical solution of a shear layer problem is considered to demonstrate the efficiency of the proposed method.

As noted by Kouznetsova et al. (2004b), the second–order multi–scale computational homogenization can study problems with the presence of moderate localization bands and size effects. This proposed DG–based FE^2 scheme is used to study the macroscopic localization phenomenon due to the microscopic buckling of cell walls and the arising size effect in cellular materials. The application for cellular materials is detailed in chapter 6.

Chapter 6

Multi–scale computational homogenization of structures made of cellular materials

The related submitted article is given in Appendix C.

The review of the literature given in chapter 2 shows that the localization and size effect phenomena arising in cellular materials could potentially be captured by the second–order multi–scale computational homogenization scheme proposed by Kouznetsova et al. (2004b). However, this second–order scheme cannot resolve strong localization bands beyond a quadratic nature in the displacements. In spite of its limitations, this scheme can still be used to capture moderate localization bands and size effect phenomena typical of cellular materials as demonstrated in this work.

The DG–based multi–scale scheme developed in chapter 5 is used to study the in–plane behavior of structures made of the hexagonal honeycomb. As the instabilities are considered at both the macroscopic and microscopic scales, the path following method reported in Wempner (1971), Riks (1979), Bellini and Chulya (1987), Riks (1992), Fafard and Massicotte (1993), Zhou and Murray (1995) is used to solve both the macroscopic and the microscopic BVPs.

The Voronoï technique is used to generate the regular and perturbed micro–structures of hexagonal honeycomb as shown in Fig. 6.1. A regular set of points, from which the regular hexagonal layout is generated, is created and characterized by an edge length l. A perturbed set of points is then created by modifying the coordinates of each control
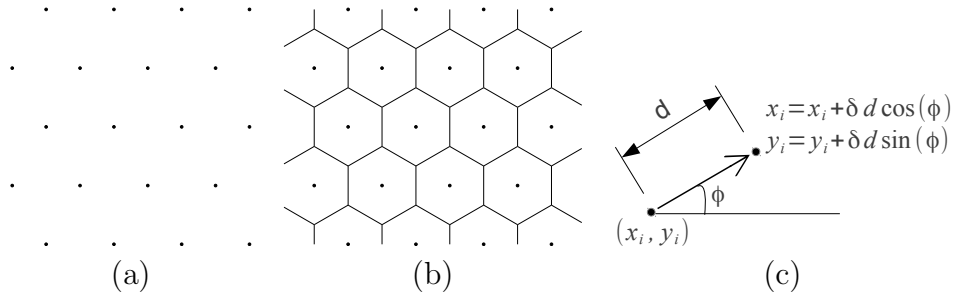
Figure 6.1: Voronoï diagram of the hexagonal honeycomb: (a) regular control points, (b) generated regular hexagones and (c) coordinate perturbation at each control point i. The coordinate perturbation is controled by ϕ, which is a random angle in $[0\ 2\pi]$, by d which is the random distance in $[0\ l]$ where l is an edge length of regular hexagon and by δ which is the control parameter defining the perturbation intensity.

point of regular one in a random way such that

$$x_i = x_i + \delta d \cos(\phi) \text{ and}$$
$$y_i = y_i + \delta d \sin(\phi), \tag{6.1}$$

where d is a random value in $[0\ l]$, ϕ is a random value in $[0\ 2\pi]$, and where δ is the control parameter which allows controlling the perturbation level of the resulting micro–structure. The same thickness t is added for all the cell walls in order to generate the complete micro–structure.

Because of the structure randomness, the micro–structures loose their periodicity leading to the non–conforming meshes. In order to enforce the periodic boundary condition in this case, the polynomial interpolation method developed in chapter 4 without the requirement of the conforming meshes is used after being extended to the second–order FE^2 scheme.

The first numerical test studies the application of the polynomial interpolation method extended to second–order boundary condition from the work of Nguyen et al. (2012). Both elastic and elasto–plastic constitutive laws are used to model the material behavior of cell walls. Under the vertical compression loading, the buckling of cell walls occurs. The loss of ellipticity of the homogenized tangent operator is observed in the elato–plastic case. The resulting macroscopic instability is expected to be captured by the proposed DG–based FE^2 scheme.

The second numerical test consists of the compression of a plate made of an hexagonal honeycomb. Both the direct and multi–scale simulations are conducted. In the multi–

scale models, because of the introduction of some randomness in the micro–structures, each macroscopic material point is associated with a local RVE which differs from the other RVEs attached to the other macroscopic positions. In order to take into account this randomness, a library of RVE meshes with a certain number of examples is generated. Each microscopic BVP located at a macroscopic position takes a random RVE mesh from the mesh library. The obtained results show that the proposed DG–based FE^2 scheme can capture the macroscopic localization band for small values of control parameter δ. The size of the RVEs within this scheme is limited by the fact that it may not be larger than the macroscopic length scale characterizing the quadratic variation in the displacements at the macroscopic scale as mentioned by Kouznetsova et al. (2004a). Using a small RVE size is acceptable for cellular materials as a single cell remains representative. For random micro–structures, choosing a small RVE size potentially leads to large variations of the homogenized properties as shown by Kanit et al. (2003). A compromise should thus be made. The results obtained with different levels of imperfection ranging from a quasi–perfect micro–structure, for which a single cell is representative, to a 30% imperfect micro–structure are analyzed. A larger value of the perturbation δ leads to a softer result on the macroscopic force–displacement behavior, which is not necessarily physical because the use of the unit cells with high randomness as the RVEs is no longer valid. Thus this approach cannot be used for structures with high degrees of imperfection, but is shown to predict with accuracy the behavior of structure made of regular micro–patterns for which a single cell can be considered as a RVE. In this case, a possible further research towards continuous–discontinuous computational homogenization schemes following the works of Massart et al. (2007), Nguyen et al. (2011) and Coenen et al. (2012) should be conducted.

The third numerical test considers the behavior of a rectangular plate with a central hole made of the elasto–plastic honeycomb. The presence of the central hole leads to a critical region with locally high strains. When the macroscopic compression displacement is large enough, microscopic buckling occurs within this region and leads to the softening behavior in which the macroscopic force decreases with an increase of the prescribed macroscopic displacement. When the cell size tends to be much smaller than the macroscopic dimensions, a classical first–order response is recovered. The capacity of the proposed method to predict the size effect existing during the softening response of structures made of cellular materials is thus demonstrated.

Chapter 7

Conclusions & perspectives

In this thesis, the main objective was to develop a multi–scale finite element framework to model the macroscopic localization due to the micro–buckling of cell walls and the size effect phenomena arising in structures made of cellular materials. Toward this end, the general review of the literature given in chapter 2 showed that such phenomena could be potentially captured by the second–order multi–scale computational homogenization scheme proposed by Kouznetsova et al. (2004b). We have thus improved this method so that it can be used for cellular materials. In particular, this work has developed the following novelties.

As the meshes of a representative volume element extracted from cellular materials are normally non–conforming and contain a large void part on the boundary, a novel method based on the polynomial interpolation method was developed to enforce the periodic boundary condition on arbitrary meshes. This method allows enforcing strongly the periodic boundary condition, without the need of conforming meshes, from the "weakest constraint" corresponding to the linear displacement boundary condition to the "strongest constraint" corresponding to the periodic boundary condition. The proposed method was shown to be easy to be implemented, and allows extracting the effective material properties of a heterogeneous structures using a representative volume element of reduced size. The polynomial interpolation method was first developed for first–order FE^2 scheme and then extended to second–order FE^2 scheme.

In order to solve the Mindlin strain gradient underlying in this second–order scheme, not only the continuity of the displacement field but also the continuity of its first derivatives must be guaranteed at the macroscopic scale. We have proposed to adapt the discontinuous Galerkin (DG) method, which is known as an excellent tool to weakly

constrain the continuities, to enforce the continuity of the displacement field and of its derivatives. A second–order DG–based FE^2 was then formulated showing that this method can be integrated into conventional parallel finite element codes without significant effort.

The proposed second–order DG–based FE^2 scheme was then used to capture the macroscopic localization due to the micro–buckling of cell walls and the size effect phenomena. As the presence of the instabilities was considered at both the macroscopic and microscopic scales, the path following method with arc–length increments was used at both scales. Some numerical applications were provided showing that this approach can predict the macroscopic localization due to the micro–buckling and the size effects existing in structures made of cellular materials.

However, our framework can only capture moderate macroscopic localization bands with a linear variation of the deformation gradient over the representative volume element as noted by Geers et al. (2010). In this case, the size of the representative volume element is smaller than the width of localization bands. In the case of sharper localization bands, *e.g.* when fracture of cell walls occurs, a possible further research towards continuous–discontinuous computational homogenization schemes following the works of Massart et al. (2007), Nguyen et al. (2011) and Coenen et al. (2012) should be conducted.
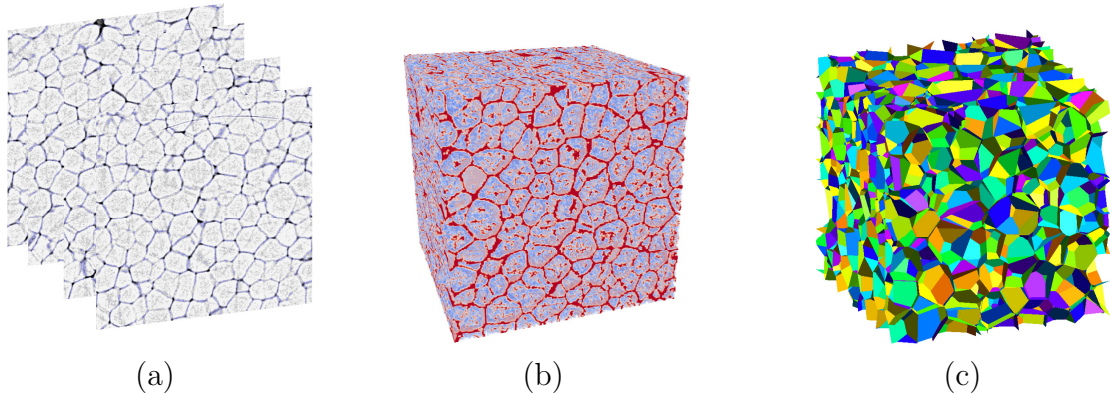

(a)   (b)   (c)

Figure 7.1: Finite element model from X–Ray tomographical images of a closed–cell polymeric foam: (a) X–Ray tomographical images from real micro–structure, (b) 3–dimensional rendering by image superposition and (c) geometrical model reconstruction by using the Laguerre tessellation (source from ARC project provided by C. Leblanc).

The computational multi–scale model developed in this thesis is currently restricted to theoretical simulations and compared with direct numerical simulations. It has not

been validated via experiments yet. However, in the context of the ARC project, a team is currently building finite element models from imaging of foamed materials, see Fig. 7.1 , and characterization tests are now conducted. Thus in the near future, with a finite element model created from tomographical images, the multi–scale computational study of real cellular materials is expected to be implemented.

The multi–scale framework presented in this thesis might be extended to study multi–physics problems such as mechanical–electromagnetic coupling during mechanical loading in which the influence of the micro–structure shape and of its evolution during macroscopic loading is accounted for.

Finally, the presented multi–scale framework can be used for material tailoring in the design of material parameters of the micro–structured materials. An objective function needs then to be specified for the optimization analysis according to the desired material properties.

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Appendix A

Annex to chapter 4: Paper A

Appendix B

Annex to chapter 5: Paper B

Appendix C

Annex to chapter 6: Paper C

Author : V.–D. Nguyen and L. Noels
Title : Computational homogenization of cellular materials
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