Homogenization Methods for Problems with

Multiphysics, Temporal and Spatial Coupling

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ABSTRACT

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There are many natural and man-made materials with heterogeneous micro- or nanostructure (fine-scale structure) which represent a great interest for industry. Therefore there is a great demand for computational methods capable to model mechanical behavior of such materials. Direct numerical simulation resolving all fine-scale details using very fine mesh often becomes very expensive. One of alternative effective group of methods is the homogenization methods allowing to model behavior of materials with heterogeneous fine-scale structure. The essence of homogenization is to replace heterogeneous material with some equivalent effectively homogeneous material. The homogenization methods are proven to be effective in certain classes of problems while there is need to improve their performance, which includes extension of the range of applicability, simplification, usage with conventional FE software and reducing computational cost.

In this dissertation methods extending the range of applicability of homogenization are developed. Firstly, homogenization was extended of the case of full nonlinear electromechanical coupling with large deformations, which allows to simulate effectively behavior of electroactive materials such as composites made of electroactive polymers. Secondly, homogenization was extended on wave problems where dispersion is significant and should be accounted for. Finally, the homogenization was extended on the case where the size of microstructure. The distinctive feature of the methods introduced in this dissertation is that they don’t require higher order derivatives and can be implemented with
conventional FE codes. The performance of methods is tested on various examples using Abaqus.
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CHAPTER 1
INTRODUCTION

1.1. Heterogeneous materials

This thesis is devoted to the homogenization methods - modeling techniques to describe the behavior of materials with heterogeneous fine-scale (micro- or nano-) structure. Absolute majority of industrial materials fall in this category because they are heterogeneous at some scale – they have composite structure, layers, grains, various inclusions, defects, dislocations etc. At same time it is assumed that at the coarse (macroscopic) scale material is sufficiently homogeneous, the length scale of heterogeneities is assumed to be much smaller than the sample or coarse-scale wavelength[1]. In other words, fine-scale structure can be revealed within every coarse-scale point A as it is shown on the Figure 1.1.1.

Figure 1.1.1. A body made of coarse-scale homogeneous material with heterogeneous fine-scale structure.

The overall, macroscopic or coarse-scale behavior of materials is controlled by their fine-scale structure and results from interaction of hierarchical structural constituents at different levels and can be very complex[2]. Contemporary technology allows creating materials with artificially designed fine-scale structure with almost arbitrary scale and complexity. The overall properties of artificial materials can be tailored by changing fine-scale structure (mixing different materials at different scales, changing the size and shape of constituents, etc.) to meet the needs of specific applications. Materials with tunable fine-scale structure can exhibit superior performance at coarse level: multiphase fine-scale structure allows improving useful properties while reducing the effect of undesirable properties of fine-scale constituents. In such materials so called “mechanical property
amplification” – orders of magnitude increases in mechanical properties such as strength and toughness relative to their constituents is possible as it often happens in biological systems[3-5]. This occurs in non-additive manner and do not follow rules of mixture.

In this thesis the attention will be paid to a particular class of micro-heterogeneous media, namely periodic medium, which can be obtained by a spatial translations of a repetitive volume element (RVE) also called elementary unit cell (UC). The examples of such medium are composite materials(Figure 1.1.2), various frame structures such as bridge trusses, multistorey buildings, porous mediums such as powders, foams, wood, soil, materials with fracture system, perforated plates and many other[6].

![Figure 1.1.2. Periodic composite material obtained by translation of unit cell: inclusions are immersed in matrix material](image)

Global periodicity is often used, but this condition is too strong. For the purposes of homogenization more general condition, namely local periodicity[1] can be used. In local periodicity(Figure 1.1.3) unit cell is repeated only in small vicinity of a coarse-scale point and is changing from one part of the macroscopic body to another part, this allows the modeling of effects related to the non-uniform distribution of fine-scale structure such as in functionally graded materials.

![Figure 1.1.3. Global (a) and local (b) periodicity](image)
Considerable information about the behavior of a periodic structure can be obtained through the analysis of a UC independently of the size of the structure. Selection of a unit cell is an important part of analysis. Typically unit cell is not uniquely defined: one can construct same periodic structure by translating different unit cells. As shown on the Figure 1.1.4 for a plate with elliptic inclusions(cells a-e). However, sometimes particular choice of UC is better than the other in the sense that the mathematical analysis more simple, for example using symmetries of UC. The selection of the best RVE is based on considerations related to the particular application, the nature of the problem and the kind of analysis needed[7].

It is also important to make sure that the selected unit cell is irreducible, i.e. it is the smallest repetitive unit identifiable in the domain carrying all the geometric features necessary to fully define the medium[8], for example, cells f and g on Figure 1.1.4 are reducible. This makes sure that UC contains information about smallest internal length scale i.e. the size of fine-scale structure, which is important for problems with intense deformations of short wave propagation.

**Figure 1.1.4**: Various choices of unit cell

Such materials possess fascinating and sometimes unexpected properties, especially in non-linear regimes[9-12].

Due to synergy of fine-scale constituents it is possible to obtain new properties which are not available in fine-scale constituents alone. Metamaterials[13-17] represent one fascinating example of how tuning fine-scale structure provides a completely different dynamic behavior of materials. Another example is dynamic materials[18, 19]. Study of various engineering, biological and geotechnical materials also presents great interest.

Various nonlinear wave phenomena[2, 20-22], such as non-linear resonances, harmonics generation, soliton formation can be used to develop methods of non-destructive material evaluation to determine composition of a particular material, for example in geo-
technical applications, or to discover various imperfections like cracks and defects in engineering materials and various inclusions, tumors in biological tissues [2, 10, 23-25].

Microstructural materials with coupled physics, for example, composites containing electroactive elastomers, possess great potential for engineering applications especially in nonlinear regimes. Examples are electroactive elastomers, electromagnetic composites. Complex mechanical response and coupled physics in such materials presents rich possibilities to adjust their mechanical behavior, enhance their structural properties; in particular application of magnetic or electric field can change strength of material, reduce damage caused by impact, change dissipative and resonant properties, influence various non-linear phenomena, activate dynamic material etc.

Understanding the structure-property relationships in micro and nano-composites is a major problem of contemporary material science. This will allow to design materials and structures with desired properties; applications of such materials are restricted only by imagination. Attempts have even been made to state optimization problems aimed at constructing an optimal material architecture [26-34].

Efficient high-fidelity computational methods are needed to design and optimize microstructural materials and use them to construct various machines, devices, structures and to develop new non-destructive evaluation methods. Direct numerical simulation resolving all fine-scale details is typically very computationally expensive and not always possible due to materials complexity. Alternative methods which would be more manageable compared to direct numeric simulation and at same will address dependence of overall properties on the fine-scale structure are highly demanded.

1.2. Homogenization and its challenges

Effective modeling of materials with fine-scale heterogeneities can be achieved by making a distinction between coarse-scale and fine-scale within the assembly, keeping in mind what are the pieces of information that compete to each of them [7]. This is generally the approach of the so-called multi-scale methods. These techniques are based on the global-local analysis approach and are described for example in [6, 35-46]. While the local analysis focuses on the peculiarities of the domain that actually make the medium heterogeneous, the global analysis predicts the global behavior of the complete structure, without dealing with the details at the microstructural level. The distinctive idea behind global-local methods is to bridge the two analyses enriching one with the other. For
example, with loading inputs from the global problem, the local model can recover the effects of the microstructure on the mechanical response. Conversely, with geometric and constitutive characteristics from the local problem, the microstructure can be successfully embedded into the global problem[7].

A number of theories has been proposed to predict the behavior of heterogeneous materials, starting from the mixture rules to various effective medium models of Eshelby, Hashin[47], Mori and Tanaka [48], self consistent approaches of Hill[49] and Christensen[50] among many others to various mathematical homogenization methods pioneered by Babuska[51], Bensoussan[52], Sanchez-Palencia[53] and Bakhvalov[6] which are strongly focused on recovering the classical limiting behavior in effective media.

Homogenization is a computational approach where medium with rapidly oscillating material properties on a fine-scale is replaced with an equivalent homogeneous material with effective material parameters, preserving properties of heterogeneous material, smearing principle[54, 55]. This usually implies slow variation of relevant fields both on the microscale and on the macroscale, which limits the applicability of the associated expansions to low-frequency situations, e.g. Parnell and Abrahams[56] or Andrianov et al.[57]. By this approach the effect of microstructure is buried into coefficients in macroscopic equations and analysis has to be performed only on the coarse scale[58]. This idea of treating micro heterogeneous solid as a conventional homogeneous solids has attracted a lot of attention due to its simplicity and out familiarity with it[59].

![Figure 1.2.1. Limit process, transition from heterogeneous domain to equivalent homogeneous](image)

Computational aspects of homogenization have been a subject of active research starting from a seminal contribution of Guedes and Kikuchi[60] for linear elasticity problems. Later important contributions have been made to extend the theory of computational homogenization to the nonlinear regime[61-64], to improve fidelity and computational efficiency of numerical simulations[65-73] and to include coupling with thermal and electric fields, but mostly restricted by linear piezoelectric coupling which will
be discussed more detailed in Chapter 2. A number studies were devoted to extend homogenization on dynamical problems and to account the finite size of unit cell, this will be discussed in details in Chapters 3 and 4 correspondingly.

Today computational homogenization methods are very promising rapidly developing technology; some of them are matured and have been proven to be effective for certain problems, successfully verified and validated[74]. They allow to establish non-linear structure-property relations, especially in the cases where the complexity and the evolving character of fine-scale structure prohibit the use of other methods[1]. But these methods still are not widely adopted by industry, and need further developments for problems involving coupled physics and coupling between time and spatial scales, where fine-scale details should be embedded into macroscopic equations.

The conventional (first order) computational homogenization framework is demonstrated on the Figure 1.2.2. and can be described as follows[1]. The coarse-scale deformation gradient $\mathbf{F}^c$ is calculated for every material point of the macrostructure (practically only integration points) and is used to formulate boundary conditions to be imposed on the unit cell associated with this coarse-scale integration point. During unit cell problem solution, unit cell experiences fine-scale deformations, which are needed to equilibrate unit cell, while overall coarse-scale deformation gradient is held constant. After solving the unit cell problem, the coarse-scale stress tensor $\mathbf{K}^c$ is extracted by averaging fine-scale stress tensor over the volume of unit cell. This procedure gives a numerical stress-deformation relationship for every coarse-scale point[1].

![Homogenization Framework](image)

**Figure 1.2.2.** Homogenization Framework
The procedure described here is deformation-driven. The stress-driven procedure, when coarse-scale stress is given and coarse-scale deformation has to be found is also possible, but it not convenient to use in homogenization[1].

The following advantages of the computational homogenization can be mentioned[1]:
1. No explicit assumptions on the coarse-scale constitutive response are made;
2. Fine-scale structure can be very complex and phases can be characterized by arbitrary physically non-linear constitutive models
3. Coarse-scale constitutive tangent operator can be derived from the total fine-scale stiffness matrix through static condensation
4. Consistency is preserved through the scale transition
5. Methods address problems with large strains and large rotations
6. Can be applied to non-periodic structures[75]
7. Fine-scale problem can be classical boundary-value problem or molecular dynamics problem[76].

One can identify the following challenges of homogenization methods which should be overcome before these methods can find wide application in industry[1, 40, 74]

1. Limitations of the range of applicability;
2. Issues of working with conventional finite element code architectures;
3. Unacceptable computational cost.

The first challenge includes problems with coupled physics, dynamic problems, problems where size of unit cell is important and affects macroscopic behavior. All these issues will be addresses in this thesis to some extent.

The second challenge is related to implementation details. The integration of homogenization methods into existing conventional finite element codes is not trivial. One has to provide interaction between fine and coarse scale – bridging mechanism: information transfer between scales, application of appropriate boundary conditions, data storage etc. Moreover, some homogenization methods do not fit conventional finite element codes because utilize generalized continuum such as second order homogenization[77]. Some of this issues are also addressed in this thesis.

The last challenge involves efficiency of homogenization methods. Homogenization methods turn out to be very expensive. This challenge can be addressed by use of parallel computations or use various reduced homogenization models[74].
1.3. Objectives and outline of the thesis

The objective of this thesis is to discuss and address some problems of homogenization technology for the multi-scale modeling of heterogeneous microstructural materials. Homogenization methods to model the behavior of electroactive materials, to model dispersive waves and to model behavior of materials with finite size microstructure are developed.

Chapter 2 is devoted to homogenization of micro-heterogeneous solids with coupled physics(electromechanical, magnetomechanical and electromagnetic coupling). Two-scale continuum equations are derived for heterogeneous continua with full nonlinear electromechanical coupling using nonlinear mathematical homogenization theory. The resulting coarse-scale electromechanical continuum equations are free of coarse-scale constitutive equations. The unit cell (or Representative Volume Element) is subjected to the overall mechanical and electric field extracted from the solution of the coarse-scale problem and is solved for arbitrary constitutive equations of fine-scale constituents. The proposed method can be applied to analyze the behavior of electroactive materials with heterogeneous fine-scale structure and can pave the way forward for designing advanced electroactive materials and devices. Details on the formulation of the microscopic boundary value problem and the micro-macro coupling in a geometrically and physically non-linear framework are given. The implementation of homogenization in a finite element framework (in commercial FEM code Abaqus) is briefly discussed. Examples demonstrating the performance of mathematical homogenization for nonlinear electroactive composites are presented. This examples show the ability of homogenization to address the dependence of mechanical response on applied electric field as well as on the volume fraction and shape of inclusions.

Since for electric current-free regions one can introduce scalar magnetic potential and describe magnetic fields in these regions similarly to electric fields, this framework is also applicable to materials with magnetomechanical coupling (such as peizomagnetics and magnetostrictors). One just has to replace all variables describing electric fields with their magnetic counterparts.

The simplest case of electromagnetic coupling when electric currents are prescribed and are not affected by mechanical deformations also can be formally reduced to mathematical homogenization in absence of electric fields. In this case one has to add fine-scale magnetic stress when calculating coarse-scale stress.
Chapter 3 deals with homogenization for dynamic problems. An effective continuum model for dispersive composite media is developed using Mathematical Homogenization method. It is shown that coarse scale stress can be defined as a sum of volume average of the fine-scale stress and additional term representing the effect of microinertia, i.e. the local motion of microstructure. The appearance of additional term in coarse-stress results in the coarse-scale equation of motion having an additional term which is second time derivative of strain. Due to this term this model is capable to describe dispersive waves in composite materials for low-frequency range.

This model is more preferable from computational point of view compared to the higher order asymptotic homogenization models because it doesn’t have higher order spatial derivatives. In the long-wave limit the model reduces to the conventional homogenization model. The comparison to the direct numerical simulation shows that effective media equations describe properly the dispersive properties of the laminated composite. The model is used to study wave propagation in laminated media. For low-frequency range the homogenized theory gives correct dispersion curves for linear laminates. Another manifestation of the dispersive nature of the model is the formation of soliton-like waves in nonlinear hyperelastic composite.

Chapter 4 deals with finite size of microstructure. Various generalizations of classical continua methods are discussed and connection of some of them with homogenization. Then a new continuum description, Computational Continua is introduced. By this approach, the coarse-scale governing equations are stated on a so-called computational continua domain consisting of disjoint union of computational unit cells, positions of which are determined to reproduce the weak form of the governing equations on the fine scale. The label ‘computational’ is conceived from both theoretical and computational considerations.

From a theoretical point of view, the computational continua is endowed with fine-scale details; it introduces no scale separation; and makes no assumption about infinitesimality of the fine-scale structure.

From computational point of view, the computational continua does not require higher-order continuity; introduces no new degrees-of-freedom; and is free of higher-order boundary conditions.

The proposed continuum description features two building blocks: the nonlocal quadrature scheme and the coarse-scale stress function. The nonlocal quadrature scheme, which replaces the classical Gauss (local) quadrature, allows for nonlocal interactions to
extend over finite neighborhoods and thus introduces nonlocality into the two-scale integrals employed in various homogenization theories.

The coarse-scale stress function, which replaces the classical notion of coarse-scale stress being the average of fine-scale stresses, is constructed to express the governing equations in terms of coarse-scale fields only.

Perhaps the most interesting finding of the present manuscript is that the coarse-scale continuum description that is consistent with an underlying fine-scale description depends on both the coarse-scale discretization and fine-scale details. Some examples showing performance of computation continua and comparison with classical homogenization are given.

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CHAPTER 2
MULTIPHYSICS, MATHEMATICAL HOMOGENIZATION THEORY FOR ELECTROACTIVE CONTINUUM

2.1. Micro-structural materials with coupled physics

Historically, the primary goal of fabricating composite materials with tunable fine-scale structure was to reduce the weight especially for materials with aerospace applications. More recently, emphasis has been placed on materials with coupled physics. In these materials mechanical fields are coupled with other fields such as electrical and magnetic fields, thermal fields, moisture and others. Materials with coupled physics found their use in actuators, transducers and structures capable of changing their mechanical behavior depending on the environment. These are so-called “smart structures” where feedback loop comprises of sensors and actuators. The presence of biasing fields makes such materials apparently behave differently[1-4], which creates an opportunity to control the response of so-called smart structures to various excitations.

This coupling can be very complex and can occur on different levels. It is impossible to account for all variety of coupled physics in simulations therefore only most relevant fields are usually considered. Most interesting for engineering applications are electromechanical coupling and electromagnetic coupling. They allow to control mechanical response of a material by application of electric or magnetic fields and enhance structural properties of a material.

In this chapter a general homogenization framework to characterize the behavior of nonlinear electroactive materials is developed. The general governing equations and boundary conditions for heterogeneous elastic solids with full nonlinear electromechanical coupling are presented, then using asymptotic expansions for displacements and potential coarse-scale equations are derived and unit cell problem. A term which is responsible for fluctuations of electric field inside UC is separated this terms is responsible for actuation. Optimizing UC structure and increasing fluctuation inside UC one can achieve increased actuation.

Magnetomechanical coupling such as magnetostriction and piezomagnetism can be reduced to electromechanical coupling by replacing variables characterizing electric fields with parameters characterizing magnetic fields. For electromagnetic coupling situation is
more complicated and only simplest case, when electric currents are prescribed and are not affected by deformations, is considered in this chapter.

2.2. Electromechanical Coupling

Electroactive materials are materials that can change their mechanical behavior in response to the applied electric field. Due to their unique characteristics such as light weight, controllable change of shape and dimensions, electroactive materials are used for actuators, sensors and smart structures. Applications range but not limited to underwater acoustics, biomedical imaging\cite{5}, robotic manipulations, artificial muscles\cite{6-8}, active damping, resonators and filters for frequency control and selection for telecommunication, precise timing and synchronization\cite{1}, MEM and NEM devices\cite{9-11}, flow control\cite{12}, precise positioning\cite{13, 14}, conformal control surfaces\cite{15}, power electronic devices\cite{16}, computer memory applications\cite{10, 11}, tunable optics, generators for harvesting energy, tactile sensors\cite{17-20}, etc.

Especially great potential possess composites based on electroactive polymers (EAP). First EAP was discovered by Roentgen in 1880\cite{21}. During last decades there was a great progress in the field of EAP fabrication\cite{7, 22-24}.

Composites containing electroactive materials in combination with other suitable materials can be used to replace pure electroactive materials with inherent limitations as low actuation capabilities, high electric fields, fast decay and instabilities. The overall properties of such composites are extremely sensitive to fine-scale details. Various studies\cite{7, 15, 22, 25-27} have shown that electromechanical coupling can be significantly improved combining flexible electromechanical material and high dielectric modulus (or even conductive) materials. The overall response of a composite actuator can be vastly superior to that of its constituents. In particular, composites based on electroactive polymers have shown tremendous promise due to their actuation capabilities resulting from the ability to produce strains of up to 40%\cite{15, 17}, and more than 100% in elastomer actuation\cite{28, 29}. The attractiveness of polymers is not only due to their electromechanical properties, but also due to their lightweight, short response time, low noise, durability and high specific energy. Proper optimization of their fine-scale structure can lead to a vast improvement in electromechanical coupling\cite{15}.

EAPs can be classified in two broad classes: ionic and electronic. In ionic EAPs electromechanical coupling occurs due to ion motion within polymer, typical actuation
voltage ranges 1-8 V. Electric field, also referred to as Coulomb force driven electronic EAPs include electrostrictive, piezoelectric, electrostatic and ferroelectric materials and require very high electric fields, more than 100 V/µm[30]. EAPs are characterized by complex interplay of nonlinear processes with possible instabilities which requires reliable computation techniques to design devices based on EAPs.

The class of electronic EAPs includes Dielectric Elastomers, Electrostrictive Graft Elastomers and Ferroelectric Polymers[31]. *Dielectric elastomers* are characterized by large strains, up to 300%, simple fabrication, low cost, repeatability, low cost, scalability and shape conformability [29, 32-35]. The actuation in dielectric elastomers is caused by electrostatic stress and can be significantly increased by prestretch[29]. *Electrostrictive graft elastomers* consist of two components: flexible macromolecule backbone chains and a grafted polymer crystal unit[36] as shown on the Figure 2.2.1. Small crystallites can induce dipole moment in electric field. Electrostrictive graft elastomers can induce strains up to 4%. *Ferroelectric polymers* have a permanent electric polarization, created by aligned dipoles. Initially dipoles are randomly oriented and do not create polarization. Alignment can be achieved by application of electric field. The most common ferroelectric polymer is polyvinylidene fluoride (PVDF) and its copolymers.

![Figure 2.2.1. Schematical structure of Electrostrictive Graft Elastomers](image)

Ionic EAPs include ionic gels, ionic polymer metal composites, conductive polymers. In ionic gels hydrogen ions move in and out of the gel, making in dense or swollen correspondingly when voltage is applied; the positively charged surfactant molecules move towards to the cathode and form a complex with negatively charged gel causing contraction and bending of the gel[37]. An example of ionic gel is poly-acrilic acid. Ionic polymer-metal composite (IPMC) consists of ionomeric polymer sandwiched by an
interpenetrating conductive medium. It can exhibit large strains, more than 8% [38]. Conductive polymers (CPs) are the material that swell when voltage is applied as a result of oxidation or reduction depending on the polarity, causing inclusion or exclusion of ions. The reaction of oxidation-reduction causes significant volume change; they require very high currents [39].

On the modeling front, there are numerous nonlinear models [1, 40-51] capable of describing electromechanical behavior for large deformation problems. There are a number of constitutive phenomenological and micromechanical models for electromechanical materials, including electrostrictors [52-54], ferroelectric switching [55-58], surface-dominated nanomaterials [59]. So while the behavior of different phases is well understood and can be described sufficiently well, the computational cost of resolving fine-scale details is very high and is often beyond the capacity of modern computers. Thus models capable of describing the overall behavior of electroactive composites without resolving fine-scale details are needed. The phenomenological equations describing the behavior of electroactive composites are usually very complex and thus there is increasing need for multiscale-multiphysics based methods.

Numerous works can be found in the literature that employ homogenization theory to model the electromechanical coupling in composites and polycrystalline materials, but mostly restricted to linear piezoelectric coupling [5, 60-70]. Schroeder [71] developed homogenization framework for nonlinear coupling to account for ferroelectric switching in the presence of a strong electric field. For mechanical problems a number of homogenization methods accounting for large deformations and arbitrary nonlinear constitutive relations have been developed [72-82]. In present manuscript we extend the nonlinear homogenization framework proposed in [73] to nonlinear electromechanical materials with full electromechanical coupling. Mathematical formulation proposed hereby can be applied to arbitrary fine-scale structures and arbitrary constitutive models of phases. To the authors’ knowledge this is first attempt to develop a general nonlinear mathematical homogenization theory for electromechanical materials.

2.3. Mathematical model

First we present the equations describing the behavior of a deformable and polarizable body, subjected to mechanical and electrical excitations. We will restrict ourselves to the quasistatic approximation, when elastic wavelengths considered are much
shorter than electromagnetic waves at the same frequency[1, 83]. In which case the effect of electromagnetic waves is neglected and electric field depends on time through boundary conditions and coupling to the dynamic mechanical fields. The formulation follows the works of Tiersten[40] and Yang[1] and is based on full electromechanical coupling in a solid via Maxwell stress, general nonlinear constitutive equations, large deformations and strong electric fields.

Consider a deformable and polarizable body occupying volume $\Omega$ with boundary $\partial \Omega$. When the body is placed in electric field, differential material elements experience both body forces and couples due to electric field. There is a full coupling through the Maxwell stress and via the constitutive equations[1, 52]. Following Tiersten[40], the electric body force $F^E$, couple $C^E$ and power $w^E$ are used to derive the balance equations

$$F^E_j = \rho_m E_j + P_i E_{j,i}, \quad (2.1.1)$$

$$C^E_i = \varepsilon_{ijk} P_j E_k, \quad (2.1.2)$$

$$w^E = \rho_m E_i \pi_i, \quad (2.1.3)$$

where $E_j$ denotes electric field, $\rho_m$ the current mass density, $\rho_e$ the current free charge density and $\pi = P_i / \rho$, the polarization per unit mass. From (2.1.1) and (2.1.2), the governing equations can be derived[1, 40].

Gauss law

$$D_{i,i} - \rho_e = 0, \quad (2.1.4)$$

where $D_i$ denotes the electric displacement,

$$D_i = \varepsilon_0 E_i + P_i, \quad (2.1.5)$$

$P_i$ and $\varepsilon_0$ are polarization and electric constant, respectively. Since divergence of polarization determines induced charge density, the total charge density is given by

$$\rho'_e = \rho_e - P_{i,i}. \quad (2.1.6)$$

Electric field is vortex free which can be written as

$$\varepsilon_{ik} E_{k,i} = 0, \quad (2.1.7)$$

which implies that electric field can be expressed in terms of the gradient of electric potential

$$E_i = -\phi_i. \quad (2.1.8)$$

The continuity equation is given by
\[
\dot{\rho}_m + \rho_m v_{i,j} = 0
\]  
and the linear momentum balance equation is
\[
\sigma_{i,j} + \rho_m b_i + F_{i,E} = (\sigma_{i,j}^E + \sigma_{i,j}^F) + \rho_m \dot{v}_i,
\]  
where \(\sigma_{i,j}\) is Cauchy stress, is \(b_i\) the body force per unit mass (excluding electric body force); \(\sigma_{i,j}^E\) is electrostatic stress, which is related to electric force \(\sigma_{i,j}^{E,E} = F_{i,E}^E\).

The electrostatic stress \(\sigma_{i,j}^E\) can be expressed as
\[
\sigma_{i,j}^E = D_i E_j = \frac{1}{2} \varepsilon_{ik} E_k \delta_{ij} = P_i E_j + \varepsilon_0 \left( E_i E_j - \frac{1}{2} E_k E_k \delta_{ij} \right)
\]  
Divergence of \(\sigma_{i,j}^E\) is given by
\[
\nabla \cdot \sigma_{i,j}^E = D_i E_i + P_i E_i_{,j} = \rho_j E_i + P_j E_{i,j} = F_{i,E}^E.
\]  
The sum of Cauchy stress \(\sigma_{i,j}\) and the electrostatic stress \(\sigma_{i,j}^E\) gives the total stress \(\tau_{i,j} = \sigma_{i,j} + \sigma_{i,j}^E\), which is symmetric and can be decomposed into symmetric tensor
\[
\sigma_{i,j}^S = \sigma_{i,j} + P_i E_j = \sigma_{\mu}^S
\]  
and Maxwell stress tensor
\[
\sigma_{i,j}^M = \varepsilon_0 \left( E_i E_j - \frac{1}{2} E_k E_k \delta_{ij} \right) = \sigma_{\mu}^M.
\]
Using the total stress, the balance of linear momentum (2.1.10) can be rewritten as
\[
\tau_{i,j} + \rho_m b_i = \rho_m \dot{v}_i,
\]  
where dot stands for time derivative.

The angular momentum balance equation is given by
\[
\varepsilon_{ijk} \sigma_{j,k} + C_i^E = \varepsilon_{ijk} \left( \sigma_{j,k} + P_j E_k \right) = \varepsilon_{ijk} \left( \sigma_{j,k} + \sigma_{j,k}^E \right) = 0,
\]  
or
\[
\varepsilon_{ijk} \tau_{j,k} = 0,
\]  
which suggests that the total stress is symmetric.

The conservation of energy is given by
\[
\rho_m \dot{e} = \sigma_{i,j} v_{i,j} + \rho_m E_i \dot{\pi}_i.
\]  
Free energy can be introduced through Legendre transform
\[
\psi = e - E_i P_i,
\]  
and
\[ \rho_m \dot{\psi} = \sigma_{ij} v_{i,j} - P_i \dot{E}_i. \] (2.1.20)

The free energy provides the constitutive relations
\[ P_i = P_i \left( E_j, \varepsilon_{ij} \right), \] (2.1.21)\[ \sigma_{ij} = \sigma_{ij} \left( E_k, \varepsilon_{kl} \right). \] (2.1.22)

In this chapter the weak form of governing equations will be expressed in the initial configuration. Therefore, we will transform the strong form of governing equations into the initial configuration. The balance laws in the in Lagrangian description are given by
\[ \mathcal{D}_{j,j} - \rho E = 0, \] (2.1.23)
where \( \mathcal{D}_L = J F_{L,j}^{-1} D_j \) and \( \rho E = \rho E J \) are Lagrangian description of electric displacement and charge density, \( D_j = J^{-1} F_{i,L} \mathcal{D}_L. \)

Electric field is vortex free in the Lagrangian description and is given by
\[ \varepsilon_{ijk} \varepsilon_{k,j} = 0, \] (2.1.24)
where \( \varepsilon_k = E_i F_{i,k} = -\phi_i F_{i,k} = -\phi_k \) is Lagrangian description of electric field, \( E_i = \varepsilon_k F_{k,i}^{-1} \).

Equation (2.1.24) can be used implicitly to describe electric field as a gradient of electric potential.
\[ K_{iL} + B_k = \rho M v_k, \] (2.1.25)
where \( K_{iL} = J F_{L,j}^{-1} \tau_{i,j} \) and \( \rho M = \rho M J \) are the first Piola-Kirchhoff stress and material density, respectively, \( B_k = \rho M b_k \) and \( \tau_{i,j} = J^{-1} F_{i,L} K_{iL}. \) \( K_{iL} \) is nonsymmetrical tensor, satisfying condition
\[ \varepsilon_{k,i} F_{i,L} K_{iL} = 0, \] (2.1.26)
which confirms that moments resulting from electric body force acting on the infinitesimal volume are equilibrated by internal forces.

The energy balance equation is given by
\[ \rho_m \dot{\psi} = \mathcal{T}_{KL}^S \mathcal{S}_{KL} - \mathcal{Q}_k \varepsilon_{k} \dot{E}_k, \] (2.1.27)
where the second Piola-Kirchhoff stress \( \mathcal{T}_{KL}^S \) is
\[ \mathcal{T}_{KL}^S = J F_{K,L}^{-1} F_{L,j}^{-1} \sigma_{ij}. \] (2.1.28)

The Green-Lagrange strain is given by
\[ \mathcal{S}_{KL} = \left( u_{K,L} + u_{K,K} + u_{M,K} u_{M,L} \right) / 2, \] (2.1.29)
and the Lagrangian description of polarization vector $\varphi_k$ is

$$\varphi_k = J F_{k,i}^{-1} P^i, \quad P = J^{-1} F_{i,k} \varphi_k, \quad (2.1.30)$$

$$\sigma^s_{ij} = \sigma_{ij} + P E_j = J^{-1} F_{i,k} F_{k,l} S^s_{kl} \quad (2.1.31)$$

The energy balance determines constitutive equations, which can be written as

$$T^s_{KL} = T^s_{KL} \left( S_{KL}, \varphi_k \right) = \rho M \frac{\partial \varphi}{\partial S_{KL}}, \quad (2.1.32)$$

$$\varphi_k = \varphi_k \left( S_{KL}, \varphi_k \right) = -\rho M \frac{\partial \varphi}{\partial E_k}. \quad (2.1.33)$$

$K_{kl}$ and $D_k$ may be calculated from

$$K_{kl} = F_{j,k} \rho M \frac{\partial \varphi}{\partial S_{KL}} + J F_{i,l} \epsilon_0 \left( E_i E_j - \frac{1}{2} E_k E_k \delta_{ij} \right), \quad (2.1.34)$$

$$D_k = \epsilon_0 J C_{KL} E_L - \rho M \frac{\partial \varphi}{\partial E_k}.$$ 

To complete the strong form of the initial-boundary value problem is given by

$$u_i = \bar{u}_i \quad \text{on} \quad \partial \Omega^u,$$

$$\varphi = \bar{\varphi} \quad \text{on} \quad \partial \Omega^\varphi,$$

$$K_{kl} N_k = \bar{T}_k \quad \text{on} \quad \partial \Omega^T,$$

$$D_k N_k = -\bar{\omega} \quad \text{on} \quad \partial \Omega^\omega,$$

$$u_i = \bar{u}_i (0) \quad \text{at} \quad t = 0,$$

$$\frac{\partial u_i}{\partial t} = \bar{v}_i (0).$$

where $\bar{\omega}$ is surface charge density applied on the portion of the surface $\partial \Omega^\omega$ and $\bar{T}_k$ is mechanical traction applied on the portion of the surface $\partial \Omega^T$; $\bar{u}_i$ and $\bar{\varphi}$ are displacements and electric potential prescribed on the surfaces $\partial \Omega^u$ and $\partial \Omega^\varphi$, respectively, such that

$$\partial \Omega^u \cap \partial \Omega^\varphi = \partial \Omega^u \cap \partial \Omega^T = \partial \Omega$$

$$\partial \Omega^u \cap \partial \Omega^\omega = \partial \Omega^\varphi \cap \partial \Omega^\omega = \partial \Omega^T = 0 \quad (2.1.35)$$

Free energy, which determines constitutive relationships for nonlinear electroelastic materials, can be written as power series of $S_{AB}$ and $E_A [1]$:
\begin{equation}
\rho \nu \psi \left( S_{KL}, E_K \right) = \frac{1}{2} c_{2ABCD} S_{AB} S_{SD} - e_{ABC} E_A S_{BC} - \frac{1}{2} \chi_{2AB} E_A E_B + \frac{1}{6} c_{3ABCDEF} S_{AB} S_{CD} S_{EF} + \\
\frac{1}{2} k_{ABCDE} E_A S_{BC} S_{DE} - \frac{1}{2} b_{ABCD} E_A E_B S_{CD} - \frac{1}{6} \chi_{3ABC} E_A E_B E_C + \\
+ \frac{1}{24} c_{4ABCDG} S_{AB} S_{CD} S_{EF} S_{GH} + \frac{1}{6} k_{2ABCD} E_A S_{BC} S_{DE} S_{FG} + \\
+ \frac{1}{4} a_{1ABCD} E_A E_B S_{CD} S_{EF} + \frac{1}{6} k_{3ABCD} E_A E_B E_C S_{DE} - \frac{1}{4} \chi_{4ABCD} E_A E_B E_C E_D,
\end{equation}

where constants \( c_{2ABCD}, e_{ABC}, \chi_{2AB}, c_{3ABCDEF}, k_{ABCD}, \chi_{3ABC}, c_{4ABCDG}, k_{2ABCD} \),
\( a_{1ABCD}, k_{3ABCD}, \chi_{4ABCD} \) are often referred to as the fundamental material constants. The
structure of \( \psi \left( S_{KL}, E_K \right) \) depends on the symmetries of particular materials under
consideration[84, 85].

From the above strong form (2.1.34) it follows that the electric fields, \( \boldsymbol{E} \) and \( \Phi \), are
coupled to the mechanical fields, \( \mathbf{F} \) and \( \mathbf{K} \), at two levels[52]. First, is the electrostatic
coupling, when the electric fields directly generate distributed forces via Maxwell stress,
which in turn affects the mechanical equilibrium of a solid. The resulting stresses depend
on the second order terms of electric field, and while typically very small (10\(^{-5}\) \( \text{MPa} \) for a
1 \( \text{MV/m} \) field), could have a significant effect if the fluctuations of the electric field are large
(field singularities) as in the case of heterogeneous media with high contrast in the
dielectric moduli or in electrodes and conducting crack tips[86, 87]. This nonlinear
phenomenon is universal and common for both, dielectrics and conductors[83], and has no
converse effects, since the mechanical stress state does not directly influence the
electrostatic balance[40], but can affect it through the motion, when such a motion changes
electric field.

The second level of coupling occurs in the constitutive behavior of dielectric
materials, expressed by equations (2.1.21), (2.1.22) or (2.1.32), (2.1.33). Polarization
induces strain, while mechanical stress affects polarization, which introduces full coupling.
Most common electromechanical materials are piezoelectrics, ferroelectrics and
electrostrictors[88].

In piezoelectrics, there is a linear dependence between applied stress and induced
electric displacement(direct piezoelectric effect)
\begin{equation}
D_i = d_{ij} \sigma_{ij}
\end{equation}
and between applied electric field and induced strain(inverse piezoelectric effect),
\[ \varepsilon_{ij} = d_{ijk} E_k, \]  

(2.1.38)

where \( d_{ijk} \) are piezoelectric coefficients. A positive electric field results in positive strain, and vice versa, negative electric field results in negative strain.

Ferroelectric materials have spontaneous polarization \( P_s \) in absence of external electric field. The charge due to spontaneous polarization is usually masked by the charges from surroundings of the material. Direction of spontaneous polarization can be switched by external electric field. Thus ferroelectric polycrystallines are characterized by hysteresis in polarization-electric field \( P(E) \) and induced strain-electric field \( \varepsilon(E) \).

In electrostrictive materials induced strain is proportional to the square of polarization

\[ \varepsilon_{ij} = Q_{ijkl} P_k P_l, \]  

(2.1.39)

where \( Q_{ijkl} \) are electrostrictive coefficients. For mildly strong electric fields, the dependence between polarization and electric field is linear and (2.1.39) may be written as

\[ \varepsilon_{ij} = M_{ijkl} E_k E_l, \]  

(2.1.40)

where \( M_{ijkl} = \chi_{km} \chi_{ln} Q_{kmln} \) and \( \chi_{ij} \) is dielectric susceptibility. Formulation of ‘converse’ electrostrictive effect is also possible[89]. Here both, positive and negative electric fields result in positive longitudinal strain.

In both, electrostriction and electrostatic coupling the overall behavior is determined by the average of the fluctuation of the electric field (rather than its average). Therefore one can obtain large coupling with relatively small macroscopic field [7, 27]. Huang et al. [27] described a three-phase polymer based actuator with more than 8% actuation strain attained with an activation field of 20 MV/m.

2.4. Mathematical homogenization for coupled nonlinear electromechanical problem

In this section we will introduce scale separation and proceed with deriving equations for different scales from the strong form of governing equations in the Lagrangian description derived in the previous section.
Consider a body with volume $\Omega^\lambda$ and surface $\partial \Omega^\lambda$ made of heterogeneous solid with characteristic size of the heterogeneity $l$, which is much smaller than the body dimensions so that heterogeneities are considered to be “invisible”. The body is effectively homogeneous at the coarse scale; its fine-scale structure can be observed by zooming (Figure 2.4.1) at any coarse-scale point $A$. It is assumed that elastic waves induced in this body by external loads are long enough to neglect the dispersion due to the material heterogeneity, i.e. lengths of elastic waves are assumed to be much bigger than the size of heterogeneity $l$. We will denote the volume and boundary of the body on the coarse-scale by $\Omega$ and $\partial \Omega$, respectively.

To describe the dependence of various fields $\Psi^\lambda (X)$ on the coarse-scale and fine-scale coordinates we will introduce global coordinate system $X$ and local (unit cell) coordinate system $Y$ associated with fine-scale structure placed at every coarse-scale point. The two coordinates are related by $Y = X / \lambda$, $0 < \lambda << 1$. Dependence of the field $\Psi^\lambda (X)$ on the two scale coordinates is denoted as

$$\Psi^\lambda (X) = \Psi (X, Y),$$

(2.4.1)

where superscript $\lambda$ denotes existence of fine-scale details.

We assume that the body is composed of a periodic repetition of unit cells(UC) with volume $\Theta_y$. The periodicity may be global, when the whole body is a lattice consisting of unit cells $\Theta_y$ (Figure 2.4.2.a) or local, when periodicity holds only in a small neighborhood of coarse-scale point (Figure 2.4.2.b)[77]. Unit cell coordinates $Y$ in (2.4.1) are defined with respect to the initial (undeformed) fine-scale configuration. All fields depend on time, but for simplicity time dependence is omitted in the notation.
To construct the weak form of the governing equations we will need to integrate over the volume $\Omega^\lambda$. This can be carried out as long as the size of unit cell is infinitesimally small, which yields the following fundamental lemma of homogenization [90, 91]

$$
\lim_{\lambda \to 0^+} \int_{\Omega^\lambda} \Psi(\mathbf{X}, \mathbf{Y}) \, d\Omega = \lim_{\lambda \to 0^+} \left( \frac{1}{\Theta_\mathbf{Y}} \int_{\Theta_\mathbf{Y}} \Psi(\mathbf{X}, \mathbf{Y}) \, d\Theta \right) d\Omega,
$$

which also implies that the fine-scale domain $\Theta_\mathbf{Y}$ exists at every point in the coarse-scale domain (Figure 3.3.).

To derive the coarse-scale equations we will start from the equilibrium equation and Gauss law in the Lagrangian description (2.1.23), (2.1.25). As before superscript $\lambda$ denotes dependence of a quantity on fine-scale details

$$
K_{I,J}^\lambda \left( \mathbf{F}^\lambda, \mathbf{E}^\lambda \right) + B_J^\lambda \left( \mathbf{X} \right) = \rho_M^\lambda \mathbf{v},
$$

$$
D_{I,J}^\lambda \left( \mathbf{F}^\lambda, \mathbf{E}^\lambda \right) - \rho_E^\lambda \left( \mathbf{X} \right) = 0
$$

with initial and boundary conditions
\[ u_i = \bar{u}_i \text{ on } \partial \Omega^*, \]
\[ \phi = \bar{\phi} \text{ on } \partial \Omega^*, \]
\[ K_{kl} N_L = T_k \text{ on } \partial \Omega^T, \]
\[ \delta_k N_k = -\bar{\omega} \text{ on } \partial \Omega^{ao}, \]
\[ u_i^\lambda = \bar{u}_i(0) \text{ at } t = 0, \]
\[ \frac{\partial u_i^\lambda}{\partial t} = \bar{v}_i(0) \text{ at } t = 0, \]
\[ \partial \Omega^{ao} \cap \partial \Omega^{ao'} = \partial \Omega^{ao} \cap \partial \Omega^{ao'} = \partial \Omega, \]
\[ \partial \Omega^{ao} \cup \partial \Omega^{ao'} = \partial \Omega^{ao} \cup \partial \Omega^{ao'} = 0. \]

(2.4.5)

Utilizing the asymptotic expansion[92-94] of displacement and electric potential fields yields

\[ u_i^\lambda (X) = u_i(X, Y) = u_i^0(X) + \lambda u_i^1(X, Y) + \lambda^2 u_i^2(X, Y) + O(\lambda^3). \]

(2.4.7)

\[ \phi^\lambda (X) = \phi(X, Y) = \phi^0(X, Y) + \lambda \phi^1(X, Y) + \lambda^2 \phi^2(X, Y) + O(\lambda^3). \]

(2.4.8)

The size of the unit cell is of the order \( \lambda \) and in the limit it is assumed to be infinitesimally small, so that first terms in asymptotic expansions for \( u_i^\lambda(X) \) and \( \phi^\lambda(X) \) do not depend on fine-scale coordinate \( Y \). This has been shown to be a unique solution for linear elliptic problems. Note that for certain class of nonlinear problems, such as problems involving softening and localizations as well as neutronic diffusion, radiative transport problems[95], one has to consider large oscillations in the leading order term in which case the first term in asymptotic expansion will depend on fine-scale coordinates \( Y \).

Expanding every term in (2.4.7) and (2.4.8) in Taylor series around the unit cell centroid \( X = \hat{X} \) yields

\[ u_i^0(X) = u_i^0(\hat{X}) + \lambda \frac{\partial u_i^0}{\partial X_j} |_{\hat{X}} Y_j + \lambda^2 \frac{\partial^2 u_i^0}{\partial X_j \partial X_k} |_{\hat{X}} Y_j Y_k + O(\lambda^3). \]

(2.4.9)

\[ u_i^\lambda (X, Y) = u_i^0(\hat{X}, Y) + \lambda \frac{\partial u_i^0}{\partial X_j} |_{\hat{X}} Y_j + \lambda^2 \frac{\partial^2 u_i^0}{\partial X_j \partial X_k} |_{\hat{X}} Y_j Y_k + O(\lambda^3). \]

(2.4.10)

\[ \phi^0(X) = \phi^0(\hat{X}) + \lambda \frac{\partial \phi^0}{\partial X_j} |_{\hat{X}} Y_j + \lambda^2 \frac{\partial^2 \phi^0}{\partial X_j \partial X_k} |_{\hat{X}} Y_j Y_k + O(\lambda^3). \]

(2.4.11)

\[ \phi^\lambda (X, Y) = \phi^0(\hat{X}, Y) + \lambda \frac{\partial \phi^0}{\partial X_j} |_{\hat{X}} Y_j + \lambda^2 \frac{\partial^2 \phi^0}{\partial X_j \partial X_k} |_{\hat{X}} Y_j Y_k + O(\lambda^3). \]

(2.4.12)

where \( X_j - \hat{X}_j = \lambda Y_j \) was used.
Substituting the above into asymptotic expansions (2.4.7), (2.4.8) gives the modified asymptotic expansion

\[ u_i^\lambda (X) = u_i \left( \hat{X}, Y \right) = \hat{u}_i^0 \left( \hat{X} \right) + \lambda \hat{u}_i^1 \left( \hat{X}, Y \right) + \lambda^2 \hat{u}_i^2 \left( \hat{X}, Y \right) + O \left( \lambda^3 \right). \]  \tag{2.4.13}

where

\[ \hat{u}_i^0 \left( \hat{X} \right) = u_i^0 \left( \hat{X} \right), \quad \hat{u}_i^1 \left( \hat{X}, Y \right) = u_i^1 \left( \hat{X}, Y \right) + \frac{\partial u_i^0}{\partial X_j} \bigg|_{\lambda_j} \cdot Y_j, \quad \hat{u}_i^2 \left( \hat{X}, Y \right) = u_i^2 \left( \hat{X}, Y \right) + \frac{\partial u_i^1}{\partial X_j} \bigg|_{\lambda_j} \cdot Y_j + \frac{1}{2} \frac{\partial^2 u_i^0}{\partial X_j \partial X_k} \bigg|_{\lambda_j} \cdot Y_j Y_k \]  \tag{2.4.14}

and similarly for potential

\[ \varphi_i^\lambda (X) = \varphi \left( \hat{X}, Y \right) = \varphi^0 \left( \hat{X} \right) + \lambda \varphi^1 \left( \hat{X}, Y \right) + \lambda^2 \varphi^2 \left( \hat{X}, Y \right) + O \left( \lambda^3 \right). \]  \tag{2.4.15}

where

\[ \varphi^0 \left( \hat{X} \right) = \varphi^0 \left( \hat{X} \right), \quad \varphi^1 \left( \hat{X}, Y \right) = \varphi^1 \left( \hat{X}, Y \right) + \frac{\partial \varphi^0}{\partial X_j} \bigg|_{\lambda_j} \cdot Y_j, \quad \varphi^2 \left( \hat{X}, Y \right) = \varphi^2 \left( \hat{X}, Y \right) + \frac{\partial \varphi^1}{\partial X_j} \bigg|_{\lambda_j} \cdot Y_j + \frac{1}{2} \frac{\partial^2 \varphi^0}{\partial X_j \partial X_k} \bigg|_{\lambda_j} \cdot Y_j Y_k \]  \tag{2.4.16}

In the classical homogenization the spatial derivative is defined as

\[ \frac{\partial f}{\partial X_i} = \frac{\partial f \left( X, Y \right)}{\partial X_i} + \frac{1}{\lambda} \frac{\partial f \left( X, Y \right)}{\partial Y_i}. \] 

Since in the modified asymptotic expansions (2.4.13) and (2.4.15) all terms are expanded in the vicinity of the unit cell centroid \( \hat{X} \), the dependence on \( X \) was eliminated by substitution \( X = \lambda Y \), therefore the spatial derivative reduces to

\[ \frac{\partial f^\lambda \left( X \right)}{\partial X_i} = \frac{1}{\lambda} \frac{\partial f \left( \hat{X}, Y \right)}{\partial Y_i}. \]  \tag{2.4.17}

Consequently the displacement gradient may be expressed as

\[ \frac{\partial u_i^\lambda}{\partial X_k} = \frac{1}{\lambda} \frac{\partial u_i \left( \hat{X}, Y \right)}{\partial Y_k} = \frac{\partial u_i^1 \left( \hat{X}, Y \right)}{\partial Y_k} + \frac{\partial u_i^2 \left( \hat{X}, Y \right)}{\partial Y_k} + O \left( \lambda^3 \right). \]  \tag{2.4.18}

where
\[
\frac{\partial \hat{u}_i^j(\mathbf{X}, \mathbf{Y})}{\partial Y_k} = \frac{\partial u_i^j(\mathbf{X}, \mathbf{Y})}{\partial Y_k} + \frac{\partial u_i^0(\mathbf{X})}{\partial X_k} \bigg|_k,
\]
\[
\frac{\partial \hat{u}_i^j(\mathbf{X}, \mathbf{Y})}{\partial Y_k} = \frac{\partial u_i^j(\mathbf{X}, \mathbf{Y})}{\partial Y_k} + \frac{\partial u_i^1(\mathbf{X}, \mathbf{Y})}{\partial X_k} \bigg|_k + \frac{\partial u_i^0(\mathbf{X})}{\partial X_j \partial Y_k} Y_j + \frac{\partial u_i^0(\mathbf{X}, \mathbf{Y})}{\partial X_j \partial X_k} Y_j.
\]

(2.4.19)

The asymptotic expansion of the deformation gradient is given as
\[
F_{ik}^j = \delta_{ik} + \frac{\partial u_i^j(\mathbf{X}, \mathbf{Y})}{\partial X_k} = \delta_{ik} + \frac{\partial u_i^j(\mathbf{X}, \mathbf{Y})}{\partial Y_k} + \frac{\partial u_i^0(\mathbf{X})}{\partial X_k} \bigg|_k = \lambda F_{ik}^j(\mathbf{X}, \mathbf{Y}) + O(\lambda^2),
\]
where
\[
F_{ik}^j(\mathbf{X}, \mathbf{Y}) = \delta_{ik} + \frac{\partial u_i^j(\mathbf{X}, \mathbf{Y})}{\partial Y_k} = \delta_{ik} + \frac{\partial u_i^j(\mathbf{X}, \mathbf{Y})}{\partial Y_k} + \frac{\partial u_i^0(\mathbf{X})}{\partial X_k} \bigg|_k = F_{ik}^j(\mathbf{X}, \mathbf{Y}).
\]

(2.4.20)

Similarly, the electric field is given as negative derivatives of electric potential
\[
\varepsilon_j^j(\mathbf{x}) = \frac{\partial \phi_j(\mathbf{X}, \mathbf{Y})}{\partial X_j} = \frac{\partial \phi_j(\mathbf{X}, \mathbf{Y})}{\partial Y_j} = \frac{\partial \phi_j^3(\mathbf{X}, \mathbf{Y})}{\partial Y_j} + O(\lambda^2) = \varepsilon_j^j(\mathbf{X}, \mathbf{Y}) + \lambda \varepsilon_j^j(\mathbf{X}, \mathbf{Y}) + O(\lambda^2),
\]
where
\[
\varepsilon_j^j(\mathbf{X}, \mathbf{Y}) = \frac{\partial \phi_j^1(\mathbf{X}, \mathbf{Y})}{\partial Y_j} - \frac{\partial \phi_j^1(\mathbf{X}, \mathbf{Y})}{\partial X_j} \bigg|_k = \varepsilon_j^j(\mathbf{X}, \mathbf{Y}) + \varepsilon_j^j(\mathbf{X}, \mathbf{Y}),
\]
\[
\varepsilon_j^j(\mathbf{X}) = \frac{\partial \phi_j^0(\mathbf{X})}{\partial X_j} \bigg|_k, \quad \varepsilon_j^j(\mathbf{X}, \mathbf{Y}) = \frac{\partial \phi_j^1(\mathbf{X}, \mathbf{Y})}{\partial Y_j}, \quad \varepsilon_j^j(\mathbf{X}, \mathbf{Y}) = \frac{\partial \phi_j^2(\mathbf{X}, \mathbf{Y})}{\partial Y_j}. \] (2.4.24)

(2.4.25)

The coarse-scale deformation gradient \( F_{ik}^c \) and electric field \( \varepsilon_j^c \) are related to the average of the leading order deformation gradient \( F_{ik}^0(\mathbf{X}, \mathbf{Y}) \) in (2.4.21) and electric field \( \varepsilon_j^0(\mathbf{X}, \mathbf{Y}) \) in (2.4.24) over the unit cell domain.
\[ F_{ik}^C (\hat{X}) = \frac{1}{\Theta} \int_{\Omega} F_{ik}^p (\hat{X}, Y) d\Theta = \delta_{ik} + \left. \frac{\partial u_0^i(X)}{\partial x_k} \right|_{\hat{X}}. \]  
(2.4.26)

\[ E^C_j (\hat{X}) = \frac{1}{\Theta} \int_{\Omega} E^p_j (\hat{X}, Y) d\Theta = -\left. \frac{\partial \varphi^0}{\partial x_j} \right|_{\hat{X}}. \]  
(2.4.27)

where conditions \( \int_{\Omega} \frac{\partial u_0^i}{\partial Y_j} d\Theta = 0 \) and \( \int \frac{\partial \varphi^1}{\partial Y_j} d\Theta = 0 \) were employed. These conditions are satisfied when periodic of weakly periodic boundary conditions for fine-scale displacements and potential are used. This will be discussed in the next section.

Expanding stress and electric displacement in Taylor series around the leading order deformation gradient \( F^0(X, Y) \) and electric field \( \varepsilon^0(\hat{X}, Y) \) yields

\[
K_{ij} \left( F^k, \varepsilon^k \right) = K_{ij} \left( F^0, \varepsilon^0 \right) + \lambda \left. \frac{\partial K_{ij}}{\partial F_{mn}^{k\ell} \varepsilon^{k\ell}} \right|_{F^0, \varepsilon^0} F_{mn}^{k\ell} + \lambda \left. \frac{\partial \varphi^0}{\partial E_M} \right|_{F^0, \varepsilon^0} \varepsilon_M^1 + O \left( \lambda^2 \right) = \]

\[= K_{ij}^0 + \lambda K_{ij}^1 + O \left( \lambda^2 \right) \]  
(2.4.28)

\[
D_{ij} \left( F^k, \varepsilon^k \right) = D_{ij} \left( F^0, \varepsilon^0 \right) + \lambda \left. \frac{\partial D_{ij}}{\partial F_{mn}^{k\ell} \varepsilon^{k\ell}} \right|_{F^0, \varepsilon^0} F_{mn}^{k\ell} + \lambda \left. \frac{\partial \varphi^0}{\partial E_M} \right|_{F^0, \varepsilon^0} \varepsilon_M^1 + O \left( \lambda^2 \right) = \]

\[= D_{ij}^0 + \lambda D_{ij}^1 + O \left( \lambda^2 \right) \]  
(2.4.29)

Taylor expansion of stress and electric displacement around the unit cell centroid \( \hat{X} \) yields

\[
K_{ij} \left( F^k, \varepsilon^k \right) = K_{ij} \left( \hat{X}, Y \right) = K_{ij}^0 \left( \hat{X}, Y \right) + \lambda \left. \frac{\partial K_{ij}}{\partial x_k} \right|_{\hat{X}, \varepsilon^k} Y_k + K_{ij}^1 \left( \hat{X}, Y \right) + O \left( \lambda^2 \right), \]  
(2.4.30)

\[
D_{ij} \left( F^k, \varepsilon^k \right) = D_{ij} \left( \hat{X}, Y \right) = D_{ij}^0 \left( \hat{X}, Y \right) + \lambda \left. \frac{\partial D_{ij}}{\partial x_k} \right|_{\hat{X}, \varepsilon^k} Y_k + D_{ij}^1 \left( \hat{X}, Y \right) + O \left( \lambda^2 \right). \]  
(2.4.31)

Again, here the relation \( (X_i - \hat{X}_i) = \lambda Y_i \) has been utilized. Further substituting above and second time derivative of (2.4.13) into equilibrium equation (2.4.3) and Gauss law (2.4.4) and neglecting \( O \left( \lambda \right) \) terms yields

\[
\lambda^{-1} \frac{\partial K_{ij}^0 \left( \hat{X}, Y \right)}{\partial Y_j} + \frac{\partial K_{ij}^0 \left( \hat{X}, Y \right)}{\partial x_j} + \partial K_{ij}^1 \left( \hat{X}, Y \right) + B_i \left( \hat{X}, Y \right) - \rho_M \left( \hat{X}, Y \right) \frac{\partial^2 u_0^i \left( \hat{X} \right)}{\partial t^2} = 0, \]  
(2.4.32)

\[
\lambda^{-1} \frac{\partial D_{ij}^0 \left( \hat{X}, Y \right)}{\partial Y_j} + \frac{\partial D_{ij}^0 \left( \hat{X}, Y \right)}{\partial x_j} + \partial D_{ij}^1 \left( \hat{X}, Y \right) - \rho_E \left( \hat{X}, Y \right) = 0. \]  
(2.4.33)
Collecting terms of equal orders in (2.4.32), (2.4.33) yields the two-scale equilibrium equation and Gauss law

\[ O(\lambda^{-1}): \frac{\partial K_{ij}^0}{\partial Y_j} (\hat{X}, \hat{Y}) = 0, \quad \frac{\partial D_{ij}^0}{\partial Y_j} (\hat{X}, \hat{Y}) = 0. \] (2.4.34)

\[ O(\lambda^0): \frac{\partial K_{ij}^0}{\partial X_j} + \frac{\partial K_{ij}^1}{\partial Y_j} + B_i (\hat{X}, \hat{Y}) = \rho_m (\hat{X}, \hat{Y}) \frac{\partial^2 u_i^0}{\partial t^2} (\hat{X}), \] \[ \frac{\partial D_{ij}^0}{\partial X_j} + \frac{\partial D_{ij}^1}{\partial Y_j} = \rho_E (\hat{X}, \hat{Y}). \] (2.4.35)

Integrating \( O(\lambda^0) \) equations over the unit cell domain and exploiting weak periodicity conditions for fine-scale stress and electric displacement \[ \int_{\Omega} \frac{\partial K_{ij}^1}{\partial Y_j} (\hat{X}, \hat{Y}) dY = 0 \]

and \[ \int_{\Omega} \frac{\partial D_{ij}^1}{\partial Y_j} (\hat{X}, \hat{Y}) dY = 0, \] yields the coarse-scale equations

\[ \frac{\partial K_{ij}^c}{\partial X_j} (\hat{X}) \bigg|_k + B_{ij}^c (\hat{X}) = \bar{\rho}_m (\hat{X}) \frac{\partial^2 u_i^0}{\partial t^2} (\hat{X}), \] \[ \frac{\partial D_{ij}^c}{\partial X_j} (\hat{X}) \bigg|_k = \rho_E^c (\hat{X}), \] (2.4.36)

where

\[ K_{ij}^c (\hat{X}) = \frac{1}{\Theta} \int_{\Theta} K_{ij}^0 (\hat{F}, \hat{X}, \hat{Y}), \hat{g} (\hat{X}, \hat{Y}) d\Theta, \quad B_{ij}^c (\hat{X}) = \frac{1}{\Theta} \int_{\Theta} B_i (\hat{X}, \hat{Y}) d\Theta. \] (2.4.37)

\[ D_{ij}^c (\hat{X}) = \frac{1}{\Theta} \int_{\Theta} D_{ij}^0 (\hat{F}, \hat{X}, \hat{Y}), \hat{g} (\hat{X}, \hat{Y}) d\Theta, \quad \rho_E^c (\hat{X}) = \frac{1}{\Theta} \int_{\Theta} \rho_E (\hat{X}, \hat{Y}) d\Theta. \] (2.4.38)

Hereafter we will make use of an argument of the unit cell infinitesimality by which the unit cell centroid \( \hat{X} \) can be positioned at an arbitrary point \( X \). Therefore, the centroid \( \hat{X} \) can be replaced by an arbitrary point \( X \). Equations(2.4.36) with boundary conditions(2.4.5) define the coarse-scale boundary value problem.

The set of equations (2.4.34) together with periodic (or weakly periodic) boundary conditions, discussed in the next section, defines fine-scale boundary value problem.

The resulting coarse-scale equations are of the same form as initial equations (2.4.3), (2.4.4). The assumption that resulting coarse-scale equations have the same form as
original equations is often used in homogenization frameworks\cite{71, 78, 82}. Even though we have got similar equations, in mathematical homogenization we didn’t make any assumption about the form of macroscopic equations in advance. The form of coarse-scale equations is a consequence of assumptions made during derivations such as the infinitesimality of unit cell and long wave limit. This is important difference of mathematical homogenization from alternative frameworks. Accounting for additional terms in asymptotic expansion (such as accelerations, gradient terms) will result in coarse-scale equations being different from the fine-scale equations and can lead to strain gradient, nonlocal continuum \cite{91} and Chapter 4) or in appearance of additional terms, such as second space derivative of acceleration\cite{96} and Chapter 3.

2.5. Boundary conditions for the unit cell problem

In this section various boundary conditions imposed on the unit cell will be considered. The most common are the periodic boundary conditions, when the displacement and electric potential perturbations on the opposite sides of the unit cell are assumed to be equal.

Consider the asymptotic expansions for displacement and electric potential fields (2.4.13), (2.4.15)

\[
u_i^\lambda (\mathbf{X}) = u_i^0 (\hat{\mathbf{X}}, \mathbf{Y}) + \lambda \left[ \left( F_{\nu_i}^C (\hat{\mathbf{X}}) - \delta_{\nu_i} \right) Y_j + u_i^1 (\hat{\mathbf{X}}, \mathbf{Y}) \right] + O \left( \lambda^2 \right),
\]

\[
\phi^\lambda (\mathbf{X}) = \phi^0 (\hat{\mathbf{X}}, \mathbf{Y}) + \lambda \left[ -E_{\phi_j}^C (\hat{\mathbf{X}}) Y_j + \phi_j^1 (\hat{\mathbf{X}}, \mathbf{Y}) \right] + O \left( \lambda^2 \right),
\]

where (2.4.25) and (2.4.26) were used (we keep here only terms up to $O(\lambda)$, since terms $O(\lambda^2)$ do not enter unit cell and macroscopic equations). The leading order terms, which represent the rigid body translation of the unit cell and constant potential, are independent of the unit cell coordinates $\mathbf{Y}$. The $O(\lambda)$ terms describe the unit cell distortion and electric field in it. The terms $\left( F_{\nu_i}^C (\hat{\mathbf{X}}) - \delta_{\nu_i} \right) Y_j$ and $E_{\phi_j}^C (\hat{\mathbf{X}}) Y_j$ represent a uniform coarse-scale deformation and uniform coarse-scale electric field, while the terms $u_i^1 (\hat{\mathbf{X}}, \mathbf{Y})$ and $\phi_j^1 (\hat{\mathbf{X}}, \mathbf{Y})$ capture the deviations from the uniform fields induced by material heterogeneity. These terms are important for electrostriction effect\cite{15} and making these terms larger increases the electrostriction effect.
Figures 2.5.1(a) and 2.5.1(b) show the initial and deformed shape of the unit cell, respectively. The dotted line in Figure 2.5.1(b) depicts the deformed shape of the unit cell due to \( F_Y^C \left( \hat{X} \right) - \delta_{ij} \), whereas the solid line shows the contribution of the \( u_i^J \left( \hat{X}, Y \right) \) term.

\[ \begin{align*}
\text{(a) Initial unit cell} & \\
\text{(b) Deformed unit cell}
\end{align*} \]

\textbf{Figure 2.5.1:} Definition of periodic boundary conditions

At the unit cell vertices \( \partial \Theta_y \), the deviations from the uniform fields, \( u_i^J \left( \hat{X}, Y \right) \) and \( \varphi_i^J \left( \hat{X}, Y \right) \), are assumed to vanish. For the remaining points on the boundary of the unit cell, the deviations from the average \( u_i^J \left( \hat{X}, Y \right) \) and \( \varphi_i^J \left( \hat{X}, Y \right) \) are prescribed to be periodic functions. Figure 2.4 depicts two points M and S on the opposite faces of the unit cell with M and S termed as the master and slave points, respectively. The displacements of the two points are given as

\[ \begin{align*}
\hat{u}_i^J \left( \hat{X}, Y^M \right) &= \left( F_Y^C \left( \hat{X} \right) - \delta_{ij} \right) Y^M_j + u_i^J \left( \hat{X}, Y^M \right), \\
\hat{u}_i^J \left( \hat{X}, Y^S \right) &= \left( F_Y^C \left( \hat{X} \right) - \delta_{ij} \right) Y^S_j + u_i^J \left( \hat{X}, Y^S \right).
\end{align*} \]  

(2.5.1)  

(2.5.2)

Subtracting equation (2.5.2) from (2.5.1) and accounting for periodicity, i.e. \( u_i^J \left( \hat{X}, Y^M \right) = u_i^J \left( \hat{X}, Y^S \right) \), gives a multi-point constraint (MPC) equation

\[ \hat{u}_i^J \left( \hat{X}, Y^M \right) - \hat{u}_i^J \left( \hat{X}, Y^S \right) = \left( F_Y^C \left( \hat{X} \right) - \delta_{ij} \right) (Y^M_j - Y^S_j) \]  

(2.5.3)

where \( Y^M \) and \( Y^S \) represent the local coordinates of the master and slave nodes on the unit cell boundary, respectively.
Similarly, periodicity of electric potential perturbations \( \phi^1(\hat{X}, Y^M) = \phi^1(\hat{X}, Y^s) \) gives the following constraint equation
\[
\phi(\hat{X}, Y^M) - \phi(\hat{X}, Y^s) = -E^C_k(\hat{X}) (Y^M_j - Y^s_j).
\] (2.5.4)

Periodic boundary conditions can be used for periodic heterogeneous medium, when the unit cell distortion is not considerable, otherwise they are not physical. For nonperiodic medium or in the case of large unit cell distortions more general boundary conditions have to be used instead. Note that the only time when the periodicity condition was exercised was in deriving equations (2.4.26), (2.4.27). For (2.4.26), (2.4.27) to hold the following conditions must be satisfied
\[
\int_{\partial Y_j} \frac{\partial u^i(X,Y)}{\partial Y_j} d\Theta_y = 0, \quad \int_{\partial Y_j} \frac{\partial \phi^i(X,Y)}{\partial Y_j} d\Theta_y = 0.
\] (2.5.5)

Applying Green’s theorem and exploiting relations (2.4.14)b, (2.4.16)b, and (2.4.26), (2.4.27) the above reduces to
\[
\int_{\partial \Theta_y} \left( \hat{u}^i(\hat{X}, Y) - \left( E^C_k(\hat{X}) - \delta_{ik} \right) Y_k \right) N_k d\Gamma_y = 0,
\]
\[
\int_{\partial \Theta_y} \left( \hat{\phi}^i(\hat{X}, Y) - \left( -E^C_k(\hat{X}) \right) Y_k \right) N_k d\Gamma_y = 0,
\] (2.5.6)

where \( \partial \Theta_y \) is the boundary of \( \Theta_y \) and \( N_k \) are the components of the unit normal to the boundary \( \partial \Theta_y \). Equation (2.5.6) represents the so-called weak periodicity condition.

Alternatively to equations (2.5.3), (2.5.4) and (2.5.6) an essential boundary condition
\[
\hat{u}^i(\hat{X}, Y) - \left( E^C_k(\hat{X}) - \delta_{ik} \right) Y_k = 0,
\]
\[
\hat{\phi}^i(\hat{X}, Y) - \left( -E^C_k(\hat{X}) \right) Y_k = 0
\] (2.5.7)
is often exercised in practice. It corresponds to zero perturbations from coarse-scale fields on the unit cell boundary.

The essential boundary conditions can be enforced either in the strong form (2.5.7) or in the weak form as
\[
\int_{\partial \Theta_y} \left( \hat{u}^i(\hat{X}, Y) - \left( E^C_k(\hat{X}) - \delta_{ik} \right) Y_k \right) \mu_i d\Gamma_y = 0,
\]
\[
\int_{\partial \Theta_y} \left( \hat{\phi}^i(\hat{X}, Y) - \left( -E^C_k(\hat{X}) \right) Y_k \right) \mu_i d\Gamma_y = 0
\] (2.5.8)
where \( \mu_i, \mu_\phi \) are the Lagrange multipliers representing unknown tractions and surface charge density on \( \partial \Omega \). If we choose \( \mu_i = K^c_i N_j, \mu_\phi = D^c_j N_j \) where \( K^c_i, D^c_j \) are constant over \( \Omega \) and require (2.5.8) to be satisfied for arbitrary \( K^c_i \) and \( D^c_j \), we then obtain equation (2.5.6). Therefore, equation (2.5.6) will be referred to as a \textit{weak compatibility boundary condition}, while equation (2.5.7) as the \textit{strong compatibility condition}. Equation (2.5.6) is in the spirit of the work of Mesarovic[97], who imposed the unit cell to satisfy average small strains. The natural boundary condition (2.5.6) is equivalent to uniform traction and allows large boundary fluctuations[82], which in not consistent with assumptions made in asymptotic expansions.

The essential (2.5.7) and natural (2.5.6) boundary conditions can be combined in the so-called \textit{mixed boundary conditions} by requiring additionally to (2.5.6) condition

\[
\left\{ \begin{array}{l}
\tilde{u}^i \left( \hat{X}, \hat{Y} \right) \left( \hat{X} \right) Y_k \right\} N_k \, d\Gamma_y \leq \varepsilon_u,

\phi^i \left( \hat{X}, \hat{Y} \right) \left( \hat{X} \right) Y_k \right\} N_k \, d\Gamma_y \leq \varepsilon_\phi
\end{array} \right.
\]  

(2.5.9)

This condition is more restrictive than (2.5.6), but more compliant than (2.5.7), which is enforced up to a tolerances \( \varepsilon_u, \varepsilon_\phi \). The mixed BC can be implemented in various ways.

For instance, by defining double nodes on the boundary and placing a linear or non-linear spring between them[73] or by introducing a pad region surrounding unit cell[91].

The different boundary conditions can be denoted for generality

\[
g \left[ \begin{array}{l}
\tilde{u}^i \\
\phi^i
\end{array} \right] = 0 \quad \text{on } \partial \Omega_y
\]  

(2.5.10)

\textbf{2.6. Two-scale problem}

The two-scale problem, consisting of the unit cell equations (2.4.34) subjected to periodic (or other) boundary conditions (4.11) and the coarse-scale equations (2.4.36), is two-way coupled. The link between the two scales is schematically shown in Figure 2.6.1.
Figure 2.6.1. Information transfer between the coarse-scale and fine-scale problems

The fine-scale problem is driven by the overall (coarse-scale) deformation gradient $F^C(\hat{X})$ and electric field $\varepsilon^C(\hat{X})$. They are calculated for every material point of the coarse-scale problem (in practice only for integration points of the coarse mesh) and used together with (2.5.10) to formulate boundary conditions to be imposed on the unit cell. Once the unit cell problem is solved, it provides the coarse-scale problem with coarse-scale stress $\sigma^C_{ij}$ and electric displacement $D^C_j$ via (2.4.37), (2.4.38). This effectively provides a coarse-scale constitutive relationship. Additionally, the local coarse-scale consistent tangent is derived from the fine-scale stiffness. This framework is similar to computational homogenization frameworks[71, 78, 82].

This scale-bridging approach belongs to the category of information-passing (sometimes referred to as hierarchical or sequential) multiscale methods which evolve a coarse-scale model by advancing a sequence of fine-scale models in small windows (representative volume or unit cell) placed at the Gauss points of the discretized coarse-scale model.

The coupled two-scale problem is summarized below:

(a) Fine scale problem
Given \( F^C_{ik}(\hat{X},t), E^C_k(\hat{X},t) \) find \( \hat{u}^i_1(\hat{X}.Y,t), \phi^i_1(\hat{X}.Y,t) \) on \( \Theta_y \) such that:

\[
\frac{\partial K^0_j}{\partial Y_j} \left( F(\hat{X}.Y), \mathcal{E}(\hat{X}.Y) \right) = 0, \quad \frac{\partial D^0_j}{\partial Y_j} \left( F(\hat{X}.Y), \mathcal{E}(\hat{X}.Y) \right) = 0 \quad \text{on } \Theta_y
\]

\[ g \left( \begin{bmatrix} \hat{u}^i_1 \\ \phi^i_1 \end{bmatrix} \right) = 0 \quad \text{on } \partial \Theta_y \]

with general constitutive relationships

\[
K^a = f_k(F, \mathcal{E}), \quad D^a_j = f_d(F, \mathcal{E})
\]

(b) Coarse-scale problem

\[
\text{Given } K^C_{ij}, \mathcal{D}^C_{ij}, \text{find } \hat{u}^0_i(\hat{X},t), \phi^0_i(\hat{X},t) \text{ on } \Omega \text{ such that}
\]

\[
\frac{\partial K^C_{ij}}{\partial X_j} + B^C_{ij} = \overline{\rho}_x \frac{\partial^2 \hat{u}^0_i}{\partial t^2} \quad \text{on } \Omega
\]

\[
\frac{\partial \mathcal{D}^C_{ij}}{\partial X_j} - \overline{\rho}_e = 0
\]

\[
K^C_{ij} N_j = \overline{F}_i \text{ on } \partial \Omega^I; \quad \hat{u}^0_i = \overline{u}_i \text{ on } \partial \Omega^u
\]

\[
\mathcal{D}^C_{ij} N_j = \overline{\phi} \text{ on } \partial \Omega^u; \quad \phi^0_i = \overline{\phi} \text{ on } \partial \Omega^\phi
\]

\[
\hat{u}^0_i = \overline{u}_i \quad \text{at } t = 0; \quad \frac{\partial \hat{u}^0_i}{\partial t} = \overline{v}_i \quad \text{at } t = 0
\]

2.7. Finite element discretization

Both the coarse- and fine-scale problems are discretized using finite elements. The displacement and electric potential fields of the fine-scale problem \( \hat{u}^i_1(\hat{X}.Y), \phi^i_1(\hat{X}.Y) \) are approximated as

\[
\hat{u}^i_1(\hat{X}.Y) = N^i_B(Y) d^i_{ab} \left( \hat{X} \right),
\]

\[
\phi^i_1(\hat{X}.Y) = N^i_B(Y) \phi^i_B \left( \hat{X} \right),
\]

where subscript \( B \) denotes the node number, \( N^i_B(Y) \) are the unit cell shape functions and \( d^i_{ab}, \phi^i_B \) are the nodal displacements and potentials in the unit cell mesh. Let \( d^m_{ic} \left( \hat{X} \right), \phi^m_c \left( \hat{X} \right) \) be the master (independent) degrees of freedom and express \( d^i_{ab}, \phi^i_B \) by a linear combination of \( d^m_{ic} \left( \hat{X} \right) \) and \( \phi^m_c \left( \hat{X} \right) \) defined by
so that the constraint equation (2.5.10) in the discrete form is satisfied

\[ g \left[ N'_{bc}(Y) \begin{bmatrix} T^d_{bc}(\hat{X}) & 0 & d^m_{bc}(\hat{X}) \\ 0 & T^e_{bc}(\hat{X}) & \phi^m_{bc}(\hat{X}) \end{bmatrix} \right] = 0 \quad \text{on} \quad \partial \Omega \]  

(2.7.3)

Then writing the Galerkin weak form of (2.6.1) and discretizing it using (2.7.1) yields the discrete residual equation:

\[ \begin{bmatrix} \rho^d_{bc}(n+1, \Delta d^1_{ij}, n+1, \Delta \phi^1) \\ \rho^e_{bc}(n+1, \Delta d^1_{ij}, n+1, \Delta \phi^1) \end{bmatrix} = \int_{\Omega} \begin{bmatrix} T^d_{bc}(\hat{X}) & 0 \\ 0 & T^e_{bc}(\hat{X}) \end{bmatrix} \begin{bmatrix} \frac{\partial N'_{bc}}{\partial y_{ij}}(n+1) \frac{1}{n+1} [K] \end{bmatrix} d\Omega = 0 \]  

(2.7.4)

where the left subscript and superscript denote the load increment and the iteration count (for implicit method) at the coarse-scale, respectively; \( \rho^d_{bc}(n+1, \Delta d^1_{ij}, n+1, \Delta \phi^1) \) and \( \rho^e_{bc}(n+1, \Delta d^1_{ij}, n+1, \Delta \phi^1) \) are the residuals, displacement and potential increments in the \( (n+1) \)th iteration of the \( (m+1) \)th load increment, respectively. If the constitutive equations are defined in terms of the Cauchy stress and electric displacement in the current configuration it is convenient to restate the unit cell problem as follows:

Given \( w^1 \mathbf{F} \), \( w^1 \mathbf{E} \) and \( \sigma_{ij}, D_j \) find \( \Delta d^1_{ij}, \Delta \phi^1 \) such that:

\[ \begin{bmatrix} \rho^d_{bc}(n+1, \Delta d^1_{ij}, n+1, \Delta \phi^1) \\ \rho^e_{bc}(n+1, \Delta d^1_{ij}, n+1, \Delta \phi^1) \end{bmatrix} = \int_{\Omega} \begin{bmatrix} T^d_{bc}(\hat{X}) & 0 \\ 0 & T^e_{bc}(\hat{X}) \end{bmatrix} \begin{bmatrix} \frac{\partial N'_{bc}}{\partial y_{ij}}(n+1) \frac{1}{n+1} [K] \end{bmatrix} d\Omega = 0 \]  

(2.7.5)

where we have exploited the relation between the first Piola-Kirchhoff stress \( K_{ij} \), electric displacement \( D_j \) in the Lagrangian description and their current configuration counterparts, Cauchy stress \( \sigma_{ij} \) and electric displacement \( D_j \): 

\[ J \sigma_{ij} = F_{jk} K_{kj}, \]

\[ JD_j = F_{ik} D_k \]  

(2.7.6)

and \( J \) in (2.7.6) is the determinant of \( F_{ij} \).

Similarly, the coarse-scale displacements and potential \( \hat{u}^0_{ij}(\hat{X}, t), \hat{\phi}^0(\hat{X}, t) \) are discretized as
\[ \ddot{u}_i^c(\hat{X}) = N_A^c(\hat{X})d_{iA}^c, \]
\[ \ddot{\phi}_i^c(\hat{X}) = N_A^c(\hat{X})\phi_i^c, \]  

where \( N_A^c(\hat{X}) \), \( d_{iA}^c \) and \( \phi_i^c \) are the coarse-scale shape functions, nodal displacements and potential, respectively. Writing the weak form of (2.6.2) and using discretization (2.7.7) the discrete coarse-scale equations can be expressed as

\[
\text{Given } n_i B_i^c, n_i \rho_i^c, n_i \overline{T}_i \text{ and } n_i \overline{\sigma}, \text{ find } n_i \Delta d_{iA}^c \text{ and } n_i \Delta \phi_i^c \text{ such that:} \\
\begin{align*}
&n_i r_i^d c (n_i \Delta d^c, n_i \Delta \phi^c) = M_{ijA} n_i d_{jB}^c + n_i f_{iA}^{\text{int}} - n_i f_{iA}^{\text{ext}} = 0 \\
&n_i r_i^\phi (n_i \Delta d^c, n_i \Delta \phi^c) = n_i f_{iA}^{\text{int}} - n_i f_{iA}^{\text{ext}} = 0 \\
&n_i d_{iA}^c = n_i \overline{d}_{iA} \text{ on } \partial \Omega^p \\
&n_i \phi_i^c = n_i \overline{\phi}_i \text{ on } \partial \Omega^p \\
&n \leftarrow n + 1, \text{ Go to the next load increment}
\end{align*}
\]

where \( n_i r_i^d c \), \( n_i r_i^\phi \) and \( n_i \Delta d_{iA}^c, n_i \Delta \phi_i^c \) are the coarse-scale residuals, displacement and potential increments in the \( (n + 1)^{\text{th}} \) load increment, respectively, and

\[
M_{ijA} = \delta_{ij} \int_{\Omega} \rho_M N_A^c N_B^c d\Omega, \]
\[
f_{iA}^{\text{int}} = \int_{\Omega} \frac{\partial N_A^c}{\partial x_j} K_{ij}^c d\Omega, \]
\[
f_{iA}^{\text{ext}} = \int_{\Omega} N_A^c B_i^c d\Omega + \int_{\partial \Omega^e} N_A^c \overline{T}_i d\Gamma, \]
\[
f_{iA}^{\text{int}} = \int_{\Omega} \frac{\partial N_A^c}{\partial x_j} D_{ij}^c d\Omega, \]
\[
f_{iA}^{\text{ext}} = \int_{\Omega} N_A^c \rho_E^c d\Omega + \int_{\partial \Omega^e} N_A^c \overline{\sigma}_i d\Gamma, \]

where \( M_{ijA} \) is the mass, \( f_{iA}^{\text{int}} \) and \( f_{iA}^{\text{ext}} \) the internal and external forces, respectively. It is again convenient to express the coarse-scale governing equations in the deformed configuration

\[
M_{ijA} = \delta_{ij} \int_{\Omega} \rho_n N_A^c N_B^c d\Omega, \]
\[
f_{iA}^{\text{int}} = \int_{\Omega} \frac{\partial N_A^c}{\partial x_j} \sigma_{ij}^c d\Omega, \]
\[
f_{iA}^{\text{ext}} = \int_{\Omega} N_A^c b_i^c d\Omega + \int_{\partial \Omega^e} N_A^c \overline{t}_i d\Gamma, \]
\[ f_{\alpha}^{\text{ext}} = \int_{\Omega} \frac{\partial N^C_\alpha}{\partial \xi_j} D^C_j d\Omega, \]  
\[ (2.7.17) \]

\[ f_{\alpha}^{\text{int}} = \int_{\Omega} N^C_\alpha \rho^C r d\Omega + \int_{\partial\Omega^C} N^C_\alpha \bar{\sigma} d\Gamma, \]  
\[ (2.7.18) \]

where
\[ \rho_m^C = \rho_m^C / J^C, \quad b_i^C = B_i^C / J^C, \quad \rho_e^C = \rho_e^C / J^C, \quad \bar{T}_d\Gamma = \bar{T}_d\Gamma, \quad \bar{\sigma} d\Gamma = \bar{\sigma} d\Gamma. \]  
\[ (2.7.19) \]

\[ \sigma^C_{ij} = F_{ik}^C K_{ik}^C / J^C \]  
\[ (2.7.20) \]

and \( J^C \) is the determinant of \( F_{ik}^C \); \( \Omega, d\Omega, \partial\Omega, d\Gamma \) denote volume, infinitesimal volume, boundary and surface element in the current configuration.

![Diagram](image)

**Figure 2.7.1.** Unit cell configurations: (a) initial, (b) coarse-scale (intermediate), (c) fine-scale deformed (final)

We now focus on deriving a closed form expression for the overall Cauchy stress \( \sigma^C_{ij} \) and electric displacement \( D^C_j \). Substituting (2.7.6) into (2.4.37), (2.4.38) and recalling \( d\Theta = Jd\Theta^C \), we have

\[ K_{ik}^C (X^C) = \frac{1}{|\Theta_i|} \int_{\Theta_i} F_{ik}^{\text{int}} \sigma_m d\Theta, \quad D_{kj}^C (X) = \frac{1}{|\Theta_j|} \int_{\Theta_j} F_{kj}^{\text{int}} D_m d\Theta. \]  
\[ (2.7.21) \]
Inserting (2.7.21) into (2.7.20) and denoting the volume of the coarse-scale (intermediate) configuration as \( |\Theta_y^*| = \mathcal{F}|\Theta_y| \), the overall quantities can be expressed as

\[
\sigma_{ij}^C = \frac{1}{|\Theta_y^*|} \int_{\Theta_y} \Delta F_{jm}^{-1} \sigma_{mi} \, d\Theta_y,
\]

\[
D_{ij}^C = \frac{1}{|\Theta_y^*|} \int_{\Theta_y} \Delta F_{jm}^{-1} D_{mj} \, d\Theta_y.
\]

(2.7.22)

where \( \Delta F_{jm}^{-1} = f_{jm}^{-1} F_{km}^{-1} \) maps the fine-scale deformed configuration \( \Theta_y \) into the coarse-scale deformed configuration \( \Theta_y^* \) as illustrated in Figure 2.7.1.

The coarse-scale problem may be solved using either explicit or implicit time integration[98].

### 2.8. Numerical examples

In this section we will consider a numerical example illustrating the ability of the mathematical homogenization to resolve the coarse-scale behavior of heterogeneous materials with nonlinear electromechanical coupling subjected to electric field. The results of the mathematical homogenization (to be referred as MH) will be compared to the direct numeric simulation (DNS) where a very fine mesh is employed to resolve fine-scale details. For simplicity, we will consider two-dimensional problem(plane strain).

For nonlinear electromechanical material we will use a simple relaxor ferroelectric material model proposed in [52], where polarization and strain are used as independent variables. It is assumed that material is isotropic, where the stress depends linearly on total strain. The polarization induced strain \( \varepsilon_E \) depends on the square of polarization, i.e., it is electrostrictive material, where polarizations saturates to \( P_s \) at high electric fields. The internal energy function for relaxor ferroelectric was proposed by Hom and Shankar as

\[
U = \frac{1}{2} (\varepsilon - \varepsilon_E) : C (\varepsilon - \varepsilon_E) + \frac{1}{2k} \left[ P \ln \left( \frac{P + |P|}{P_s - |P|} \right) + P_s \ln \left( 1 - \left( \frac{|P|}{P_s} \right)^2 \right) \right],
\]

(2.8.1)

\( \varepsilon_E \) is polarization-induced strain defined as

\[
\varepsilon_E = Q : (PP) = (Q_{11} - Q_{12}) PP + Q_{12} |P|^2 I.
\]

(2.8.2)

\( C \) and \( Q \) are an isotropic elastic stiffness matrix and an isotropic electrostrictive strain coefficient matrix; \( k \) is material constant; coefficients \( Q_{11} \) and \( Q_{12} \) are defined so that the
longitudinal and transverse induced strains relative to polarization direction are $Q_{11} |P|^2$ and
$Q_{12} |P|^2$, respectively.

Stress and electric field are calculated from the internal energy by differentiation

$$\sigma = \frac{\partial U}{\partial \varepsilon} = C : (\varepsilon - Q : (PP)), \quad \text{(2.8.3)}$$

$$E = \frac{\partial U}{\partial P} = -2 (\varepsilon - Q : (PP)) : C : Q \cdot P + \frac{1}{k} \arctanh \left( \frac{|P|}{P_s} \right) \frac{P}{|P|} \quad \text{(2.8.4)}$$

The first term in (2.8.4) represents the converse electrostrictive effect, while the second term represents the stress-free dielectric behavior. Polarization can be written in more compact form as

$$P = P_s \tanh \left( k \frac{|R|}{|R|} \right), \quad \text{(2.8.5)}$$

where

$$R = E + 2 (\varepsilon - Q : (PP)) : C : Q \cdot P = E + 2 \sigma : Q \cdot P. \quad \text{(2.8.6)}$$

Therefore, electric displacement will be

$$D = \varepsilon_o E + P = \varepsilon_o E + P_s \tanh \left( k \frac{|R|}{|R|} \right) \frac{R}{|R|}. \quad \text{(2.8.7)}$$

For a given strain and electric field (which are known from the previous iteration), one can solve (2.8.5) for induced polarization and then use (2.8.3) to calculate stress. The Jacobian for the constitutive model can be derived from (2.8.5) and (2.8.3) as

$$\begin{bmatrix} d\sigma \\ dD \end{bmatrix} = \begin{bmatrix} C - 4C : Q \cdot P \cdot Z \cdot (Q \cdot P)^T : C & -2C : Q \cdot P \cdot Z \\ 2Z \cdot (Q \cdot P)^T : C & \varepsilon_o I + Z \end{bmatrix} \begin{bmatrix} d\varepsilon \\ dE \end{bmatrix}, \quad \text{(2.8.8)}$$

where

$$Z = \left[ I - H \cdot \begin{bmatrix} 2 (\varepsilon - Q : (PP)) : C : Q - 4 (Q \cdot P)^T : C : Q \cdot P \end{bmatrix}^{-1} \cdot H \right], \quad \text{(2.8.9)}$$

$$H = P_s \tanh \left( k \frac{|R|}{|R|} \right) \left[ \frac{I}{|R|} - \frac{RR}{|R|^2} \right] + \frac{kP \cdot RR}{\cosh^2 \left( k \frac{|R|}{|R|} \right)} \cdot \frac{|R|^2}{k^2}. \quad \text{(2.8.10)}$$

<table>
<thead>
<tr>
<th>Y(GPa)</th>
<th>$\nu$</th>
<th>$Q_{11}$($m^3/C^2$)</th>
<th>$Q_{12}$($m^3/C^2$)</th>
<th>$Ps$($C/m^2$)</th>
<th>$k$($m/MV$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>115</td>
<td>0.26</td>
<td>$1.33 \times 10^{-4}$</td>
<td>$-6.06 \times 10^{-3}$</td>
<td>0.2589</td>
<td>1.16</td>
</tr>
</tbody>
</table>

Table 2.1. Model parameters for PMN-PT-BT at 5°C
Numerical values of model parameters for PMN-PT-BT at 5°C are given in Table 2.1. Dependence of polarization and induced strain on electric field is presented in Figure 2.8.1.

The above model is valid for small strains, so consequently we consider a problem where induced strains are small, in which case stress, strain, electric displacement and electric field coincide in initial and deformed configurations.

### 2.8.1 Actuator example

This example demonstrates the ability of mathematical homogenization to model the dependence of coarse-scale behavior on fine-scale details.

Consider a beam with top half made of electroactive material and lower half made of material with no electromechanical coupling(Figure 2.8.2). The electroactive material is a periodic composite with unit cell consisting of matrix material and horizontal electroactive fiber. Both materials have the same mechanical properties (linear isotropic material with Young modulus $E$ and Poisson ratio $\nu$ ), with fiber additionally having electromechanical coupling – electrostriction with parameters given in Table 2.1. Unit cell dimensions are 100 µm x100 µm.

The left side of the beam is mechanically fixed and grounded. A potential 36kV (this potential corresponds to the saturation of polarization) is applied to the right hand side of the beam.
Figure 2.8.2. Actuator: a) geometry of the beam, b) a square unit cell consisting of matrix and electrostrictive horizontal fiber, c) deformed beam.

Figure 2.8.3. Comparison of displacements of the point A for DSN and homogenization for fractions of electroactive material.
When voltage is applied, the electrostrictive material in the upper half of the beam extends due to electrostriction effect and the beam will bend as shown on Figure 2.8.2.c. This permits using the beam as an actuator.

We considered three cases with different fiber thicknesses $a$: $a=100\mu m$ (i.e. the whole unit cell consists of electrostrictive material), $a=60\mu m$ and $a=40\mu m$. Deflections of the point A as function of pseudo time (pseudo time parameterizes load) for different fiber thicknesses $a$ found by DNS-simulation are shown in Figure 2.8.3.a. It can be seen that different fiber sizes result in different actuation capabilities for the same loading, i.e., coarse-scale response is sensitive to the fine-scale details.

The purpose of homogenization is to capture this dependence. Figure 9 shows also the comparison of DNS simulation with MH for different values of $a$. The MH simulations were performed for two different meshes with 96 elements and with 192 elements to study the convergence of MH solution to DNS solution. For $a=40\mu m$, the error between DNS and MH was 4.8% for 96 element mesh and 1.3% for 192 element mesh. For $a=60\mu m$, the error was 4.9% and 1.4%, respectively. For $a=100\mu m$, error was 5%. These results suggest that the mathematical homogenization is capable of reproducing the reference solution and captures the dependence of the coarse-scale response on fine-scale details.

2.8.2 Beam bending

Now consider the whole beam (with same dimensions as previously) made of an electrostrictive material subjected to a linearly varying traction $F = 0.25 \cdot 10^5 E + 5 \cdot Y$ Pa, as shown in Figure 2.8.4. The left side of the beam is mechanically fixed and grounded. Electric potential $\phi$ is applied to the right hand side of the beam. Again, the unit cell consists of matrix and fiber as depicted in Figure 2.8.2.b. with $a=40\mu m$. The matrix is assumed to be hyperelastic material with stress depending exponentially on the first invariant of the strain $I_1 = \varepsilon_{11} + \varepsilon_{22}$.

[Diagram of beam with mechanical load applied to the left end]

Figure 2.8.4. Beam with mechanical load applied to the left end.
The application of electric field changes the mechanical properties of the beam which results in different deflections under the same loading. We compare the results of DNS and MH to show the ability of MH to capture the change of mechanical properties due to biasing fields.

Figure 2.8.5 shows the deflection of point A as function of pseudo time for the two cases. In the first case the applied potential was $\varphi=36$ kV. The result of DNS simulation is depicted by red line and MH (192 elements) simulation is depicted with a green line. The difference between DNS and MH at time $t=0.5$ was 5.6% for 96 elements and 1.6% for 192 elements. In the second case the right end of the beam was grounded, $\varphi=0$. The result of DNS simulation is depicted by blue line and MH (192 elements) simulation is depicted by magenta line. The difference between DNS and MH simulation at time $t=0.5$ was 5.2% for 96 elements and 1.5% for 192 elements.

![Figure 2.8.5. Comparison the DNS and MH simulations for beam bending.](image)

It can be seen that the mathematical homogenization is capable of capturing the change of mechanical properties due to biasing electric fields and reproduces the reference solution with good approximation.

### 2.8.3 Wave propagation in a layered beam

Finally, consider wave propagation in a beam consisting of vertical layers of matrix material with Young modulus $Y= 8.96E+9$Pa and Poisson ratio $\nu=0.3$, and electroactive
fibers with same parameters as in previous examples (Fig. 2.8.6a). The unit cell size has same dimensions as in previous examples, however fiber is oriented in vertical direction and its thickness $a=19.6 \, \mu m$. The beam has length $8.0 \times 10^{-3} \, m$ and thickness $4.0 \times 10^{-4} \, m$. The right end of the beam is constrained; the top and bottom surfaces are constrained in y-direction.

**Figure 2.8.6.** a) Layered beam, b) displacement boundary conditions $u(t)$ (measured in $\mu m$) prescribed at left end of the beam and corresponding velocity $v(t)$.

Displacement compressive impulse of the form

$$u(t) = \begin{cases} \sqrt{\frac{t - \frac{T_{imp}}{2\pi}}{T_{imp}}} \sin \left( \frac{2\pi t}{T_{imp}} \right), & t \leq T_{imp} \\ \sqrt{\frac{v}{T_{imp}}}, & t > T_{imp} \end{cases}$$

is applied in horizontal direction to the left end of the beam (Fig. 2.8.6b), where $T_{imp} = 1.0 \times 10^{-6} \, s$, $v = 1.0 \, m/s$. This boundary condition induces longitudinal compression wave in the beam. Two cases are compared: when both ends of the beam are grounded and
when potential $\phi = 16.0\text{kV}$ is applied to the left end of the beam (potential is applied before displacement). The application of electric field induces biasing stress field in the beam, which results in increasing of the peak of the stress wave. The comparisons of the stress wave profile at time $t=3.0\mu\text{s}$ for DNS and MH simulations are shown on Fig. 2.8.7. Mathematical homogenization solution is in good correspondence with reference solution for both cases.

2.9. Magnetomechanical coupling

Because there is no macroscopic currents in the volume of non-conductive magnetic media, one can introduce scalar magnetic potential and equations describing magnetizable non-conducting media will fully coincide with equations describing polarizable media. One just has to replace all variables describing electric fields with corresponding quantities describing magnetic fields. Again, as in the case of electromechanical coupling, there are two levels: through Maxwell stress tensor (magnetostatic coupling) and through constitutive relations. The constitutive relations are non-linear in general.

Magnetostriiction and piezomagnetism are magnetic analogues of electrostriction and piezoelectricity. The first effect corresponds to induced deformation which doesn’t have quadratic dependence of the magnitude of applied magnetic field and does not depend on its direction. The second effect corresponds to magnetization of some noncentro-symmetrical crystals when they are deformed.

Natural piezomagnetism is a very rare phenomena, electrostriction of much more common phenomena, it’s utilized in magnetostrictive transducers. It is cause for many interesting phenomena. One is the effect of internal deformations (which can be caused by structural defects for example) on the magnetization curve of a ferromagnetic. Another interesting effect is magnon-phonon interaction – coupling between oscillations in deformations and in spin system of a crystal[49].

2.10. Conclusions and future work

In this chapter Mathematical Homogenization theory have been extended for the case of materials with full nonlinear electromechanical coupling, including coupling through Maxwell stress, which is substantial in the presence of strong electric field, and especially important in the case of electrostrictive materials. The framework proposed in this
The manuscript is applicable to arbitrary fine-scale structures and arbitrary constitutive models of phases and allows large deformations, large electric fields and large distortions of UC.

Macro-scale equations were derived without a priori assumptions on their form using asymptotic expansions. This is an unique feature of the proposed Mathematical Homogenization framework in comparison to the alternative frameworks that can be found in the literature. The form of the coarse-scale equations is a consequence of assumptions made during derivations such as the infinitesimality of unit cell and long wave limit. Accounting for additional terms in asymptotic expansion (such as accelerations, gradient terms) will result in change of coarse-scale equations being different from fine-scale equations.

The examples presented in this manuscript show that Nonlinear Mathematical Homogenization captures well the coarse-scale behavior of heterogeneous electroactive composite and its dependence on the fine-scale details.

At the same time the method shares the shortcomings common to the first order homogenization methods; it is insensitive to the absolute size of the UC because of assumption of UC infinitesimal[91]. This lack of accuracy increases with the unit cell size and the magnitude of strains and electric fields inhomogeneities.

The study of dynamic problems with coupled physics is of big interest. Of particular are studies of wave propagation in the media with periodic resonant structures. It would be interesting to explore if mathematical homogenization can capture the negative effective refractive indexes as it was found in metamaterials. Another approach would be to ascertain whether the present formulation can be used to control band gaps by biasing fields and will it allow extending effective band gaps for use in various devices (for sub wavelength imaging, wave attenuation etc). The other interesting phenomenon, which possibly may be studied using mathematical homogenization is the controlled response of smart structures to various impacts. Depending on the impact a control strategy may be developed to obtain the desired response from the smart structure. This phenomenon might be utilized in development of smart armor and other structures. Fine-scale structure optimization aimed at optimizing coarse-scale properties, in particular for electroactive polymers containing composites, is another useful application of the method. The asymptotic expansion would allow to isolate the term \( \phi'((\hat{X},Y,t)) \), responsible for
electrostrictive and electrostatic coupling. Making this term larger will permit increasing the actuation.

References


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CHAPTER 3
HOMOGENIZATION FOR WAVE PROBLEMS, MICROINERTIA

3. 1. Introduction

This chapter is concerned with linear and non-linear wave phenomena in micro-heterogeneous solids and application of homogenization to describe these phenomena. Homogenization procedure discussed in the previous chapter belongs to the class of conventional homogenization theories, it is based on the utilization of the classical continuum model, i.e. micro-heterogeneous materials are modeled as effectively homogeneous classical solids, which allows to drastically simplify the analysis. This approach has its area of applicability, it is adequate for low rates of loading and for short observation times, and can be very effective in this area.

As it was mentioned, the fundamental assumption of the conventional homogenization approach is that the size of a heterogeneity is infinitesimally small, i.e. the ratio of the the unit cell size to the macroscopic size of the sample approaches zero, $l / L \to 0$. This is actually never true; the size of microstructure is always finite. Neglecting this fact one neglects also all effects related to the finite size of the UC, thus only the averaged motion of the material is described, and the local motion in the UC is totally ignored. Unit cell problem is assumed to be quasistatic[1] and time appears only in macroscopic equations, which prevents propagation of the microstructural dynamics on the coarse scale. This conventional representation of heterogeneous solids is adequate only for low rate loading, when the wavelength of the disturbance is large compared to the size of the unit cell.

However, for long observation times and for high rates of loading, when wavelength of disturbance becomes comparable with the characteristic size of heterogeneities, the inertia associated with the local motion (microinertia) may become quite significant and cannot be neglected. The dominant feature that has been observed in the experiments and simulations is that of dispersion, which is typical for materials with microstructure[2-10] and cannot be predicted by the effective medium model derived by classical homogenization. This is because internal material interfaces in a heterogeneous material cause reflection and refraction of stress waves, giving rise to dispersion and attenuation of waves within material microstructure Bedford[11]. Macroscopically it is expressed in that...
higher frequencies components of a signal propagate slower then low frequency components, this results in deformation of wave front while wave moves in solid. This effect becomes more pronounced when time of observation increases.

In nonlinear regimes things become even more complicated: such effects as shock waves, nonlinear resonances, generation of sub- and super-harmonics, formation of solitons e.t.c. [3, 9, 10, 12-16]. Some typical phenomena and some material classes will be considered in Section 2 of this chapter. An example of soliton-like waves formation in nonlinear layered composite, also called stegotons Leveque[17] will be considered later in Section 3.3.

In classical homogenization one accounts only for spatial variability in material properties. However, for dynamic applications one has to account for temporal variability in the material properties. In dynamic problems time appears as an additional independent variable on microscale and typically it is a fast-varying variable. Therefore, one needs somehow account for this fast fine-scale dynamics. The straightforward approach would be simulate UC over the some period of fast time and then average response over the time and over the UC volume, but this approach is very expensive. Another approach is to account this fine-scale dynamical effects in some overall manner, i.e. to consider a system with hidden motions[18].

As is was mentioned in Chapter 1 developing of homogenization methods capable to address all these phenomena is a challenge which is not overcome yet.

3.2. Some wave phenomena in microstructural materials and classes of materials

In this section we will consider some phenomena and some classes of materials where dispersion plays a significant role.

3.2.1. Dispersion

When wave travels through material with substructure it crosses material interfaces of constituents. At every interface successive reflections and refractions of the local waves lead to dispersion and attenuation of the global wave field, Figure 3.2.1. The higher frequency components of a signal experience more reflections and refractions while they propagate through the heterogeneous solid and thus experience stronger attenuation. Thus, effectively high frequency components propagate with delay comparing to the low
frequency components, i.e. phase speed decreases with frequency increase. Macroscopically it leads to the deformation of wave profile.

![Figure 3.2.1](image)

**Figure 3.2.1.** Refraction and Reflection at an interface, from [19].

### 3.2.2. Phononic band gaps

A further decrease in the wavelength increases scattering of elastic waves on heterogeneities. In periodic elastic structures a complicated structure of the so-called pass and stop frequency bands reveals[20], often referred to as acoustic or phononic bands. Thus, a periodic composite plays the role of a *discrete wave filter*. If the frequency of the signal falls within a stop band, a stationary wave is excited and neighboring heterogeneities (e.g. particles) vibrate in alternate directions. On a macrolevel, the amplitude of the global wave is attenuated exponentially, so no propagation is possible[5].

These general properties are defined for infinite unbounded media. In finite composites there is a selective reflection phenomenon. A wave belonging to pass a band will be partially reflected and partially transmitted in bounded composite, the amount of the reflection is defined by a matching problem at the composite boundary[5].

Experimental observations of the stop bands in heterogeneous elastic structures have been reported among others by Tamura et al.[21], Martinez-Sala et al.[22], Montero de Espinosa et al.[23], Torres et al.[24], Liu et al.[25], Penciu et al.[26] and Russell et al.[27]. Silva[28] established major qualitative aspects on simple discrete and 1d continuous systems. He showed how parameters (ratio of impedances, ration of times required to the wave to travel across the different media) define the width of the pass and stop bands. Ruzzene and Baz [29] studied the control of bandgaps using shape memory inserts. The elastic modulus of inserts can be varied which allows to introduce impedance mismatch necessary and change pass and stop bands. Huang and Wu[30] analyzed the influence of
temperature on the band gaps structure. They showed that the elastic bandgaps can be enlarged or reduced by adjusting the temperature of the band structure and that the temperature effects potentially can be used for fine-tuning of the phononic bandgap frequency. Cheng et al.[31] report the first observation of a hypersonic bandgap in face-centred-cubic colloidal crystals formed by self-assembly of polystyrene nanoparticles with subsequent fluid infiltration. Depending on the particle size and the sound velocity in the infiltrated fluid, the frequency and the width of the gap can be tuned. C. M. Reinke et al.[32] investigated the optimal conditions for bandgap formation in square-lattice phononic crystal. Zou et al.[33] studied the dependences of the widths and starting frequencies of the first bandgaps n the filling fraction and the ratio of length to width of the embedded section are calculated for different polarized directions of the piezoelectric ceramics and different phononic structures in a two-dimensional composite structure consisting of rectangular piezoelectric ceramics placed periodically in an epoxy substrate. They showed that the band structure depends strongly on the polarized directions, the phononic structures, the filling fraction and the ratio of length to width, respectively and that one can control the band structure in engineering according to need by choosing these parameters of the system.

3.2.3. Metamaterials

Acoustic metamaterials are composites containing components capable to exhibit resonances when excited by incident acoustic wave or possibly by electromagnetic fields[34], their effective elastic constant are negative, thus this materials posses similar properties as electromagnetic metamaterials. This phenomenon is not found for any naturally occurring material. Interesting and promising property for microwave applications that can be shown by acoustic metamaterials is the negative refractive index. In particular, they can be used in the construction of superlenses providing resolution several times better than the diffraction limit[35, 36]. Acoustic metamaterials can be used also for sound focusing and confinement[37].

Milton et al proposed a curvilinear transformations transforming equations of motion to a general form where density is anisotropic, and stress is coupled not only to strain but also to velocity, likewise momentum is coupled not only to velocity, but additionally to strain. It is argued that this equations should apply to any material containing microstructure below the scale of continuum modeling. If composites could be designed
with the required moduli then it could be possible to design elastic cloaking devices where an object is cloaked from elastic waves of given frequency[38].

Liu et al[39] fabricated sonic crystals with local resonant structures, demonstrating spectral gaps with lattice constants two orders of magnitude smaller than the relevant sonic wavelength. Review of mechanical models of acoustic metamaterials can be found in[40]. By varying the size and geometry of the structural unit one can tune the frequency ranges over which the effective elastic constants are negative[39]. Moreover one can tune already fabricated metamaterial by applying electric or magnetic field, if components contain electroactive materials, in particular hyperelastics. Due to extensions hyperelastic can change its stiffens and thus resonant properties will be also changed. This seems to be very promising perspective and here homogenization methods can help a lot.

For the case when resonators are much smaller than the operating wavelength it turns out that metamaterials can be homogenized. Zhou and Hu[31] calculated effective mass density, bulk modulus and shear modulus as functions of corresponding parameters of components and scattering coefficients for metamaterials made of coated spheres. Effective parameters can take negative values, thus homogenized model is capable to describe specific properties of metamaterials. This model is valid for low filling factors.

3.2.4. Dynamic materials

Another interesting material class is Dynamic Materials. Dynamic Materials are heterogeneous formations assembled from materials which are distributed on a microscale in space and in time[18, 41].

Optimal material design for static or non-smart applications generally results in the formation of composites where the design variables, such as material density, stiffness, yield force, and other structural parameters are position dependent, but invariant in time. The structures that result from these designs are the ordinary composite materials, and their properties depend on the individual properties of the constituent materials and the microgeometry of the mixture. The effective property of a dynamic material, however, also depends on the temporal arrangement, so that by varying the spatiotemporal parameters in the material mixture, we can effect a range of responses. The performance of structures can be improved by using spatio-temporal composite materials which match the time dependent environment of dynamic problems.
In [18] the inverse problem of mechanics was stated about funding such material distribution which will result in peculiar required motion. In particular one can require that waves propagates in this material with some prescribed velocity. Under certain conditions it is possible to isolate completely a certain part of a body from long-wave disturbances by activating a dynamic material via the design of material properties[42-44].

Lurie showed analytically that by appropriately controlling the design factors of a dynamic composite, it is possible to selectively screen large domains in space–time from the invasion of long wave disturbances. Weekes[41] presented some numerical examples to illustrate this screening effect for one-dimensional dynamic elastic composite.

For materials experiencing dynamic loads and corresponding surges of stress waves or undesirable impulses, for example, it is important to have a means of screening certain crucial parts of the structure or mechanism from the effects of such surges.

This problem formally reduces to a problem of control of the coefficients in a hyperbolic system of equations. By appropriately controlling the design factors of a dynamic composite, it is actually possible to selectively screen large domains in space–time from the invasion of long wave disturbances [13,16]. With an ordinary static composite, this screening effect is impossible.

In study [18] authors separate two classes of dynamic materials. The first-type materials are obtained by instantaneous or gradually changing the material parameters of various parts of a system (masses, rigidities, self-inductance, capacitance, etc.) with no relative motion of these parts. Such a method is termed the activation, and the corresponding materials are called the dynamic materials of the first type or activated dynamic materials[41].

In the second class, the entire system or its certain parts are presumed to be set in motion, which is predetermined or excited by a certain method. Such a method is called the kinetization, and the corresponding materials are called the dynamic materials of the second type or kinetic dynamic materials. One builds a dynamic material by setting some parts of the system into actual motion to displace materials in other regions, resulting in a material whose properties are space and time dependent. In most cases both methods are used to create a dynamic material.
3.2.5. **Nonlinear Waves**

Nonlinear phenomena in materials with heterogeneous microstructure are more complex and diverse. The analytical and experimental study of such materials even more complicated and computational methods play more important role. Some of the typical nonlinear phenomena will be mentioned below.

Waves almost without dispersion with small but finite nonlinearity are studied by classical non-linear acoustics. Typical problems are Riemann(simple) waves, weak discontinuities, parametric antennas, nonlinear sound beams, acoustic interaction in crystals e. t. c.

For weak nonlinearity, when stress can be expanded in powers of strain, for example, in 1 d case

\[ \sigma = M^1 \varepsilon + M^2 \varepsilon^2 + M^3 \varepsilon^3 + ... \]

local wave speed can be obtained as a series

\[ c = \sqrt{\rho^{-1} \frac{d \sigma}{d \varepsilon}} = c_0 \left[ 1 + \frac{1}{2} \left( \frac{1}{M^2} \right) + \frac{1}{2} \left( \frac{3}{M^3} - \frac{1}{2} \right) \varepsilon^2 + ... \right] \]

In general it follows from this equation that propagating wave of finite magnitude experiences the shape distortion up to overturn, which means formation *shock wave*. Wave evolves differently for quadratic and cubic nonlinearities; wave evolution for quadratic and cubic nonlinearities is show schematically on Figures 3.2.2 and 3.2.3[10].

**Figure 3.2.2.** Shockwave formation, from[14].

**Figure 3.2.3.** Shock wave and discontinuity formation, from[10].
For dispersive media situation changes: shock waves do not form in such media, instead due to combination of dispersion and non-linearity so-called solitary waves are formed. In homogeneous media these waves propagate as a whole without changing shape despite nonlinearities[14, 45-47].

![Solitary waves in dispersive nonlinear material](image1)

**Figure 3.2.4.** Solitary waves in dispersive nonlinear material, from[14].

Media with strong nonlinearities is subject of nonlinear acoustics. Water with bubbles, porous solids, and solids with soft inclusions and cracks, water or resin-like solids (some geotechnical materials for example) are characterized by strong nonlinearities and often demonstrate strong dispersion[10], can generate a wide range of harmonics and subharmonics. This materials often posses non-analytical relationship between stress and strain, in particular, may have hysteresis. The study of this effects is very promising to develop non-destructive material evaluation methods, in particular presence of cracks in material can lead to nonlinear resonance, while intact specimen has linear resonance[10], Figure.3.2.6. Crack possess very strong non-classical non-linearity and can increase nonlinear response of material by orders, while change in wave speed or dissipation are very small.

![Non-classical material example](image2)

**Figure 3.2.5.** Non-classical material example, from[10]
3.3. Attempts to address dynamic problems

How to account for this fine-scale phenomena without exhausting computational resources has been a topic of considerable interest in a scientific and engineering communities. The most common approach to accounting for the dispersion phenomenon is by enriching continuum description in some way[48, 49]. The effective stiffness theory developed by Achenbach and Herrmann[50] is one of the first dispersive continuum models for composites. Subsequently, several higher-order homogenization-based theories were proposed (see Bedford and Stern[51], Hegemier, Gurtman and Nayfeh[52], and Boutin and Auriault[53]).

Boutin and Auriault [53] demonstrated that the terms of higher order successively introduce effects of polarization, dispersion and attenuation. Various self-consistent schemes were employed for the purposes of dynamic homogenization by Sabina and Willis [54], Kanaun and Levin [55, 56]. Santosa and Symes[57] developed dispersive effective medium theory using Bloch wave expansion, which is in essence a representation of the solution in terms of the eigenmodes. Surveys of various higher order continuum models in elastodynamics of composites can be found [58].

Most of the higher-order homogenization theories introduce multiple spatial scales and higher order terms in the asymptotic expansion. However, while higher order terms in the asymptotic expansion are capable of capturing dispersion effects, they introduce secular terms which grow unbounded in time[59-61]. When the observation time is small, higher order terms introduce the necessary correction to the leading order term capable of resolving the dispersion effect. However, as the time window increases, the higher order terms become close to or larger than the leading order term owing to the existence of secularity. Consequently, the asymptotic expansion breaks down as it ceases to be valid.
The secularity of the asymptotic expansion can be eliminated by introducing slow time scale aimed at capturing long-time effect of dispersion in addition to the fast spatial scale aimed at spatial resolution of the microstructure (see [59-61]). As a variant to the space-time homogenization theory [59-61], nonlocal dispersive model has been developed by adding various order equilibrium equations[62, 63]. The resulting equation is independent of slow time scales, but contains fourth-order spatial derivative and thus requires C^1 continuous finite element formulation. For the case of constant mass density, the fourth-order spatial derivative term can be approximated by a mixed second-order derivative in space and time.

The mathematical framework developed for the dispersive continuum theories [5, 53-63] have been limited to linear problems. Nonlinear dispersive formulations are very rare. Among the very few exceptions are the works of Molinari and Mercier[64], Wang and Jiang[65] and Leveque and Yong[17]. While the latter focusses on mathematical analysis of one-dimensional model problems, the effect of micro-inertia in[64, 65] is incorporated in the coarse-scale equations of motion by expressing the fine-scale velocity in terms of the coarse-scale rate of deformation in the context of the Hamilton’s principle. A similar approach was used by Wang and Sun [66] to obtain dispersion curves.

For high-frequency range one can apply Floquet-Bloch approach[5, 20], where unknown solution is represented as an effective wave modulated by a spatially periodic functions, which describes the effect of composite microstructure. This leads to spectral eigenvalue problem which allows to determine the structure of phononic bands. For one-dimensional problems it is often possible to derive exact dispersion equations[28, 29, 67, 68], while in two- and three-dimensional cases the following approximate approaches can be used[5]:

- the plane-wave (PW) expansions method[5, 69-77];
- the Korringa–Kohn–Rostoker method (also known as the multiple scattering theory[25, 78, 79];
- the Rayleigh multipole expansions method and its generalizations[80-87].

McIver[88] used the method of matched asymptotic expansions to obtain the dispersion relation and predict the appearance of band gaps for a doubly periodic array of rigid scatterers of arbitrary shape.
High-frequency homogenization using two-scale asymptotic methods in a combination with the Floquet–Bloch approach was proposed by Allaire and Conca[89] Cherednichenko and Guenneau[90], and Craster at al.[6].

In the next section of this chapter homogenized model capable to describe dispersive waves in composites for low-rate loadings is presented, this section is based on the paper[91]. The model doesn’t have higher order derivatives as in the case of higher order homogenization models[5, 59], instead it has second spatial derivative of acceleration, at same time for linear cases contrary to model of [66] our model gives same results as higher order homogenization case, in 1d they can be shown to be equivalent[59]. The other difference is that this model is shown to be adequate for some nonlinear composites.

Reduced order homogenized model, which is more preferable for practical calculations, because all necessary information regarding UC may be precomputed in advance is presented. Also implementation details of the direct homogenization and reduced order model are discussed.

1d and 3d examples of wave propagations in layered composite and composite with cylindrical fibers are presented. 3d exmeples were implemented in Abaqus, where to we used user element subroutine to include additional terms in stress. Comparison with DNS simulations shows good performance of the proposed model.

3.4. Low frequency homogenization

3.4.1. Motivation

This approach focuses on the case where the shortest wavelength is several times larger than the characteristic size of the microstructure, and the observation window is large: precisely the regime where dispersion is significant. As we are interested in general purpose computational framework, we want to develop a formulation that will possess the following characteristics:

(i) **Generality**: valid for nonlinear problems;

(ii) **Compatibility with standard finite element code architecture**: use of standard $C^0$ continuity formalism with no higher order boundary conditions; and

(iii) **Computational efficiency**: capable of systematically reduce computational complexity of solving nonlinear unit cell problem.

The fine-scale inertia effect will be accounted for by formulating a *quasi-dynamic unit cell problem* where the fine-scale inertia effect is represented by so-called *inertia*
induced eigenstrain. Solution of the nonlinear quasi-dynamic unit cell problem gives rise to either modification of the coarse-scale mass matrix in the implicit solvers or internal force in the explicit solvers. Similarly to the classical homogenization theory, scale-separation is assumed, but higher order homogenization is not pursued to avoid higher order coarse-scale gradients, higher order continuity and higher order boundary conditions.

Asymptotic expansions of displacements, inertia and test functions are introduced in SubSection 3.4.2, which when combined with governing equations stated on the fine scale lead to the derivation of the coarse-scale problem. The formulation of the quasi-dynamic unit cell problem is given in SubSection 3.4.3. A closed-form solution for linear periodic heterogeneous medium, which coincides with the space-time solution obtained in [59-61], is given in SubSection 3.4.4. To reduce the computational complexity of solving the unit cell problem, residual-free dispersive formulation is introduced in SubSection 3.4.5 and residual-free unit cell problem is formulated in SubSection 3.4.6. Solution of the nonlinear model problem is given in SubSection 3.4.7. Implicit and explicit integration schemes are formulated in SubSection 3.4.8. In the implicit scheme, the effect of dispersion is introduced in the enhanced mass matrix, whereas in the explicit formulation, dispersion enters the internal force calculation. This is because the dispersive effect vanishes by mass lumping. Numerical examples for both the 1D model problem and 3D heterogeneous medium with layered and fibrous composite microstructure are given in SubSections 3.4.9,3.4.10.

In this chapter small deformation equations defined over the composite (fine-scale) domain $\Omega^\zeta$ are considered

\[
\begin{align*}
\sigma_{i,j}^\zeta (x,t) + b_{i}^\zeta (x,t) &= \rho^\zeta \dot{u}_{i}^\zeta (x,t) \quad \text{on } \Omega^\zeta \\
\sigma_{ii}^\zeta (x,t) &= L_{ijkl}^\zeta (x) \varepsilon_{ij}^\zeta (x,t) - \mu_{ii}^\zeta (x,t) \quad \text{on } \Omega^\zeta \\
\varepsilon_{ij}^\zeta (x,t) &= u_{(i,j)}^\zeta (x,t) = \frac{1}{2}(u_{i,j}^\zeta + u_{j,i}^\zeta) \quad \text{on } \Omega^\zeta \\
u_{i}^\zeta (x,t) &= \bar{u}_{i}^\zeta (x,t) \quad \text{on } \partial \Omega^\zeta \\
\sigma_{i,j}^\zeta (x,t) n_{j}^\zeta (x) &= t_{i}^\zeta (x,t) \quad \text{on } \partial \Omega^\zeta \\
u_{i}^\zeta (x,0) &= \bar{u}_{i}^\zeta (x) \end{align*}
\]  

(3.4.1)

where $\sigma^\zeta$, $u^\zeta$, $\varepsilon^\zeta$, $\mu^\zeta$, $b^\zeta$, $\rho^\zeta$ are stress, displacement, total strain, inelastic part of strain (or eigenstrain), body force and density, respectively; $\zeta$ denotes existence of fine-scale features. Summation convention over repeated indices is employed. Eq. (3.4.1)a is
equation of motion; (3.4.1)b the constitutive relation with \( L^\varepsilon \) being the elastic constitutive tensor; (3.4.1)c is small deformation kinematic relation; (3.4.1)d,e are essential and natural boundary conditions defined over the composite domain essential and natural boundaries, \( \partial \Omega^e \) and \( \partial \Omega^n \), respectively; and (3.4.1)f are initial conditions. We impose traction continuity along the interface between the fine-scale constituents \( s^\varepsilon \), where \( s^\varepsilon \) denotes the two sides of the interface

\[
\left[t^\varepsilon \right]_{s^\varepsilon} = 0
\]  

(3.4.2)

Note that large rotations can be accounted for by writing equation (3.4.1) in the corotational frame.

In absence of body forces, the weak form of equation (3.4.1) can be written as

\[
\int_{\Omega^e} w^\varepsilon_i \sigma^\varepsilon_{ij} \, d\Omega^e + \int_{\Omega^n} w^\varepsilon_i \rho \ddot{u}^\varepsilon_i \, d\Omega^e = \int_{\partial \Omega^e} w^\varepsilon_i t^\varepsilon_i \, d\Gamma^e
\]

\( \forall w^\varepsilon_i \in W^\varepsilon = \{ w^\varepsilon_i \in C^0(\Omega^e), w^\varepsilon_i = 0 \text{ on } \partial \Omega^e \} \)

(3.4.3)

where \( w^\varepsilon_i \) denotes the weight (or test) function.

### 3.4.2. The Coarse-Scale Problem

In the present manuscript spatial scale separation is assumed. In the spirit of the mathematical homogenization theory two spatial coordinates are introduced: the coarse-scale coordinate \( x \) and the unit cell coordinate \( y = x/\zeta \) with \( 0 < \zeta \ll 1 \). Spatial derivatives appearing in equations in (3.4.1) and (3.4.3) obey the following chain rule:

\[
\partial_{x_i} = \partial_{x_i} + \partial_{x_i}/\zeta
\]

(3.4.4)

We now introduce various asymptotic expansions starting with displacements

\[
u^\varepsilon(x, y, t) = u^c(x, t) + \zeta u^{(1)}(x, y, t) + O(\zeta^2)
\]

(3.4.5)

where \( u^c \) and \( u^{(1)} \) are the coarse- and fine-scale displacements, respectively.

Using the two-scale spatial derivative rule (3.4.4), the strain field is given as

\[
\begin{align*}
\varepsilon^c_{ij}(x, y, t) &= \varepsilon^f_{ij}(x, y, t) + O(\zeta) \\
\varepsilon^{(1)}_{ij}(x, y, t) &= \varepsilon^f_{ij}(x, t) + u^{(1)}_{(x, y)}(x, y, t) \\
\varepsilon_{ij}(x, t) &= u^{(1)}_{(x, y)}(x, t) = \left\{ \varepsilon^f_{ij}(x, y, t) \right\}_0
\end{align*}
\]

(3.4.6)

where superscripts \( f \) and \( c \) denote the fine-scale and coarse-scale fields, respectively. The angle bracket operator denotes the averages over spatial domain.
Similarly to the strain field, the stress field is decomposed into the coarse-scale and the fine-scale perturbation fields

\[
\sigma^c (x,y,t) = \sigma^f (x,y,t) + O(\zeta)
\]

\[
\sigma^f (x,y,t) = \sigma^c (x,y,t) + \sigma^f (x,y,t)
\]

\[
\sigma = \left\langle \sigma^f \right\rangle_o; \quad \left\langle \sigma^f \right\rangle_o = 0
\]

where the superscript * denotes the fine-scale perturbation. In the proposed dispersive model the inertia force assumes the following expansion

\[
\rho^c \ddot{u}^c_i (x,y,t) = \rho^f \ddot{u}^f_i (x,y,t) + \zeta \rho^{(1)} \ddot{u}^{(1)}_i (x,y,t) + O(\zeta^2)
\]

where \(\rho^c\) is the coarse-scale density defined by \(\rho^c = \left\langle \rho^c \right\rangle_o\) and \(\rho^{(1)} \ddot{u}^{(1)}_i\) is the fine-scale inertia which assumes the following decomposition

\[
\rho^{(1)} \ddot{u}^{(1)}_i (x,y,t) = \rho^c \dddot{h}^{mn}_i (x,y,t) \dddot{\omega}^{mn} (x,t)
\]

where \(\dddot{h}^{mn}_i (x,y,t)\) is \(y\)-periodic tensor function normalized as

\[
\left\langle \dddot{h}^{mn}_i (x,y,t) \right\rangle_o = 0
\]

The weight (or test) function in the weak form (3.4.3) is expanded similarly to the displacements (3.4.5) as

\[
w^c (x,t) = w^c (x,t) + \zeta w^{(1)} (x,y,t) + O(\zeta^2)
\]

where the fine-scale test function \(w^{(1)}\) is \(y\)-periodic function satisfying the following normalization condition

\[
\left\langle w^{(1)} \right\rangle_o = 0
\]

Applying the two-scale spatial differentiation rule (3.4.4) to the weight function asymptotic expansion yields

\[
w^c_{(i,j)} (x,t) = w^c_{(i,j)} (x,t) + w^{(1)}_{(i,j)} (x,y,t) + \zeta w^{(1)}_{(i,j)} (x,y,t) + O(\zeta^2)
\]

Integration of the two-scale functions over the composite domain and its boundary are defined as

\[
\int_{\Omega^c} \left\langle \cdot \right\rangle d\Omega = \lim_{\zeta \to 0} \int_{\Omega} \left\langle \frac{1}{\zeta} \right\rangle_{\zeta} d\Omega
\]

\[
\int_{\Omega^c} \left\langle \cdot \right\rangle d\Gamma = \lim_{\zeta \to 0} \int_{\Omega} \left\langle \frac{1}{\zeta} \right\rangle_{\zeta} d\Gamma
\]
which follows from the usual unit cell infinitesimaly assumption.

Applying the two-scale integration scheme (3.4.15) to the weak form over the composite domain (3.4.3), then inserting (3.4.14), (3.4.11), (3.4.13) and neglecting terms of the order $O(\zeta^3)$ and higher yields

$$
\int_{\Omega} w_{(i,j),s}^f \sigma_{ij}^f \, d\Omega + \int_{\Omega} w_{(i,j),s}^c \rho^c \ddot{u}_{ij}^c \, d\Omega + \int_{\Omega} \left[ w_{(i,j),s}^{(1)} \sigma_{ij}^f \right]_{\partial\Omega} + \zeta^2 \rho^c \dot{\varepsilon}_{mn}^c \left< w_{(i,j),s}^{(1)} \tilde{h}_m^c \tilde{h}_n^c \right>_{\partial\Omega} \, d\Omega =
$$

$$
= \int_{\partial\Omega'} w_{i}^f \left< t_i^c \right>_{\partial\Omega'} d\Gamma + \int_{\partial\Omega'} \left< w_{i}^{(1)} t_i^c \right>_{\partial\Omega'} d\Gamma
$$

(3.4.16)

$$
\forall w^c \in W^c = \{ w^c \in C^0(\Omega), \dot{w}^c = 0 \text{ on } \partial\Omega^c \}
$$

$$
\forall w^{(1)} \in W^{(1)} = \{ w^{(1)} \in C^0(\Theta), y\text{-periodic}, \left< w^{(1)} \right>_{\partial\Omega} = 0, \dot{w}^{(1)} = 0 \text{ on } \partial\Theta^c \}
$$

Integrating (3.4.16) by parts gives

$$
\int_{\Omega} w_{i}^f \left[ \sigma_{ij,s}^c - \rho^c \ddot{u}_{ij}^c \right] \, d\Omega + \int_{\Omega} \left[ \left< w_{i}^{(1)} \sigma_{ij,s}^f \right>_{\partial\Omega} - \zeta^2 \rho^c \dot{\varepsilon}_{mn}^c \left< w_{i}^{(1)} \tilde{h}_m^c \tilde{h}_n^c \right>_{\partial\Omega} \right] \, d\Omega =
$$

$$
= \int_{\partial\Omega'} w_{i}^c \left[ t_i^c - \tilde{t}_i^c \right] d\Gamma; \quad \forall w^c \in W^c, \forall w^{(1)} \in W^{(1)}
$$

(3.4.17)

where $t_i^c = \sigma_{ij,s}^c n_j^c$, and the fine-scale traction is assumed to be constant over the $\partial\Theta$, $t_i^c = \tilde{t}_i^c$.

The first and second terms in the Eq. (3.4.17) correspond to the coarse-scale and unit cell problems, respectively. Here we have two ways to proceed. One approach is to account for the inertia term in both the unit cell and coarse-scale problems. Thus assuming arbitrariness of $w^{(1)} \in W^{(1)}$ yields the dynamic unit cell problem and the classical coarse-scale problem

$$
\sigma_{ij,s}^f = \zeta^2 \rho^c \dot{\varepsilon}_{mn}^c \tilde{h}_m^c \tilde{h}_n^c; \quad \sigma_{ij,s}^c = \rho^c \ddot{u}_{ij}^c; \quad \tilde{t}_i^c = t_i^c
$$

(3.4.18)

This variant introduces two-way coupling even for linear problems where the unit cell problem (3.4.18a) has to be continuously reanalyzed for different coarse-scale acceleration gradients.

As an alternative to be pursued in the present manuscript, we will seek for an approximation of the unit cell problem that would not depend on the coarse-scale solution for linear problems. This will be accomplished by eliminating the inertia term from the fine-scale problem, which would yield the classical quasi-static unit cell problem

$$
\sigma_{ij,s}^f = 0
$$

(3.4.19)
and by constructing the test function $w_i^{(1)}$ as

$$w_i^{(1)}(x, y, t) = h_i^W(x, y, t)w_{(k, s)}^e(x, t)$$

(3.4.20)

with inertia influence function $h_i^W \in W^\Theta$ constructed from the solution of so-called quasi-dynamic unit cell problem (to be discussed in Section 3.4.3).

Thus, substituting (3.4.19) into (3.4.16) and (3.4.17) yields the weak form of the coarse-scale problem

$$
\int_{\Omega} w_i^{e} \left( \sigma_{ij} + D_{ijmn} \tilde{\varepsilon}_{mn}^e \right) d\Omega + \int_{\Omega} w_i^{e} \rho^e \ddot{u}_i^{e} d\Omega = \int_{\partial\Omega} w_i^{e} \tilde{\tau}_i^{e} d\Gamma
$$

(3.4.21)

where so-called dispersion tensor $D$ is defined by

$$D_{ijmn}(x, t) = \varepsilon^2 \rho^e \left\{ h_{ij}^W(x, y, t) \tilde{h}_{mn}^{\omega}(x, y, t) \right\}_{\omega}$$

(3.4.22)

Integrating by parts the first term in (3.4.21) and imposing arbitrariness of $w^e$ yields the following strong form of the coarse-scale problem

$$
\frac{\partial}{\partial x_j} \sigma_{ij} + \zeta^2 D_{ijkl} \tilde{\varepsilon}_{kl}^{e} - \rho^e \ddot{u}_i^{e} = 0 \quad \text{on} \quad \Omega
$$

$$
\sigma_{ij} + \zeta^2 D_{ijkl} \tilde{\varepsilon}_{kl}^{e} n_j = \tilde{\tau}_i^{e} \quad \text{on} \quad \partial\Omega
$$

(3.4.23)

Equation (3.4.23) suggests redefinition of the coarse-scale stress for high frequency dynamic problems as

$$\sigma_{ij}^{e} = \sigma_{ij} + \zeta^2 D_{ijkl} \tilde{\varepsilon}_{kl}^{e}$$

(3.4.24)

### 3.4.3. The Unit Cell Problem

The effect stress wave propagating in a unit cell will be introduced via inertia-induced strain $\varepsilon_{kl}^{e}$, which is assumed to be proportional to the material density

$$\varepsilon_{kl}^{e}(x, y, t) = \frac{\rho y}{\rho^e} f_{kl}^{e}(x, t)$$

(3.4.25)

where the coarse-scale function $f_{mn}^{e}(x, t)$ is assumed to depend on $\tilde{\varepsilon}_{kl}^{e}$ so that in absence of $\tilde{\varepsilon}_{kl}^{e}$, $f_{mn}^{e} \equiv 0$. In other words, inertia acts as an eigenstrain, which changes the shape and/or volume of the material element.

We further consider constitutive relation (3.4.1) expressed in term of instantaneous constitutive tensor $L^{e}$ as
\[ \dot{\sigma}_{ij}^f(x,t) = L_{ijkl}^f(x,t) \dot{e}_{ij}^f(x,t) \] (3.4.26)

Assuming small deformations (or co-rotational frame), the rate form of the fine-scale problem (3.4.19) is given by

\[ \dot{\sigma}_{ij}^{f,r} = 0. \] (3.4.27)

Consider now decomposition of the symmetric fine-scale velocity gradient \( \dot{u}_{ij}^{(1)}(x,y,t) \) into two parts. One that is driven by the coarse-scale strain; the other that is governed by the function that depends on the coarse-scale acceleration \( f_{mn}^x x,t \)

\[ \dot{u}_{ij}^{(1)}(x,y,t) = \hat{H}_{ij}^{kl}(x,y,t) \dot{\varepsilon}_{kl}^c(x,t) + \varepsilon_{ij}^c(x,y,t) + \zeta h_{mn}^{du}(x,y,t) f_{mn}^x(x,t) \] (3.4.28)

where \( \hat{H}_{ij}^{kl}(x,y,t) \) is \( y \)-periodic tensor, which depends on both the linear and nonlinear material behavior.

Substituting (3.4.28) into (3.4.6), the fine-scale strain rate \( \dot{\varepsilon}_{kl}^f x,y,t \) is given by

\[ \dot{\varepsilon}_{kl}^f x,y,t = I_{klmn} + \hat{H}_{klmn}^x x,y,t + \left( \frac{\rho}{\rho^e} I_{klmn} + \zeta h_{mn}^{du} x,y,t \right) f_{mn}^x(x,t) \] (3.4.29)

Further inserting (3.4.29) into (3.4.26) and (3.4.27) and requiring it to be satisfied for arbitrary coarse-scale fields \( \dot{\varepsilon}_{kl}^c \) and \( f_{mn}^x \) yields the two influence functions problems

\[ \begin{bmatrix} L_{ijkl} y_t \left( I_{klmn} + \hat{H}_{klmn}^x x,y,t \right) \right]_{y_j} = 0 \] (3.4.30)

Equation (3.4.30)a is a classical nonlinear quasi-static unit cell problem (see for instance [92]). It will be further reformulated. We will refer to equation (3.4.30)b as a quasi-dynamic unit cell problem to reflect the fact that the inertia term is represented implicitly via the eigenstrain term. Observing the two equations in (3.4.30) it can be seen that the influence functions, \( \hat{H}_{ij}^{kl}(x,y,t) \) and \( h_{mn}^{du} \), are related by

\[ \zeta h_{kq}^{mn}(x,y,t) x,y,t = \hat{H}_{kq}^{mn}(x,y,t) + \frac{\Delta \rho}{\rho^e} I_{klmn} \] (3.4.31)

\[ \Delta \rho y = \rho^e - \rho y \]
and therefore only the quasi-static unit cell boundary value problem has to be solved, whereas \( \tilde{h}_{k}^{mn} \) can be subsequently computed from (3.4.31)a.

We now focus on reformulation and solution of the quasi-static unit cell problem (3.4.30)a. For the quasi-static unit cell problem, the fine-scale displacements

\[
\dot{u}_{i}^{(1)}(x,y,t) = H_{i}^{kl}(x,y,t)\dot{e}_{kl}(x,t)
\]

(3.4.32)
can be rewritten as

\[
u_{i}^{(1)}(x,y,t) = H_{i}^{kl}(y)\dot{e}_{kl}(x,t) + f_{j}^{\mu}(x,y,t); \quad f_{j}^{\mu} = f_{j}^{\mu}(\mu^{'})
\]

(3.4.33)

where \( H_{i}^{kl}, f_{j}^{\mu} \) are \( y \)-periodic tensor functions corresponding to the coarse-scale strain \( \varepsilon^{\varepsilon} \) and eigen strain \( \mu^{\varepsilon} \) dependent responses, respectively, such that \( f_{j}^{\mu} = 0 \) for \( \mu^{'}, \theta \) . Comparing the incremental form of (3.4.33) with its the rate form (3.4.32), \( \dot{H}_{i}^{kl} \) can be approximated as

\[
\dot{H}_{i}^{kl}(x,y,t) \approx H_{i}^{kl}(x,y) + \frac{\partial f_{j}^{\mu}}{\partial \varepsilon_{kl}}(x,y,t)
\]

(3.4.34)

where for second order accuracy the derivative in (3.4.34) is computed at the mid-step. Combining the fine-scale displacement expression (3.4.33) with strain decomposition (3.4.6), constitutive relation (3.4.1)b and fine-scale equilibrium (3.4.19) yields

\[
\{ L_{ijkl}^{\varepsilon}(x)\left[ I_{kln} + H_{k(y)}^{mn}(x,y) \right] \}_{ij} \dot{\varepsilon}_{mn}(x,t)
\]

\[
\{ L_{ijkl}^{\varepsilon}(x)\left[ f_{(k,l)}^{\mu}(x,y,t) - \mu_{j}^{\mu}(x,y,t) \right] \}_{ij} = 0
\]

(3.4.35)

Further requiring equilibrium equation (3.4.35) to be satisfied for arbitrary coarse-scale strain and eigenstrains yields

\[
\{ L_{ijkl}^{\varepsilon}(x)\left[ I_{kln} + H_{k(y)}^{mn}(x,y) \right] \}_{ij} = 0
\]

\[
\{ L_{ijkl}^{\varepsilon}(x)\left[ f_{(k,l)}^{\mu}(\mu^{\varepsilon}) - \mu_{j}^{\mu}(x,y,t) \right] \}_{ij} = 0
\]

(3.4.36)

Consider now an additive decomposition of \( \tilde{h} \) into constant and variable functions in \( (x,t) \), denoted by \( h(x,y) \) and \( k(x,y,t) \), respectively

\[
\tilde{h}_{i}^{mn}(x,y,t) = \frac{1}{\varepsilon} \left( h_{i}^{mn}(y) + k_{i}^{mn}(x,y,t) \right)
\]

\[
\left< h_{i}^{mn}(y) \right>_{\varepsilon} = 0; \quad \left< k_{i}^{mn}(x,y,t) \right>_{\varepsilon} = 0
\]

(4.3.7)
where \( h \) and \( k \) are of order \( O \ \zeta \), and \( h \sim O \ 1 \), so the dispersion coefficient (3.4.22) has a quadratic dependence on the microstructural size, i.e. \( D \sim O \ \zeta^2 \).

Substituting (3.4.37) into (3.4.31) and (3.4.33) and assuming linear material, \( t^{\mu} = 0 \), yields the relation between \( h \) and \( H \).

\[
h_{i(y,y)}^{kl}(y) = H_{i(y,y)}^{kl}(y) + \frac{\Delta \rho(y)}{\rho^e} I_{ol}\quad (3.4.38)
\]

The tensor function \( k \) follows from

\[
k_{i}^{mn} = \frac{\partial \Delta f_{i}^{\mu}}{\partial \Delta \varepsilon_{mn}^{e}} = \frac{\partial \Delta f_{i}^{\mu}}{\partial \Delta \mu_{ij}^{e}} \frac{\partial \Delta \mu_{ij}^{e}}{\partial \Delta \varepsilon_{mn}^{e}}\quad (3.4.39)
\]

provided that equation (3.4.36)b can be solved for \( \frac{\partial \Delta f_{i}}{\partial \Delta \mu_{ik}^{e}} \). Note that the derivative \( \frac{\partial \Delta \mu_{ik}^{e}}{\partial \Delta \varepsilon_{mn}^{e}} \) can be computed from the constitutive relation. Details will be given in Section 3.4.5.

### 3.4.4. Linear Model Problem

Consider a one-dimensional unit cell problem (Figure 3.4.1) consisting of two elastic phases \( \rho_1, E_1 \) and \( \rho_2, E_2 \); \( \alpha_1 \) and \( \alpha_2 \) are the corresponding volume fractions such that

\[
\alpha_1 + \alpha_2 = 1.
\]

![Figure 3.4.1. The 1D model unit cell](image)

The quasi-dynamic unit cell problem (3.4.30)b for the linear model problem is given by

\[
E \ y \left( \frac{\rho \ y}{\rho^e} + h_{y} \ y \right) = 0 \quad (3.4.40)
\]

A closed-form solution of (3.4.40) is
\[ h \cdot y = \begin{cases} -\alpha_1 \Lambda(y + l) & -l \leq y < -\alpha_1 l \\ \alpha_2 \Lambda y & -\alpha_1 l \leq y \leq \alpha_1 l \\ -\alpha_1 \Lambda(y - l) & \alpha_1 l < y \leq l \end{cases} \quad l^{\text{ext}} = 2l \]  

(3.4.11)

where \( \Lambda \) is the \textit{normalized acoustic impedance variation} given by

\[ \Lambda = \frac{E_x \rho_x - E_z \rho_z}{\rho^* (\alpha_1 E_x + \alpha_2 E_z)} \]  

(3.4.12)

The dispersion coefficient (3.4.22) for the model problem is given by

\[ D = \frac{1}{12} \rho^* (\alpha_1 \alpha_2) \Lambda^2 \left( l^{\text{ext}} \right)^2. \]  

(3.4.33)

It can be seen that there are two major factors affecting the dispersion coefficient: (i) the square of the unit cell size \( l^{\text{ext}} \) in the physical domain and (ii) the square of the normalized impedance variation \( \Lambda \). Incidentally, the dispersion coefficient in (3.4.33) is identical to the one obtained by other formulations [5],[59-63].

The resulting strong form of the coarse-scale problem is given by

\[ E^{*} \frac{d^2 u^*}{dx^2} + D \frac{d^2 u^*}{dx^2} = \rho^* \ddot{u}^*, \]  

(3.4.44)

where \( E^* = \left( E(y) \left( 1 + H_{\gamma}(y) \right) \right)_0 = E_x E_z / (\alpha_1 E_x + \alpha_2 E_z) \).

To quantify the dispersion \( D \), consider harmonic wave \( u^* = u_0 e^{i(y-x)} \) and substitute it into (3.4.44), which yields

\[ -E^{*} + D k^2 c^2 = -\rho^* c^2 \]  

(3.4.45)

from which the phase velocity speed \( c \) and angular frequency \( \omega = kc \) are determined

\[ c = \sqrt{\frac{E^{*}}{\rho^* + k^2 D}}, \quad \omega = \frac{k^2 E^{*}}{\rho^* + k^2 D} \]  

(3.4.46)

Note that due to appearance of the dispersive coefficient the wave speed depends on wave number \( k \) caused by wave reflections from the interfaces of dissimilar materials. It can be seen that dispersion effectively increases material density for high wave numbers and thus slows down propagation of high frequency waves.

The exact dispersion equation for the model has been derived by many authors (see for instance [93, 94])

\[ \cos (k l) = \cos (k_1 l_1) \cos (k_2 l_2) - \frac{1}{2} \left( \frac{z_1}{z_2} + \frac{z_2}{z_1} \right) \sin (k_1 l_1) \sin (k_2 l_2) \]  

(3.4.47)
where \( l_i = \alpha l_i \), \( z_i = \sqrt{E_i \rho_i} \), \( k_i = \sqrt{\rho_i / E_i} \omega \).

Figure 3.4.2 depicts the wave dispersion curves for the model problem with the following material parameters: \( \alpha = 0.2 \), \( E_2 / E_1 = 100.0 \), \( \rho_2 / \rho_1 = 3.0 \), \( z_2 / z_1 = 17.32 \), \( D = 0.0446 \).

![Dispersion curves for model problem](image)

Figure 3.4.2. Dispersion curves for model problem

It can be seen that for the unit cell size 5 times smaller than the wave length there is little dispersion. The dispersive formulation provides considerable improvement over nondispersive theory for larger unit cells. Yet, the quality of the solution (in comparison to the exact solution) predicted by the above dispersive formulation degrades with increase in the unit cell size.

### 3.3.5. Residual-free Dispersive Homogenization

Consider the following definition of \( \mu \)

\[
 f^\mu_i (x, y, t) = \int_{\Theta} g_i^{kl} (y, \tilde{y}) \mu_{kl}^\prime (x, \tilde{y}, t) d\tilde{\Theta} \tag{3.48}
\]

which corresponds to the fine-scale displacement decomposition [95-98]

\[
 u_i^{(1)} (x, y, t) = H_i^{kl} (y) \epsilon_{kl}^r (x, t) + \int_{\Theta} g_i^{kl} (y, \tilde{y}) \mu_{kl}^\prime (x, \tilde{y}, t) d\tilde{\Theta} \tag{3.49}
\]

where \( g_i^{kl} \) is \( y \)-periodic tensor function.

In the reduced order homogenization approach [95-98], the eigenstrain representing inelastic deformation, is discretized as a piecewise function over volume partitions \( \theta^{(\sigma)} \)
\[ \mu' (x,y,t) = \sum_{a=1}^{n} N^{(a)} (y) \mu^{(a)} (x,t) ; \quad \mu^{(a)} (x,t) = \left\{ \mu' (x,y,t) \right\}_{a \in a}, \] (3.450)

\[ N^{(a)} (y) = \begin{cases} 1 & y \in \Theta^{(a)} \\ 0 & y \notin \Theta^{(a)} \end{cases} \bigcup_{a=1}^{n} \Theta^{(a)} = \Theta ; \bigcap_{a=1}^{n} \Theta^{(a)} = \emptyset \]

Substituting (3.450) into (3.449) and introducing \( y \)-periodic tensor \( S_{i}^{kl(a)} (y) \) yields

\[ u_{i}^{(1)} (x,y,t) = H_{i}^{kl} (y) e_{st}^{(x)} (x,t) + \sum_{a=1}^{n} S_{i}^{kl(a)} (y) \mu_{is(t)}^{(a)} (x,t) \]

\[ S_{i}^{kl(a)} (y) = \int_{\Theta} S_{i}^{kl} (y,\tilde{y}) N^{(a)} (\tilde{y}) d\Theta \] (3.451)

\[ f_{i}^{\mu} (x,y,t) = \sum_{a=1}^{n} S_{i}^{kl(a)} (y) \mu_{is(t)}^{(a)} (x,t). \]

The resulting constitutive relation (3.41)b is given

\[ \sigma_{j}^{(x,y,t)} = L_{ijkl} (y) \left( I_{klmn} + H_{n,\{k,\gamma\}}^{mn} (y) \right) e_{ms}^{(x)} (x,t) + \sum_{a=1}^{n} L_{ijkl} (y) \left( S_{n,\{k,\gamma\}}^{mn(a)} (y) - I_{klnm}^{(a)} (y) \right) \mu_{mn}^{(a)} (x,t). \] (3.452)

Here, \( L_{ijkl} (x,y) = L (y) \) and \( 1^{(a)} (y) = N^{(a)} (y) \). Integrating (3.452) over the unit cell domain yields coarse-scale stress (3.48)c

\[ \sigma^{e} (x,t) = \bar{L} (x) e^{(x,t)} + \sum_{a=1}^{n} \bar{A}^{(a)} (x) \mu^{(a)} (x,t) \]

\[ \bar{L}_{ijkl}^{mn} (x) = \left\{ L_{ijkl} (y) \left( I_{klmn} + H_{n,\{k,\gamma\}}^{mn} (y) \right) \right\}_{\Theta} \]

\[ \bar{A}_{ijkl}^{mn} (x) = \left\{ L_{ijkl} (y) \left( S_{n,\{k,\gamma\}}^{mn(a)} (y) - I_{klnm}^{(a)} (y) \right) \mu_{mn}^{(a)} (x,t) \right\}_{\Theta}. \] (3.453)

Substituting (3.451)c into (3.36)b and assuming arbitrariness of eigenstrain \( \mu^{(a)} \) yields the boundary value problem for the eigenstrain influence function

\[ \left[ L_{ijkl} S_{k,\{l,\gamma\}}^{mn(a)} (y) - I_{klnm}^{(a)} (y) \right]_{\Theta} = 0 \] (3.454)

subjected to periodicity and normalization conditions on \( S^{(a)} \). Subsequently, the influence function \( k \) in (3.39) is given by

\[ k_{ij}^{mn} (x,y,t) = \sum_{a=1}^{n} S_{i}^{kl(a)} (y) \frac{\partial \Delta \mu^{(a)}_{ij} (x,t)}{\partial \Delta e_{ms}^{(x)} (x,t)} \] (3.455)

Finally, the dispersion coefficient (3.22) can be decomposed into linear and nonlinear parts, \( D = D^{lin} + D^{nonlin} \), defined as
\[
\left(D_{ijm}^{lin}\right)^{lin} = \rho^c \left\{ h^{ij}_{mm} \right\}_0; \\
\left(D_{ijm}^{nonlin}\right)^{nonlin} = \rho^c \left[ \left\{ k^{ij}_{mm} \right\}_0 + \left\{ h^{ij}_{mm} \right\}_0 + \left\{ k^{ij}_{sm} \right\}_0 \right].
\] 

(3.4.56)

For implementation purpose, it is convenient to express the nonlinear dispersion coefficient as

\[
\left(D_{ijm}^{nonlin}\right)^{nonlin} = \sum_{a=1}^\infty \sum_{\beta=1}^\infty \frac{\partial \Delta \eta_{\mu_{ijm}}^{(a)}}{\partial \Delta \epsilon_{\alpha_{mm}}} R_{\alpha_{\beta}}^{(a\beta)} + \sum_{a=1}^\infty Q_{\beta_{\alpha}}^{(a\alpha)} \frac{\partial \Delta \eta_{\mu_{ijm}}^{(a)}}{\partial \Delta \epsilon_{\alpha_{mm}}} + \sum_{a=1}^\infty Q_{\beta_{\alpha}}^{(a\alpha)} \frac{\partial \Delta \eta_{\mu_{ijm}}^{(a)}}{\partial \Delta \epsilon_{\alpha_{mm}}}
\]

(3.4.57)

\[R_{\alpha_{\beta}}^{(a\beta)} = \rho^c \left\{ s^{(a\beta)}(x) \right\}_0; \quad Q_{\beta_{\alpha}}^{(a\alpha)} = \rho^c \left\{ h^{(a\alpha)}(x) \right\}_0.\]

Note that tensor coefficients \(D^{lin}, R^{(αβ)}, Q^{(α)}\) and the overall properties \(\overline{L}, \overline{A}^{α}\) are computed prior to the coarse-scale analysis.

**3.3.6. Residual-free Unit Cell Problem**

Let us define an average strain and stress over partition \(\Theta^β\)

\[\varepsilon^{(β)}_i(x, t) = \left\{ \varepsilon^{(β)}_i(x, y, t) \right\}_{q_{t}^{(β)}}; \quad \sigma^{(β)}_i(x, t) = \left\{ \sigma^{(β)}_i(x, y, t) \right\}_{q_{t}^{(β)}} \]

(3.4.58)

Substituting (3.4.51)a and (3.4.6)a into (3.4.58) yields

\[\varepsilon^{(β)}_i(x, t) = E^{(β)}_i(x, t) \varepsilon^{(β)}_m(x, t) + \sum_{\alpha=1}^{\infty} P^{(β)}_\alpha(x) \mu^{(β)}_\alpha(x, t)\]

\[E^{(β)}_i = \left\{ I_{ijm} + H^{(β)}_{(i, j)} \right\}_{q_{t}^{(β)}}; \quad P^{(β)}_\alpha = \left\{ s^{(β)}_{\alpha} \right\}_{q_{t}^{(β)}} \]

(3.4.59)

where the tensor coefficients \(E^{β}, P^{β}\) are computed from (3.4.54) prior to the solution of the coarse-scale problem.

Applying the averaging operator \(\left\{ \right\}_{q_{t}^{(β)}}\) to the stress-strain relation (3.4.1)b and exploiting the fact that \(L^{(β)}\) is constant over \(\Theta^β\) gives

\[\mu^{(β)}_i(x, t) = \varepsilon^{(β)}_i(x, t) - M^{(β)}_{ijkl} \sigma^{(β)}_{ij}(x, t)\]

\[\frac{\partial \Delta \eta^{(β)}_{\mu_{ijkl}}}{\partial \Delta \epsilon^{(β)}_{\alpha_{mm}}} = I_{ijkl} - M^{(β)}_{ijkl} \frac{\partial \Delta \sigma^{(β)}_{\mu_{i}}}{\partial \Delta \epsilon^{(β)}_{ijkl}} \]

(3.4.60)

where \(M^{β}\) is elastic compliance (or inverse of \(L^{β}\)) of phase partition \(β\).

The an incremental form of the reduced order unit cell problem follows from (3.4.59).
\[ r_{ij}^{(\rho)} \left( \Delta \varepsilon_{mn}^{(\rho)} \right) = \Delta \varepsilon_{ij}^{(\rho)} - E_{ijm}^{(\rho)} \Delta \varepsilon_{mn}^{(\rho)} - \sum_{u=1}^{n} P_{uj}^{*m(u\mu)} \Delta \mu_{mn}^{(\mu)} = 0 \] \tag{3.4.61}

\[ J_{ijmn} = \frac{\partial \Delta \varepsilon_{ij}^{(\rho)}}{\partial \Delta \varepsilon_{mn}^{(\rho)}} = I_{ijmn} \delta_{\rho \tau} - P_{ij}^{*i(\rho \tau)} \frac{\partial \Delta \mu_{ij}^{(\mu)}}{\partial \Delta \varepsilon_{ij}^{(\rho)}} \] where \( \Delta \varepsilon' \) is computed by the coarse-solver, and \( \Delta \mu^{(\mu)} \) is a specified in (3.4.60) by the fine-scale constitutive law (see [95-98] for details).

The nonlinear dispersion coefficient in (3.4.57) follows from

\[ \frac{\partial \Delta \mu_{ij}^{(\mu)}}{\partial \Delta \varepsilon_{ij}^{(\rho)}} = \frac{\partial \Delta \mu_{ij}^{(\mu)}}{\partial \varepsilon_{ij}^{(\rho)}} \] \tag{3.4.62}

where the term in (3.4.62) follows from the solution of the residual-free unit cell problem (3.4.61) which gives

\[ E_{ijm}^{(\rho)} = \sum_{u=1}^{n} \left( I_{ijm}^{(\rho)} \delta_{\mu \nu} - P_{ij}^{*i(\rho \nu)} \frac{\partial \Delta \mu_{ij}^{(\mu)}}{\partial \varepsilon_{ij}^{(\rho)}} \right) \frac{\partial \Delta \varepsilon_{ij}^{(\rho)}}{\partial \varepsilon_{ij}^{(\rho)}} = \sum_{u=1}^{n} J_{ijm}^{(\rho \nu)} \frac{\partial \Delta \varepsilon_{ij}^{(\rho)}}{\partial \varepsilon_{ij}^{(\rho)}} \] \tag{3.4.63}

### 3.3.7. Nonlinear Model Problem

Consider the following nonlinear 1D model problem in Figure 3.3.1. Material parameters for the two phases are \( L^1 \rho^1 \), \( K^1 \) and \( L^2 \rho^2 \), \( K^2 \) where \( K^i \) is hardening parameter as defined in equation (3.4.67). Volume fractions for the two phases are equal and the unit cell length is \( l^{uc} = 2l \). In the following, we derive a closed-form dispersion coefficient (3.4.56) for the model problem.

Solving the fine scale problems (3.4.40), (3.4.54) yields

\[ \tilde{\zeta} \hat{h} \ y = \begin{cases} - \lambda + C \ (y + l) & - l \leq y < -l / 2 \\ \lambda + C \ y & -l / 2 \leq y \leq l / 2 \\ - \lambda + C \ (y - l) & l / 2 < y \leq l \end{cases} \]

\[ \lambda = \frac{L^2 \rho^2 - L^1 \rho^1}{\rho^c \ (L^1 + L^2)}; \quad C = \frac{\partial \Delta \mu^1}{\partial \Delta \varepsilon^1} - \frac{\partial \Delta \mu^2}{\partial \Delta \varepsilon^2} \] \tag{3.4.64}

\[ b^{(1)} = \frac{L^1}{L^1 + L^2}; \quad b^{(2)} = \frac{L^2}{L^1 + L^2} \]

Solution of the residual-free equation (3.4.63) gives (3.4.62) from which the coefficient \( C \) can be found. Note that if \( \frac{\partial \Delta \sigma^{\alpha}}{\partial \Delta \varepsilon^{\alpha}} = 0 \) then \( C = 0 \), otherwise it is
\[ C = \frac{2b^{(1)}b^{(2)} \phi^{(1)} - \phi^{(2)}}{1 - b^{(1)}\phi^{(1)} - b^{(2)}\phi^{(2)}} \quad \phi^{(\beta)} = \frac{\partial \Delta \mu^{(\beta)}}{\partial \Delta \varepsilon^{(\beta)}}, \quad (3.4.65) \]

The resulting dispersion coefficient is given by
\[ D = \rho^c \left( \xi \frac{h}{2} \right) = \frac{\rho^c}{48} \lambda + C^2 \left[ \lambda^2 - 1 \right]. \quad (3.4.66) \]

Now, consider the constitutive behavior described by the exponential law [17]
\[ \sigma^{(\beta)} = \exp \left[ \left( K^{(\beta)} \varepsilon^{(\beta)} - 1 \right) L^{(\beta)} \right] = 1. \quad (3.4.67) \]

The resulting eigenstrain field (3.4.60) is given by
\[ \mu^{(\beta)} = \varepsilon^{(\beta)} + 1 - \exp \left[ K^{(\beta)} \varepsilon^{(\beta)} \right] \quad \frac{\partial \mu^{(\beta)}}{\partial \varepsilon^{(\beta)}} = 1 - K^{(\beta)} \sigma^{(\beta)} + 1 \]
\[ \phi^{(\beta)} = \left. \frac{\partial \Delta \mu^{(\beta)}}{\partial \Delta \varepsilon^{(\beta)}} \right|_{\varepsilon^{(\beta)} = 0} \approx \left. \frac{\partial \mu^{(\beta)}}{\partial \varepsilon^{(\beta)}} \right|_0 = 1 - K^{(\beta)} \sigma^{(\beta)} + 1 \quad (3.4.68) \]

For \( \partial \Delta \sigma^a / \partial \Delta \varepsilon^a \neq 0 \), the coefficient \( C \) is
\[ C = \frac{K^{(2)} \sigma^{(2)} + 1 - K^{(1)} \sigma^{(1)} + 1} {K^{(2)} \sigma^{(2)} + 1 + K^{(1)} \sigma^{(1)} + 1}. \quad (3.4.69) \]

Exploiting the traction continuity condition (3.4.2) \( a^1 = \sigma^2 \) yields
\[ C = \frac{K^{(2)} - K^{(1)}}{K^{(2)} + K^{(1)}}, \quad \lambda + C = \frac{\rho^c K^{(2)} - \rho^p K^{(1)}}{\rho^c K^{(2)} + K^{(1)}} \quad \lambda = \frac{\rho^c - \rho^p}{2\rho^c}. \quad (3.4.70) \]

Finally, a closed-form dispersion coefficient (3.4.66) for the model problem is given by
\[ D = \frac{1}{48\rho^c} \left( \frac{\rho^c K^{(2)} - \rho^p K^{(1)}}{K^{(2)} + K^{(1)}} \right)^2 \quad (3.4.71) \]

### 3.3.8. Implicit and Explicit Formulations

Consider discretization of the coarse-scale displacement, test function and strain
\[ u^c = N d; \quad w^c = N e; \quad \varepsilon^c = B d \quad (3.4.72) \]

where \( N, B, d \) are the shape function matrix, its gradient and nodal displacement vector, respectively.
Discretizing the weak form (3.4.21) using finite element discretization (3.4.72) yields
\[ \mathbf{f}^{\text{int}} + \mathbf{m}^D \ddot{\mathbf{d}} + \mathbf{M} \dddot{\mathbf{d}} = \mathbf{f}^{\text{ext}} \] (3.4.73)
where
\[ \mathbf{f}^{\text{int}} = \int_B \mathbf{B}^T \mathbf{\sigma} \, d\Omega; \quad \mathbf{f}^{\text{ext}} = \int_{\partial\Omega'} \mathbf{N}^T \mathbf{T} \, d\Gamma; \quad \mathbf{M} = \rho^e \int_{\Omega'} \mathbf{N}^T \mathbf{N} \, d\Omega \] (3.4.74)
are the usual internal force, external force and consistent mass matrices and
\[ \mathbf{m}^D = \int_B \mathbf{B}^T \mathbf{D} \mathbf{B} \, d\Omega \] (3.4.75)
is the dispersion matrix.

It is interesting to point that lumping of dispersion matrix \( \mathbf{m}^D \) results in zero matrix and therefore the discrete system of equation
\[ \tilde{\mathbf{M}} \dddot{\mathbf{d}} + \mathbf{f}^{\text{int}} = \mathbf{f}^{\text{ext}} \]
\[ \tilde{\mathbf{M}} = \mathbf{M} + \mathbf{m}^D \] (3.4.76)
can be employed in the context of implicit integration methods only.

For explicit methods, the effect of dispersion has to be accounted for in the stress field (see (3.4.24))
\[ \tilde{\mathbf{f}}^{\text{int}} = \int_B \mathbf{B}^T \mathbf{\sigma} \, d\Omega \] (3.4.77)
\[ \tilde{\mathbf{\sigma}}^e = \mathbf{\sigma}^e + \mathbf{D} \mathbf{B} \dddot{\mathbf{d}} \]

The resulting acceleration in the explicit method follows from
\[ \dddot{\mathbf{d}} = \tilde{\mathbf{M}}^{-1} (\mathbf{f}^{\text{ext}} - \tilde{\mathbf{f}}^{\text{int}}) \] (3.4.78)
where \( \tilde{\mathbf{M}} \) is lumped (or diagonal) matrix. Note that acceleration \( \dddot{\mathbf{d}} \) appearing in (3.4.77) is taken from the previous increment.

Comparison of different approaches for implicit and explicit method are given in Section 2.4.9. For 3D implicit implementation, we used ABAQUS Standard with Hilbert-Hughes-Taylor integration method and user-defined element (UEL) subroutine to account for the dispersion (3.4.75) in the mass matrix. For 3D explicit solution, we used ABAQUS Explicit and VUEL subroutine to account for the dispersion in the internal force (3.4.77).

For linear coarse-scale elements the mass matrix has been lumped whereas for quadratic elements consistent mass matrix has been considered.
3.3.9. Nonlinear model problem

To demonstrate the performance of the proposed model we consider some numerical examples. In this section we will present 1d examples comparing performance of classical direct homogenization and proposed dispersive direct homogenization. In the next section we will consider 3d examples obtained by reduced order homogenization.

As first example, consider periodic 1d structure consisting of two alternating linear materials with parameters

\[ \alpha_1 = 0.2, \quad \frac{E_2}{E_1} = 100.0, \quad \frac{\rho_2}{\rho_1} = 3.0, \quad \frac{z_2}{z_1} = 17.32, \quad E_d = 0.0446 \]

is depicted on the Figure 3.4.3.

\[
\begin{align*}
\text{matrix} & \quad \text{fiber} & \quad \text{matrix}
\end{align*}
\]

Figure. 3.4.3. UC for periodic 1d structure consisting of two alternating materials.

Dispersive curve for this material was obtained previously in model problem Figure. 3.4.2, Figure. 3.4.4 depicts dynamics response for one-dimesional model problem. The total length of the medium is \( L = 1.0 \, m \). The thicknesses of materials are \( l_1 = 0.002 \, m \) and \( l_2 = 0.008 \, m \), respectively. The specimen is subjected to traction impact loading on the right \( q(t) = q_o a_o t^4 (t - T)^4 \left( 1 - h(t - T) \right) \), \( q_o = 500 E + 3 \, Pa \), \( T = 30 E - 6 \, sec \), \( H(t - T) \) is Heaviside step function, \( a_o \) is scaled such that \( 0 \leq q(t) \leq q_o \). The left face is fixed.
Figure 3.4.4. Comparison of displacement time history of the point with coordinates $x=0.5$, for $T=30\times 10^{-6}\text{ s}$. 

Figure 3.4.5 Comparison of displacement time history of the point with coordinates $x=0.5$, for $T=15.71\times 10^{-6}\text{ s}$

Figure 3.4.5 depicts dynamics response for one-dimensional model problem. The total length of the medium is $L = 1.0 \text{ m}$. The thicknesses of materials are $l_1 = l_2 = 0.01 \text{ m}$, respectively. The specimen is subjected to traction impact loading on the right
\[ q(t) = q_0 a_0 t^4 (t - T)^4 \left[ 1 - h(t - T)^4 \right] , \quad q_0 = 50E + 3 \text{ Pa} , \quad T = 15.71E - 6 \text{ sec} , \quad H(t - T) \text{ is Heaviside step function}, \quad a_0 \text{ is scaled such that } 0 \leq q(t) \leq q_0 . \text{ The left face is fixed.} \\

Material parameters: \rho_1 = \rho_2 = 8000 \text{ K g }/\text{ m}^3, \quad E_1 = 200 \text{ GPa}, \quad E_2 = 5 \text{ GPa}, \quad E_o = 0.06 .

These two pictures show that dispersive direct homogenization gives considerably better time history for displacements than classical direct homogenization.

Dispersive nature of the proposed model can be demonstrated very clearly on the example of a non-linear material. It is well known that in nonlinear dispersive media combination of dispersion and nonlinearity results in a soliton formation. Couple words about solitons. The solitary strain waves were the subject of active theoretical investigation since 1970s in works[45, 99, 100] to mention few. More detailed reviews can be found in[3, 47, 101]. Experimental observations of strain waves were documented only after 1988. Interestingly, solitons can be observed in homogeneous non-dispersive bars with variable cross section[47]. Additionally to theoretical interest to strain solitons as a new phenomena in solids, there were multiple attempts of practical utilization of this phenomena such as application to third order elastic moduli measurements, to non-destructive evaluation techniques, to fracture and strain elenry transitions etc.

In non-linear composites a similar phenomena can be observed: a long-wavelength pulse disintegrates into a series of solitary waves. These solitary waves(also known as stegotons[17, 102]) interact as solitons, passing through one another, but do not preserve their shape when propagate, instead the wave shape is constantly modulating while it propagates through the laminate, they also possess some scaling properties. The width of stegotons is only a few layers wide and depends on the impedance difference of the constituents and unit cell size. Solitary waves in periodic nonlinear laminates were first observed in[102] and their scaling properties were studied in work by LeVeque and Yong[17], they also proposed a homogenized model, which, however, has higher order spatial derivatives of stress.

We will test our dispersive model on the example of non-linear laminate. As before, consider a heterogeneous material with unit cell consisting of two elastic materials as shown of Figure 3.3.3, but now suppose that both, matrix and fiber materials have non-linear stress-strain relationship, assume exponential dependence for concreteness.
Figures 3.4.6 and 3.4.7 depict comparisons of DNS simulation and dispersive direct homogenization simulation for dynamic response of a nonlinear 1d composite structure subjected to a displacement impulse of the form

\[
u = \begin{cases}
\bar{u} \left( \frac{T_{\text{imp}}}{2\pi} \sin \left( \frac{2t\pi}{T_{\text{imp}}} \right) + t \right), & t < T_{\text{imp}}, \\
\bar{u}T_{\text{imp}}, & t \leq T_{\text{imp}}.
\end{cases}
\]

which is same as used in[17]. Figures show that proposed dispersive model adequately describes stegotons formation and their dependence on the unit cell size, \( T_{\text{imp}} = 20 \), \( \bar{u} = 0.2 \)

Figure 3.4.6. Comparison of DNS and MI solutions for stress wave propagation in 1d nonlinear periodic structure with UC=1.0.

Figure 3.4.7. Comparison of DNS and MI solutions for stress wave propagation in 1d nonlinear periodic structure with UC=2.0.
Contrary, the non-dispersive model fails to describe stegoton formation, Figure 3.4.8. Instead a shock wave is formed and then it turns over and splits on multiple waves having no physical meaning and results are independent of the unit cell size.

![Figure 3.4.8. Comparison of DNS and Homogenization without dispersion](image)

![Figure 3.4.9. Comparison of DNS(red), Dispersive model with dispersive term in mass(blue) and Dispersive model when acceleration is extrapolated (green).](image)

3.3.10. 3D Examples

Consider a bar containing 120 unit cells along its axis, aligned in x-direction as shown in Figures 3.4.10 and 3.4.11. The unit cell is a cube of size equal to one. Two types of unit cell microstructures are considered: layered (Figure 3.4.10) and fibrous (Figure 3.4.11) with fiber radius of 0.36. The former is considered with Poisson ratio equal zero to closely mimic the one-dimensional simulation results. The left face of the bar is fixed in the axial direction with one of the nodes fully constrained to eliminate rigid body motion. The right face of the bar is subjected to prescribed displacement pulse $\vec{U}_x(t)$, such that at
time \( t = 0 \), \( \bar{U}_x(0) = 0 \) and at time \( t = 20 \), \( \bar{U}_x(20) = -2 \) for layered microstructure and \( \bar{U}_x(20) = -1.2 \) for fibrous composite. Here non-dimensional values are used.

Material behavior is described by the exponential law with material parameters for each phase listed in Table 3.4.1. For the layered composite we consider Poisson’s ratio \( \nu = 0 \) to mimic the 1D problem, whereas for the fibrous composite, we use \( \nu = 0.23 \).

<table>
<thead>
<tr>
<th>Material</th>
<th>K</th>
<th>density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
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<td>1</td>
</tr>
<tr>
<td>Inclusion</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

**Table 3.4.1** Material parameters for layered composite

The reduced order dispersive formulation has been implemented in ABAQUS via user-defined 8 and 20 hexahedral elements with full or reduced integration, respectively. The size of the user-defined coarse-scale element is either equal to the unit cell size or half of it.

The reference solution is obtained by direct numerical simulation (DNS). A single-scale mesh is constructed using either linear tetrahedral elements (T) (see Figure 3.4.10b), which coincides with the unit cell mesh, or using linear hexahedral elements (H), (see Figure 3.4.10c).

![Figure 3.4.10](image)

**Figure 3.4.10.** Layered composite (colors denote different phases): (a) A reference mesh for direct numerical simulation (DNS); (b) dispersive coarse-scale mesh; (c) nondispersive coarse-scale mesh; (d) unit cell mesh.

The nondispersive homogenization solution was obtained using first order homogenization with model reduction [95-98]. Note that the proposed dispersive formulation coincides with the nondispersive solution when dispersion coefficient is zero. The nondispersive model can be implemented in ABAQUS as a user-defined material without the need for user-defined element.
Figure 3.4.11. Fibrous composite (colors denote different phases): (a) A reference hexahedral mesh for direct numerical simulation (DNS-H); (b) A reference tetrahedral mesh for direct numerical simulation (DNS-T), (c) nondispersive coarse-scale mesh; (d) unit cell mesh.

For the fibrous composite problem (Figure 3.4.11), the coarse-scale element was an 8-node hexahedral, with full integration; the mass matrix was lumped by row summation for explicit and implicit methods.

Comparison of nodal velocities as obtained with direct numerical simulation and dispersive homogenization models at times $t=40, 80, 120$ are shown in Figure 3.4.12. Figure 3.4.13 depicts the axial stress (top) and strain (middle) profiles at $t=120$ as well as velocity (bottom) profile at $t=102$ as obtained with direct numerical simulation (DNS), dispersive and nondispersive homogenization models. For the three models implicit integration scheme was employed.

Figure 3.4.12. Layered composite bar. Comparison of nodal velocities as obtained with direct numerical simulation and dispersive homogenization models at times $t=40, 80, 120$. 
Figure 3.4.13. Layered composite bar. Axial stresses (top), strains (middle) at t=120 and velocity (bottom) profiles at t=102 as obtained with direct numerical simulation (DNS), dispersive and nondispersive homogenization models.

It can be seen that the solution obtained by the dispersive model is in good agreement with the direct numerical simulation while the classical nondispersive model shows spurious oscillations. The difference in the displacement profile (not shown) between the dispersive and nondispersive models is very minor; however, it leads to visible difference in stress, strain and velocity profiles.
Results (see Figure 3.4.14) obtained by the implicit and explicit implementations for the dispersive homogenization model are in good agreement.

![Graph showing velocity profile](image)

**Figure 3.4.14.** Layered composite bar. Velocity profile at t=120 as obtained with dispersive homogenization method using implicit and explicit integration methods.

For fibrous composite, Figure 3.4.15 compares the velocity profile as obtained with a direct numerical simulation, dispersive and non-dispersive homogenization. The coarse-scale mesh is modeled with 20-node serendipity elements, one coarse-scale element per unit cell (see Figure 3.4.11c). Implicit integration method with consistent mass matrix has been used.

![Graph showing stress profile](image)

**Figure 3.3.15.** Fibrous composite bar at time t=120. Axial stress profiles as obtained with direct numerical simulation DNS, nondispersive and dispersive homogenization models.
It can be seen that dispersive homogenization model is in reasonable agreement with the DNS whereas dispersive homogenization model predicts spurious oscillations.

3.3.11. Summary of Low Frequency Model

A general purpose nonlinear dispersive continuum model has been developed using mathematical homogenization method. We show that the coarse-scale stress can be defined as a sum of the classical volume average of the fine-scale stress and additional term representing the effect of micro-inertia, i.e. the local motion of microstructure in the low-frequency range.

The proposed model can be considered as complimentary to the high frequency models [6], which will be considered in the next section. The computational overhead in accounting for the dispersion effect in either explicit or implicit scheme is very minor, and therefore the proposed model is superior from the computational cost of view to the models derived using higher order asymptotic homogenization that necessitates consideration of higher order spatial derivatives. In the long-wave limit the model reduces to the conventional homogenization model.

Our dispersive model predicted coarse-scale fields (velocity, stress) substantially more accurately than the classical non-dispersive model. We showed that in the low-frequency range our dispersive model gives correct dispersion curves for periodic linear medium. Another manifestation of the dispersive nature of the proposed model is its ability to predict formation and evolution of soliton-like waves in nonlinear periodic medium.

References


CHAPTER 4

COMPUTATIONAL CONTINUA

4.1. Introduction

Development of new materials in the past decade spurred renewed interest in nonlocal and generalized continuum theories. These generalizations of the classical local continuum description were conceived to account for subscale details in the continuum description and to deal with nonlocal nature of fracture and localization. Generalized and nonlocal continuum theories are equipped with material microstructure information in the form of enhanced kinematics, balance and constitutive equations or their nonlocal (integral) representation.

Generalized continuum models can be classified into two main categories [1]: higher-grade continua and higher-order continua. Higher-grade continuum is characterized by higher-order spatial derivatives of the displacement field [2-8], whereas higher-order continuum is endowed with additional degrees-of-freedom independent of the usual translational degrees-of-freedom ranging from 3 rotational degrees-of-freedom in the Cosserat or polar continuum [9] to 12 degrees-of-freedom in the micromorphic continuum [10] and more in the so-called multiscale micromorphic continuum [11]. For background information, one can refer to review articles of Green and Naghdi[12], Askes and Aifantis[13] and monographs of Eringen [14], Erofeev[15], Maugin et al[16], Altenbach et al[17].

The link between the generalized continua, on one hand, and homogenization theories on the other, was shown to exist by several investigators [18-23]. The unit cell (UC) or the representative volume element (RVE) in the first-order homogenization theories [24-32] experiences (or is subjected to) a constant macroscopic deformation gradient independent of its size. This is an anomaly that becomes unacceptable as the UC size and/or strain gradients become sufficiently large. Higher-order theories [33, 34], on other hand, are equipped with a mechanism of subjecting the UC to ‘true’ macroscopic deformation. For example, in second-order theories, the macroscopic deformation gradient is idealized to vary linearly over the UC domain. Yet, despite the noteworthy performance in some localization problems [35-37], higher-order homogenization theories are not without shortcomings. From theoretical point of view, they still hinge on the two-scale integration scheme (see Equation (29)), which assumes infinitesimality of the UC although
the coefficients of the enriched coarse-scale continua depend on the size of the UC. Moreover, these theories require consideration of higher-order boundary conditions. While higher-order homogenization and generalized continua theories are equipped with enriched kinematics, which approximate the fine-scale deformation, they remain local in nature. Trostel [38] and Forest and Sievert [1] referred to these type of continuum models as local, whereas Bazant and Jirasek[39] classified both the generalized continua and nonlocal gradient models as weakly nonlocal. From computational point of view, the generalized continua models require consideration of additional degrees-of-freedom in combination with hybrid formulations, or alternatively, impose $C^1$ continuity requirement.

Various nonlocal theories of either integral or gradient type include a nonlocal kernel function whose support provides an internal length scale. The integral formulation reduces to the gradient type by truncating the series expansion of the nonlocality kernel[40]. By virtue of truncation, the nonlocal gradient models assume that nonlocal interactions are limited to close neighborhood. In the earlier works, nonlocality was introduced in the nonlocal approximations of fields and balance equations [41, 42] with later works focusing on nonlocality in internal variables [43, 44], which is closely related to the gradient plasticity theories[45]. The nonlocal theories reduce to those of the generalized continua or higher-order homogenization theory when the coarsescale problem size is much larger than the scale of heterogeneity. Selection of nonlocal kernels and the magnitude of the internal length scale are still controversial issues. It is also unclear how to construct nonlocal kernels that would have a sufficient degree of generality for a wide range of problems in heterogeneous media. For problems for which nonlocal interactions are well understood, computational difficulties related to higher-order continuity and boundary conditions can be partially alleviated by a reproducing kernel strain regularization of implicit gradient models [46]. Also, noteworthy are more recent variations of higher order and nonlocal continuum theories that bring certain microstructural information to the macroscopic equation of motion [47-51].

The primary goal of this chapter is to develop a coarse-scale continuum description, which is consistent with an underlying fine-scale description, for heterogeneities of finite size. The so-called Computational Continua (CC) developed here possesses the fine-scale features, but without introducing scale separation, which can be mathematically justified provided that the fine-scale structural details are infinitesimally small. From computational
point of view, the *Computational Continua does not require higher-order continuity, introduces no new degrees-of-freedom and is free of higher-order boundary conditions.*

The proposed continuum description features

(i) *nonlocal quadrature scheme* defined over *Computational Continua domain* consisting of disjoint union of computational UCs, positions of which are determined to reproduce the weak form of the governing equations on the fine scale; and

(ii) *the coarse-scale stress function*, which replaces the classical definition of coarse-scale stress being the average of fine-scale stresses and thus allowing to restate the governing equations of continua in terms of coarse-scale fields only. We distinguish between the classical notion of the UC defined in the rescaled (stretched) coordinate system positioned at the coarse-scale element Gauss quadrature points and the computational UCs defined in the physical domains whose locations are chosen to provide variational consistency with the fine-scale governing equations.

Consider a strong form of the boundary value problem on a composite domain $\Omega^\zeta_X$ with boundary $\partial \Omega^\zeta_X$ given as

$$\frac{\partial P_{ij}^\zeta \left( F^\zeta \right)}{\partial X_j} + B_i^\zeta = 0 \quad \text{on} \quad \Omega^\zeta_X$$

(4.1.1)

$$F_{ik}^\zeta = \delta_{ik} + \frac{\partial u_i^\zeta}{\partial X_k}$$

(4.1.2)

$$P_{ij}^\zeta \tilde{N}^\Omega_j = T_i^\Omega of \quad \partial \Omega^\zeta_X$$

(4.1.3)

$$u_i^\zeta = \bar{u}_i \quad \text{on} \quad \partial \Omega^\zeta_X$$

(4.1.4)

$$\partial \Omega^\zeta_X \cup \partial \Omega^\zeta_X = \partial \Omega^\zeta_X \cap \partial \Omega^\zeta_X = 0$$

(4.1.5)

where $P^\zeta$ denotes the First Piola-Kirchhoff stress tensor; $F^\zeta$ the deformation gradient; $B^\zeta$ and $T^{\alpha\zeta}$ the body force and traction vectors, respectively; $N^\Omega$ the unit normal to the boundary $\partial \Omega^\zeta_X$. Lower case subscripts $i$ and $j$ denote spatial dimensions except for subscripts $X$ and $x$ that refer to the initial and deformed configurations, respectively. The superscript $\zeta$ denotes existence of fine-scale features. Summation convention over repeated subscripts is employed except for the subscripts $X$ and $x$.

As a prelude to introducing the Computational Continua formulation, Section 4.2. establishes the relation between the generalized continua and the mathematical
homogenization theory and points out to their limitations. To our knowledge, this is an original attempt to derive the governing equations of the generalized continua for large deformation problems from asymptotic homogenization method. The computational continua formulation is presented in Section 4.3, which is self-contained. It includes the formulation of the coarse- and fine-scale problems, the nonlocal quadrature scheme defined over computational continua domain consisting of disjoint union of computational UC domains, the derivation of the coarse-scale stress function and the finite element discretization of the two-scale problem including treatment of weakly periodic boundary conditions. Numerical examples conclude the Chapter in Section 4.4. Conclusions and future research directions are discussed in Section 4.5.

4.2. Homogenization, Generalized Continua and their Limitations

In the mathematical homogenization theory various fields are assumed to depend on two coordinates: \( X \) - the coarse-scale coordinate in the initial domain \( \Omega_x \) and \( Y \) – the fine-scale coordinate in the initial unit cell \( \Theta_y \) domain. The two coordinates are related by \( Y = \frac{X}{\zeta^\alpha} \) with \( 0 < \zeta^\alpha \ll 1 \) and \( \alpha = 1 \) in the classical theory. The initial composite domain \( \Omega_x^\zeta \) is defined as a product space \( \Omega_x \times \Theta_y \).

Coordinates in the deformed (or current) configuration are \( x \) and \( y \) corresponding to the deformed composite domain \( \Omega_x^\zeta \), the coarse-scale domain \( \Omega_x \), and the unit cell domain \( \Theta_y \). Dependence of various fields on the two scale coordinates is denoted by \( P^\zeta = P(X,Y) \), \( B^\zeta = B(X,Y) \), \( T^{\Omega\zeta} = T^{\Omega}(X,Y) \) and \( u^\zeta(X) = u(X,Y) \).

In the mathematical homogenization theory, displacements are expanded as

\[
 u^\zeta(X) = u^0(X) + \zeta^{\alpha} u^1(X,Y) + \zeta^{2\alpha} u^2(X,Y) + O(\zeta^{3\alpha})
\]  (4.2.1)

where it is assumed that the size of the unit cell is infinitesimally small and therefore the leading-order displacement \( u^0(X) \) is considered to be constant over the unit cell domain. For large unit cell distortions, \( u^0(X) \) is no longer constant over the unit cell domain and therefore equation (4.2.1) has to be modified as described below.

We proceed by expanding \( u^0(X) \) in the Taylor’s series around the unit cell centroid \( X = \hat{X} \)
\[ u_i^o (X) = u_i^o (\hat{X}) + \frac{\partial u_i^o}{\partial X_j} (X_j - \hat{X}_j) + \frac{1}{2} \frac{\partial^2 u_i^o}{\partial X_j \partial X_k} (X_j - \hat{X}_j)(X_k - \hat{X}_k) + \cdots \] (4.2.2)

In the classical theory it is assumed that coarse-scale displacements \( u_i^o (X) \) and its various order derivatives are \( O(1) \) functions. Here we consider existence of high coarse-scale gradients

\[ \frac{\partial^{n+1} u_i^o}{\partial X_j \ldots \partial X_k} = O\left( \delta^{-\alpha n} \right) \] for \( n = 0, 1 \) and \( 0 < \alpha \leq 1 \) (4.2.3)

such that

\[ \frac{\partial u_i^o}{\partial X_j} (X_j - \hat{X}_j) = \ell' O(\delta^u) \quad ; \quad \frac{\partial^2 u_i^o}{\partial X_j \partial X_k} (X_j - \hat{X}_j)(X_k - \hat{X}_k) = \ell' O(\delta^{2u}) \] (4.2.4)

where \( \ell' \) is dimensional characteristic parameter. For the second order theory considered here we will assume that higher order terms in (4.2.2) remain of order \( O(\delta^{2u}) \) and higher.

From (4.2.3) and (4.2.4) follow that \( X_j - \hat{X}_j = \delta^u Y_j \) and thus \( u_i^o (X) \) can be written as

\[ u_i^o (\hat{X}, Y) = u_i^c (\hat{X}, Y) + \ell' O(\delta^{2u}) \] (4.2.5)

where \( u_i^c (\hat{X}, Y) \) is termed as a coarse-scale displacement given by

\[ u_i^c (\hat{X}, Y) = u_i^o (\hat{X}) + \delta^u \frac{\partial u_i^o}{\partial X_j} Y_j + \frac{1}{2} \delta^{2u} \frac{\partial^2 u_i^o}{\partial X_j \partial X_k} Y_j Y_k \] (4.2.6)

Similarly, higher order terms \( u_i^o (X, Y) \), for \( n \geq 1 \) are expanded around \( X = \hat{X} \) as

\[ u_i^o (X, Y) = u_i^c (\hat{X}, Y) + \delta^u \frac{\partial u_i^c}{\partial X_j} Y_j + \delta^{2u} \frac{1}{2} \frac{\partial^2 u_i^c}{\partial X_j \partial X_k} Y_j Y_k + \ell' O(\delta^{3u}) \] (4.2.7)

Substituting (4.2.6) and (4.2.7) into (4.2.1) gives

\[ u_i^c (X) = u_i^c (\hat{X}, \hat{Y}) = u_i^c (\hat{X}, Y) + \delta^u u_i^1 (\hat{X}, Y) + \]

\[ + \delta^{2u} \left\{ u_i^2 (\hat{X}, Y) + \frac{\partial u_i^1}{\partial X_j} Y_j \right\} + \ell' O(\delta^{3u}). \] (4.2.8)

Spatial derivative of \( f(\hat{X}, Y) \) is given by

\[ \frac{\partial f^c}{\partial X_j} = \frac{1}{\delta^u} \frac{\partial f(\hat{X}, Y)}{\partial Y_j}. \] (4.2.9)
The deformation gradient can be expressed as
\[ F_{ik}^0 = \delta_{ik} + \frac{\partial u_i^0}{\partial X_k} + 1 \frac{\partial u_{ik}}{\partial Y_i} = F_{ik}^0(\hat{X},Y) + \zeta^a F_{ik}^1(\hat{X},Y) + O(\zeta^{-2a}) \] (4.2.10)
where \( \delta_{ik} \) is Kronecker delta and
\[ F_{ik}^0(\hat{X},Y) = F_{ik}^c(\hat{X},Y) + F_{ik}^\alpha(\hat{X},Y) \] (4.2.11)
\[ F_{ik}^c(\hat{X},Y) = \delta_{ik} + \frac{\partial u_i^0}{\partial X_k} \] (4.2.12)
\[ F_{ik}^\alpha(\hat{X},Y) = \frac{\partial u_i^1(\hat{X},Y)}{\partial Y_k} \] (4.2.13)
\[ F_{ik}^1(\hat{X},Y) = \frac{\partial u_i^2}{\partial Y_k} + \frac{\partial u_i^1}{\partial X_k} \] (4.2.14)

In the present manuscript the First Piola-Kirchhoff stress \( P^i_j(F^\gamma) \) formulation is adopted due to its conjugacy with the deformation gradient. Expanding \( P^i_j(F^\gamma) \) around the leading order deformation gradient \( F_{ik}^0 \) yields
\[ P^i_j(F^\gamma) = P^i_j(F^0) + \zeta^a \frac{\partial P^i_j}{\partial F_{mn}^c} F_{mn}^1 + O(\zeta^{-2a}) \] (4.2.15)
\[ = P^i_j(\hat{X},Y) + \zeta^a P^i_j(\hat{X},Y) + O(\zeta^{-2a}) \]

Further expanding equation (4.2.15) in Taylor series around the centroid \( X = \hat{X} \) yields
\[ P^i_j(\hat{X},Y) = P^i_j(\hat{X},Y) + \frac{\partial P^i_j}{\partial X^k} \left(X_k - \hat{X}_k\right) + \zeta^a P^i_j(\hat{X},Y) + \nabla \left(\frac{\partial P^i_j}{\partial X^k} |_{X = \hat{X}} (X_k - \hat{X}_k)\right) + \ldots \] (4.2.16)

Substituting (4.2.16) into equilibrium equation (4.1.1) yields the two-scale residual equations
\[ r^i_j(\hat{X},Y) = \frac{\partial P^i_j}{\partial Y_j} = 0 \] (4.2.17)
\[ r^c_j(\hat{X},Y) = \frac{\partial P^i_j}{\partial X_j} + \frac{\partial P^i_j}{\partial Y_j} + B_j = 0 \] (4.2.18)
We now focus on the derivation of the weak form starting with a unit cell problem (4.2.17)a. Let $W_{\Theta_y \times \Omega_y}$ be the space of $C^n$ continuous weakly $Y$-periodic weight functions on $\Theta_y$ defined as

$$W_{\Theta_y \times \Omega_y} = \left\{ w^i \left( Y \cdot \hat{X} \right) \text{ defined in } \Theta_y \times \Omega_y, C^n(\Theta_y), \text{ weakly } Y - \text{periodic} \right\} \quad (4.2.18)$$

Multiplying (4.2.17)a by $w^i$ and integrating by parts yields the weak form of the unit cell problem

$$\int_{\Theta_y} \frac{\partial w^i}{\partial Y_j} P^i_j \left( \hat{X}, Y \right) d\Theta = 0 \quad \forall w^i \in W_{\Theta_y \times \Omega_y} \quad (4.2.19)$$

where we assumed weak periodicity of $P^i_j$ defined as

$$\int_{\Theta_y} w^i P^i_j \left( \hat{X}, Y \right) N^i_j d\Gamma = 0 \quad \forall w^i \in W_{\Theta_y \times \Omega_y} \quad (4.2.20)$$

We now turn to the derivation of the coarse-scale weak form. Let $\Psi(X,Y)$ be a two-scale function defined by interpolation form the unit cell centroids

$$\Psi(X,Y) = \sum_I \Psi(\hat{X}_I, Y) \varphi_I(X) \quad (4.2.21)$$

where $\hat{X}_I$ denotes the coordinates of the unit cell centroid $I$; and $\varphi_I(X) \in C^n(\Omega_x)$ possesses interpolation property $\varphi_I(\hat{X}_I) = \delta_{Ii}$.

We define a smooth coarse-scale residual $r^C(X,Y)$ as

$$r^C(X,Y) = \frac{\partial P^0_s(X,Y)}{\partial X_j} + \frac{\partial P^1_s(X,Y)}{\partial Y_j} + B^C(X,Y) \quad (4.2.22)$$

where

$$P^s_{ij}(X,Y) = \sum_I P^s_I \left( \hat{X}_I, Y \right) \varphi_I(X) \quad \text{for } s = 0,1 \quad (4.2.23)$$

The integral of the oscillatory two-scale function over composite domain $\Omega_x^\varepsilon$ is defined in the usual way as

$$\lim_{\varepsilon \to 0} \int_{\Omega_x^\varepsilon} \Psi(X,Y) \ d\Omega = \lim_{\varepsilon \to 0} \int_{\Omega_x^\varepsilon} \left( \frac{1}{|\Theta_y|} \int_{\Theta_y} \Psi(X,Y) d\Theta \right) d\Omega \quad (4.2.24)$$

To construct the coarse-scale weak form we define the space of $C^1(\Omega_x)$ continuous functions as

$$W_{\Omega_x} = \left\{ w^0 \text{ defined in } \Omega_x, w^0 \in C^1(\Omega_x), w^0 = 0 \text{ on } \partial \Omega_x^\varepsilon \right\} \quad (4.2.25)$$
and construct the coarse scale test function \( w^c(X,Y) \) as

\[
w^c(X,Y) = w^0(X) + \zeta^a \frac{\partial w^0_i(X)}{\partial X_j} Y_j
\]

(4.2.26)

The coarse-scale weak form is obtained by integrating the product of \( r^c(X,Y) \) and \( w^c(X,Y) \) over composite domain \( \Omega^c \), which yields

\[
\lim_{\zeta^c \to 0} \int_{\Omega^c} \frac{w^c_i(X,Y) r^c(X,Y) d\Omega}{\Theta^c} = \\
= \int_{\Theta^c} \left( \frac{1}{\Theta^c} \int_{\Theta^c} \left( w^0_i(X) + \zeta^a \frac{\partial w^0_i(X)}{\partial X_k} Y_k \right) \frac{\partial p^0_j(X,Y)}{\partial X_j} d\Theta \right) d\Omega + \\
+ \int_{\Theta^c} \left( \frac{1}{\Theta^c} \int_{\Theta^c} \left( w^0_i(X) + \zeta^a \frac{\partial w^0_i(X)}{\partial X_k} Y_k \right) \frac{\partial p^1_j(X,Y)}{\partial Y_j} d\Theta \right) d\Omega + \\
+ \int_{\Theta^c} \left( \frac{1}{\Theta^c} \int_{\Theta^c} \left( w^0_i(X) + \zeta^a \frac{\partial w^0_i(X)}{\partial X_k} Y_k \right) B_j(X,Y) d\Theta \right) d\Omega
\]

(4.2.27)

Denoting

\[
\bar{p}_j = \frac{1}{\Theta^c} \int_{\Theta^c} p^0_j d\Theta; \quad \bar{q}_{aj} = \frac{1}{\Theta^c} \int_{\Theta^c} p^0_a Y_j d\Theta
\]

(4.2.28)

\[
\bar{b}_j = \frac{1}{\Theta^c} \int_{\Theta^c} b_j d\Theta; \quad \bar{t}_j^i = \frac{1}{\Theta^c} \int_{\Theta^c} t^i_j d\Omega; \quad \bar{T}_j^i = p^\alpha N_j^i
\]

(4.2.29)

\[
\bar{b}_j = \frac{1}{\Theta^c} \int_{\Theta^c} b_j Y_j d\Theta; \quad \bar{T}_j^i = \frac{1}{\Theta^c} \int_{\Theta^c} t^i_j Y_j d\Omega
\]

(4.2.30)

and integrating the coarse-scale spatial derivatives of \( \bar{p}_j \) and \( \bar{q}_{aj} \) by parts yields the leading order coarse-scale weak form

\[
\int_{\Omega^c} \frac{\partial w^0_i}{\partial X_k} \bar{p}_j d\Omega + \zeta^a \int_{\Omega^c} \frac{\partial^2 w^0_i}{\partial X_k \partial X_k} \bar{q}_{aj} d\Omega = \\
= \int_{\partial \Omega^c} w^0_i \bar{T}_j d\Gamma + \int_{\Omega^c} w^0_i \bar{b}_j d\Omega + \zeta^a \int_{\partial \Omega^c} \frac{\partial w^0_i}{\partial X_k} \bar{T}_j d\Gamma + \zeta^a \int_{\Omega^c} \frac{\partial w^0_i}{\partial X_k} \bar{b}_j d\Omega
\]

(4.2.31)

where \( \partial \Omega^c \) is portion of the boundary where \( \bar{T}_j \) is prescribed. In the above we assumed weak \( Y \)-periodicity conditions of \( p^1_j \) and \( p^\alpha_j Y_j \)

\[
\int_{\partial \Omega^c} p^1_j N_j^\alpha d\Gamma = 0; \quad \int_{\partial \Omega^c} p^\alpha_j N_j^\alpha Y_j d\Gamma = 0
\]

(4.2.32)

In summary, we seek for the trial function \( u^c \in U_{\Omega^c \times \theta} \) where
\[
U_{\Omega_X \times \Theta_Y} = \begin{cases} 
\tilde{u} \text{ defined for } (X,Y) \in \Omega_X \times \Theta_Y, \text{ weakly } Y \text{-periodic}, \\
C^b(\Theta_Y) \text{ and } C^1(\Omega_X) \text{ in } \tilde{u} = \overline{u} \text{ on } \partial \Omega_X 
\end{cases}
\]

that satisfies the weak form of the coarse-scale problem (4.2.31) and the UC problem (4.2.19) subjected to the weak periodicity conditions (4.2.20) and (4.2.32).

Equation (4.2.31) defines the weak form of the second-grade continuum boundary value problem [36, 52]. The strong form of the higher order/grade continua can be obtained by appropriate integration by parts of the weak form (4.2.31). It involves higher-order derivatives and thus requires \(C^1\) continuity. The second-order continuum can be constructed by defining coarse-scale displacement gradients as independent fields and then requiring the two to be equal in the weak sense. While such a formulation alleviates computational difficulties arising from \(C^1\) continuity requirement, it introduces additional degrees-of-freedom and requires mixed or multi-field formulation [35]. At a more fundamental level, the two theories hinge on the two-scale integration scheme (4.2.24), which assumes infinitesimality of the UC.

### 4.3. Second-order computational continua

In this section, we develop a second-order continuum formulation that is free of the theoretical and the computational limitations discussed in the previous section. The so-called second-order computational continua to be derived hereafter will make no assumption about infinitesimality of the UC, will require \(C^0\) continuity only and will involve no additional degrees-of-freedom. Furthermore, we will make no assumption about scale decomposition, but will introduce a UC local coordinate system \(\chi\) in the physical UC domain, which is related to the stretched coordinate by \(\chi = \zeta^a Y\). Both the test and the trial functions will be decomposed into oscillatory weakly periodic functions and smooth coarse-scale functions. In addition to various mathematical homogenization theories, such a decomposition has been used in various local enrichment methods including enriched elements[53, 54], variational multiscale method [55], the s-version of the finite element method [56] with application to strong [57] and weak [58] discontinuities, the multigrid-like methods [59, 60] and the extended finite element method [61, 62].
4.3.1. Nonlocal quadrature

To construct the coarse-scale weak form, it is necessary to integrate functions on a composite domain $\Omega^c_x$ with finite size fine-scale details for which the two-scale integration scheme (4.2.24) is no longer valid. The trivial solution is to (4.2.24) by a sum of integrals over UC domains. However, such an integration scheme is not practical for problems involving numerous UCs. Furthermore, it would give rise to cumbersome integration over coarse-scale finite element domains whose boundaries do not coincide with UC boundaries. To circumvent these difficulties, we introduce the so-called nonlocal quadrature scheme by which the integration over composite domain $\Omega^c_x$ is replaced by integration over the so-called computational continua domain $\Omega^c_x$ consisting of a disjoint union [63] (sometimes called direct sum or free union) of computational unit cell (CUC) domains $\Theta_{x_i}$ denoted as

$$\Omega^c_x = \bigcap_{i=1}^{N} \Theta_{x_i}$$

where $x_i$ denotes the coordinates of centroid of the computational unit cell domain $\Theta_{x_i}$. Note that if $\Theta_{x_i} \cap \Theta_{x_j} = 0, \forall i \neq j$ then the disjoint union reduces to a regular union.

The nonlocal quadrature scheme is then defined as

$$\int_{\Omega^c_x} \Psi(X) d\Omega = \sum_{i=1}^{N} \int_{\Theta_{x_i}} \tilde{\omega}(\tilde{x}_i, \tilde{z}) \Psi(\tilde{x}_i, \tilde{z}) d\Theta$$

(4.2.35)

where $\tilde{\omega}(\tilde{x}_i, \tilde{z})$ is defined as

$$\tilde{\omega}(\tilde{x}_i, \tilde{z}) = \frac{J^c(\tilde{x}_i, \tilde{z}) W_i}{|\Theta_{x_i}|}$$

(4.2.36)

where $W_i$ denotes the nonlocal quadrature weight; $|\Theta_{x_i}|$ the volume of the computational unit cell domain $\Theta_{x_i}$; $J^c(\tilde{x}_i, \tilde{z})$ the Jacobean that maps a coarse-scale element into bi-unit cube (square, interval). $W_i$ and $\tilde{x}_i$ are chosen to exactly evaluate integrals (4.2.35) on the composite domain with integrand $\Psi(X)$ approximated by a polynomial of order $m$. The pair $(W_i, \tilde{x}_i)$ depend on the computational unit cell size relatively to the coarse-scale finite element size as will be subsequently discussed.
We first consider the nonlocal quadrature scheme for integrating smooth functions in one dimension followed by the generalization to multidimensions in the remaining of this section. Discussion about smoothness of $\Psi(X)$ is given in Section 4.3.2 (see Remark 4).

Consider a one-dimensional domain $[a,b]$ mapped into a parent element domain $[-1,1]$ as shown in Figure 4.3.1.

**Figure 4.3.1.** Nonlocal Quadrature: Physical (top) and parent element (bottom) domains. Unit cell domains are shown in the brackets. $\bar{X}_i, \zeta_i$ denote positions of quadrature points in the physical and parent element domains, respectively; $\Theta$ and $\Theta’ = \Theta / J’$ are the size of the unit cell in the physical and parent element domains, respectively; $J’ = (b - a) / 2$ is element Jacobean.

The goal is to find quadrature weights and sampling points that would exactly integrate polynomials of a given order. Applying the nonlocal quadrature scheme (4.2.35) to one-dimensional element domain yields

$$I’ = \int_{-1}^{1} J’ \Psi(\xi) ~ d\xi = \sum_{i=1}^{\tilde{N}} \frac{W_i}{\Theta} \int_{-\Theta/2}^{\Theta/2} J’ \Psi(\bar{X}_i) + \chi ~ d\chi$$

(4.2.37)

where $\tilde{N}$ is number quadrature points in the element domain. Applying element mapping to the unit cell domain yields

$$I’ = \sum_{i=1}^{\tilde{N}} \frac{W_i}{\Theta / J’} \int_{-\Theta/J’/2}^{\Theta/J’/2} J’ \Psi(\xi_i + \eta) ~ d\eta$$

(4.2.38)
Further denoting $\Psi' \xi = J' \Psi \xi$ and $\Theta' = \Theta / J'$ equation (4.2.37) can be rewritten as

$$I' = \int_{-1}^{1} \Psi' \xi \, d\xi = \sum_{i=1}^{N} \frac{W_i}{\Theta'} \int_{-\Theta'/2}^{\Theta'/2} \Psi' \xi_i + \eta \, d\eta$$  \hspace{1cm} (4.2.39)

Let us now approximate the integrand $\Psi' \xi$ by a polynomial function

$$\Psi' \xi = \sum_{j=1}^{\infty} \alpha_j \xi^{j-1}$$  \hspace{1cm} (4.2.40)

Substituting polynomial expansion (4.2.40) into the quadrature scheme (4.2.37) yields

$$I' = \sum_{i=1}^{N} \frac{W_i}{\Theta'} \int_{-\Theta'/2}^{\Theta'/2} \sum_{j=1}^{\infty} \alpha_j \xi_i + \eta \, d\eta$$  \hspace{1cm} (4.2.41)

A closed-form integration of the above yields

$$I' = \sum_{i=1}^{N} W_i \left( \alpha_1 + \alpha_2 \xi_i + \alpha_3 \left( \frac{\Theta_i}{12} + 1 \right) + \alpha_4 \left( \frac{\xi_i}{4} \right) + ... \right)$$

$$= \alpha_1 \sum_{i=1}^{N} W_i + \alpha_2 \sum_{i=1}^{N} W_i \xi_i + \alpha_3 \left( \frac{\Theta_i}{12} + \sum_{i=1}^{N} W_i \xi_i^2 \right) + \alpha_4 \left( \sum_{i=1}^{N} W_i \left( \frac{\xi_i^3}{4} \right) + ... \right)$$  \hspace{1cm} (4.2.42)

On the other hand, exact integration of (4.2.40) gives

$$I' = \int_{-1}^{1} \Psi' \xi \, d\xi = \int_{-1}^{1} \sum_{i=1}^{\infty} \alpha_i \xi^{i-1} = 2\alpha_1 + 0\alpha_2 + \frac{2}{3}\alpha_3 + 0\alpha_4 + ...$$  \hspace{1cm} (4.2.43)

Requiring the nonlocal quadrature to exactly integrate polynomials for arbitrary $\alpha_i$ yields nonlinear system of equations from which the quadrature weights and positions of the computational unit cells can be determined. For instance, for two-point nonlocal quadrature we get

$$\begin{bmatrix}
\xi_1 \\
\xi_2 \\
\xi_3 \\
\xi_4
\end{bmatrix}
\begin{bmatrix}
\xi_1 \\
\xi_2 \\
\xi_3 \\
\xi_4
\end{bmatrix}
=
\begin{bmatrix}
1 \\
1 \\
1 \\
1
\end{bmatrix}
\begin{bmatrix}
W_1 \\
W_2 \\
W_3 \\
W_4
\end{bmatrix}
= \begin{bmatrix}
2 \\
0 \\
2/3 \\
0
\end{bmatrix}$$  \hspace{1cm} (4.2.44)

which yields

$$\xi_{1,2} = \pm \sqrt{\frac{1}{3} - \frac{\Theta_i^2}{12}}; \quad W_{1,2} = 1$$  \hspace{1cm} (4.2.45)
Remark 1: As expected in the limit as $\Theta' \to 0$ the above reduces to the usual Gauss quadrature, hereafter to be referred as local quadrature. When the unit cell size is equal to one half of the element size, $\Theta' = 1$, we get $\xi_{1,2} = \pm 0.5$. As the unit cell size further increases the two sampling points move towards the origin, and when the size of the unit cell coincides with that of the element we get $\xi_{1,2} = 0$, which is equivalent to having one quadrature point in the middle of the interval with quadrature weight equal to 2. Note that while nonlocal one-point quadrature element maintains full rank (provided that the unit cell is fully integrated), it should be used only if the unit cell size is close to that of the element. Also, it can be seen that $\Theta' \leq 2$, i.e. the unit cell must be smaller than element.

Remark 2: For three-point nonlocal quadrature the weights quadrature points are

$$W_{1,3} = \frac{5}{3} \cdot \frac{4 - \Theta'}{48 + 7\Theta' - 40\Theta'^2} \quad \xi_{1,3} = \pm \frac{1}{2} \sqrt{\frac{48 + 7\Theta' - 40\Theta'^2}{5} \cdot \frac{4 - \Theta'}{4}}$$

$$W_2 = 2 - 2W_{1,3} \quad \xi_2 = 0$$

Note that when $\Theta' = 0$ we have $W_{1,3} = 5/9$ and $\xi_{1,3} = \pm 0.774596692$, which reduces to the local three-point Gauss quadrature. For $\Theta' = 1$ the three-point nonlocal quadrature reduces to two-point nonlocal quadrature with $W_{1,3} = 1, W_2 = 0$ and $\xi_{1,3} = \pm 0.5$. The three-point nonlocal quadrature should be limited to $\Theta' \leq 1$ to avoid negative values of weights.

Remark 3: The formula for nonlocal quadrature in multidimensions remains the same as defined by equation (4.2.35), but evaluation of sampling points and weights needs to be further addressed. For elements whose edges (faces in 3D) are parallel to those of the unit cell, position of quadrature points and weights in each space direction $a$ of the parent element $(\bar{W}_{a}, \bar{\xi}_{a})$ can be determined by $\Theta_{a}' = \Theta_{a} / J_{a}'$ where $\Theta_{a}$ and $J_{a}'$ are the length of the unit cell and one half of the element length along the axis $\bar{\xi}_{a}$, respectively. When edges (faces in 3D) are not parallel, it is necessary to define an effective unit cell domain $\Theta_{a}'$ as described below. Consider a quadrilateral element and a unit cell in the physical (left) and parent (right) element domains as shown in Figure 4.3.2.
Figure 4.3.2: Definition of the effective unit cell size in the parent element domain

Note that a rectangular CUC in the physical domain becomes distorted following element mapping. Thus, an effective rectangle (brick) CUC has to be defined whose edges (faces) are parallel to those of the parent element. Such an effective CUC can be determined to have the same centroid, the same area (volume) and the same ratio between the moments of inertia. An alternative to constructing quadrature scheme in multidimensions by tensor product of one-dimensional quadrature is to directly derive quadrature weights and sampling points in multidimensions. This can be accomplished by integrating the monomials in the Pascal triangle (pyramid) exactly and by the nonlocal quadrature scheme. This forms a system of non-linear equations for the unknown quadrature positions and weights that can be solved for each element in the preprocessing stage. We will elaborate on this variant in our future work.

4.3.2 Coarse-scale stress function

We now focus on derivation of the coarse-scale weak form. Consider the coarse-scale weak form

\[
\int_{\Omega_x} w^c \left( \frac{\partial}{\partial X_k} P_{ik}^\xi + B_i^\xi \right) d\Omega = 0
\]  

(4.2.46)

where the coarse-scale test function \( w^c \) is \( C^0 \) continuous on \( \Omega_x \) and satisfies homogeneous boundary conditions on \( \Omega_x \); for the second order theory considered here \( w^c \) is bi-linear on the computational unit cell \( \Theta_{x_j} \) and has computable first and second order derivatives at the centroid of the computational unit cell.
\[ w^c_i (\mathbf{X}_j, \mathbf{X}) = w^c_i (\mathbf{X}_j) + \frac{\partial w^c_i}{\partial \mathbf{X}_j} \mathbf{X}_j \mathbf{X}_k + \frac{1}{2} \frac{\partial^2 w^c_i}{\partial \mathbf{X}_j \partial \mathbf{X}_k} \mathbf{X}_j \mathbf{X}_k \]

Integrating by parts the divergence terms and then applying the nonlocal quadrature scheme yields

\[ \sum_{i=1}^{\tilde{N}} \int_{\tilde{\Omega}_i} \tilde{\omega} \tilde{\mathbf{X}}_j, \mathbf{X} \left( \frac{\partial w^c_i}{\partial \mathbf{X}_j} \right)_{\mathbf{X}_j} + \frac{\partial^2 w^c_i}{\partial \mathbf{X}_j \partial \mathbf{X}_k} \mathbf{X}_j \mathbf{X}_k \right) P_{ik}^c (\mathbf{X}_j, \mathbf{X}) d\Theta = \]

\[ = \int_{\partial \tilde{\Omega}_i} \tilde{\omega} \tilde{\mathbf{X}}_j, \mathbf{X} \left( T^o_i d\Gamma + \int_{\tilde{\Omega}_i} w^c_i \mathbf{X} \mathbf{B}^c_i d\Omega \right) \]

We now define the so-called coarse-scale stress function to address the computational challenge of integrating over unit cell domains \( \Theta, \mathbf{x} \), when the size of the heterogeneity is much smaller than the size of the unit cell domain. We decompose \( P_{ik}^c (\mathbf{X}_j, \mathbf{X}) \) into the coarse-scale stress \( P_{ik}^c (\mathbf{X}_j, \mathbf{X}) \) and the fine-scale perturbation \( P_{ik}^r (\mathbf{X}_j, \mathbf{X}) \) as

\[ P_{ik}^c (\mathbf{X}_j, \mathbf{X}) = P_{ik}^c (\mathbf{X}_j, \mathbf{X}^c) + P_{ik}^r (\mathbf{X}_j, \mathbf{X}) \]

where

\[ P_{ik}^c (\mathbf{X}_j, \mathbf{X}) = \tilde{P}_{ik} \tilde{\mathbf{X}}_j, \mathbf{X} + Q_{ikj} \tilde{\mathbf{X}}_j, \mathbf{X}_j \]

The first term in (4.2.50) represents the constant part of the coarse-scale stress, whereas the second term describes its linear variation. The two constants, \( \tilde{P}_{ik} \tilde{\mathbf{X}}_j, \mathbf{X} \) and \( Q_{ikj} \tilde{\mathbf{X}}_j, \mathbf{X}_j \), will be determined to satisfy the following conditions

\[ \int_{\tilde{\Omega}_i} \tilde{\omega} \tilde{\mathbf{X}}_j, \mathbf{X} P_{ik}^r (\mathbf{X}_j, \mathbf{X}) d\Theta = 0 \]

\[ \int_{\tilde{\Omega}_i} \tilde{\omega} \tilde{\mathbf{X}}_j, \mathbf{X} P_{ik}^r (\mathbf{X}_j, \mathbf{X}) \mathbf{X}_j d\Theta = 0 \]

Combining (4.2.49)-(4.2.51) yields

\[ \beta \tilde{\mathbf{X}}_j, \tilde{P}_{ik} \tilde{\mathbf{X}}_j, \mathbf{X} + \beta \tilde{\mathbf{X}}_j, \mathbf{X} Q_{ikj} \tilde{\mathbf{X}}_j, \mathbf{X}_j = \int_{\tilde{\Omega}_i} \tilde{\omega} \tilde{\mathbf{X}}_j, \mathbf{X} P_{ik}^c (\mathbf{X}_j, \mathbf{X}) d\Theta \]

\[ \beta \tilde{\mathbf{X}}_j, \tilde{P}_{ik} \mathbf{X}_j, \mathbf{X} + \beta \tilde{\mathbf{X}}_j, \mathbf{X} Q_{ikj} \mathbf{X}_j, \mathbf{X}_j = \int_{\tilde{\Omega}_i} \tilde{\omega} \tilde{\mathbf{X}}_j, \mathbf{X} P_{ik}^c (\mathbf{X}_j, \mathbf{X}) \mathbf{X}_j, d\Theta \]

where

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\[
\beta \tilde{X}_i = \int_{\alpha_{x_i}} \omega \tilde{X}_i \cdot \chi \, d\Theta; \quad \beta \tilde{X}_i \chi = \int_{\alpha_{x_i}} \omega \tilde{X}_i \chi \, d\Theta;
\]
\[
\beta_{ij} \tilde{X}_i = \int_{\alpha_{x_{ij}}} \omega \tilde{X}_i \chi \, d\Theta.
\]

Equation (4.2.52) comprises a system of linear equations from which \( \tilde{P}_{ik} \tilde{X}_i \) and \( Q_{ik} \tilde{X}_i \) can be determined. It is instructive to point out that in case of constant Jacobean \( J^i(\tilde{X}_i) \), \( \beta_i = 0 \) and \( \tilde{P}_{ik} \tilde{X}_i \) reduces to the average stress

\[
\tilde{P}_{ik} \tilde{X}_i = \frac{1}{\Theta} \int_{\Theta_{x_i}} P_{ik}(\tilde{X}_i, \chi) \, d\Theta
\]

and

\[
Q_{ik} \tilde{X}_i \frac{1}{\Theta} \int_{\Theta_{x_i}} \chi \, d\Theta = Q_{ik} \tilde{X}_i \frac{1}{\Theta} \int_{\Theta_{x_i}} P_{ik}(\tilde{X}_i, \chi) \, d\Theta
\]

where \( \alpha_i = \frac{l_i^2}{12} \) and \( l_i \) is the unit cell length in the \( i \)-direction.

Substituting (4.2.50) into (4.2.48) and exploiting (4.2.51) and (4.2.47) yields the computational continua weak form

\[
\sum_{i=1}^{N} \int_{\Theta_{x_i}} \omega \tilde{X}_i \cdot \chi \frac{\partial w^{c}_{i}(X_{i}, \chi)}{\partial \chi} P_{ik}(\tilde{X}_i, \chi) \, d\Theta = \int_{\Theta_{x_i}} w^{c}_{i} X \cdot T_{i}^{c} \, d\Gamma + \int_{\Theta_{x_i}} w^{c}_{i} X \cdot B_{i}^{c} \, d\Omega
\]

Remark 4: The integrand on the left hand side of equation (4.2.56) is a smooth function defined over computational continua domain, which is a disjoint union of computational unit cell domains. Thus the original integral (4.2.35) of an oscillatory fine-scale function over a composite domain \( \Omega_{x}^{c} \) has been replaced by integration of smooth coarse-scale function over computational continua domain. Thus the nonlocal quadrature scheme smoothness requirement is met by virtue of replacing the integration of the oscillatory function \( \Psi^{c}(X) \in \Omega_{x}^{c} \) by integration of smooth coarse-scale function \( \Psi^{c}(X) \in \Omega_{x} \).

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4.3.3 Computational unit cell problem

The computational unit cell problem is constructed by defining a space of test functions over computational unit cell domains as

\[ W_{\omega_{x_i}} = \left\{ w^i \left( \boldsymbol{X}, \tilde{X}_i \right) \right\} \text{ defined in } \Theta_{\tilde{x}_i}, \quad C^0 \left( \Theta_{\tilde{x}_i} \right), \text{ weakly } \boldsymbol{X} - \text{periodic} \]  

and requiring the equilibrium equation (4.1.1) to be satisfied in the weak sense

\[ \int_{\omega_{x_i}} w^i \left( \frac{\partial}{\partial \tilde{X}_k} P^\delta_k + B^\delta_i \right) d\Theta = 0 \quad \forall w^i \in W_{\omega_{x_i}} \]  

Integration by parts of the above yields

\[ \int_{\omega_{x_i}} \frac{\partial w^i}{\partial \tilde{X}_k} P^\delta_k d\Theta = 0 \quad \forall w^i \in W_{\omega_{x_i}} \]  

where the weak periodicity is defined as

\[ \int_{\omega_{x_i}} w^i P^\delta_k d\Theta - \int_{\omega_{x_i}} w^i \tilde{\chi}_k d\Theta = 0 \quad p = 0, 1, \ldots m \]  

In (4.2.60)b the body force \( B_i^\gamma \left( \boldsymbol{X} \right) \) was approximated by a polynomial function of order \( m \) over the computational unit cell domain. At a minimum we will require (4.2.60)b to be satisfied for \( p = 0, 1, 2 \).

The weak periodicity conditions (4.2.60) can be satisfied provided \( w^i \) (and \( u^i \)), \( P^\delta_k \) are periodic functions. This apparently is not trivial for problems where the coarse-scale deformation gradient \( F^C_{jk} \left( \bar{X}_i, \boldsymbol{X} \right) \) varies in \( \Theta_{\tilde{x}_i} \). In this case \( u^i \left( \bar{X}_i, \boldsymbol{X} \right) \) is no longer periodic even though some investigators \([86,87]\) assumed periodicity. This lack of periodicity can be attributed to the following. Consider the usual decomposition \( u^i = H_{ijk} \left( \boldsymbol{X} \right) F^C_{jk} \left( \bar{X}_i, \boldsymbol{X} \right) \) where \( H_{ijk} \left( \boldsymbol{X} \right) \) is \( \boldsymbol{X} - \text{periodic} \). If \( F^C_{jk} \) is not a function of \( \boldsymbol{X} \) then \( u^i \) is periodic. Otherwise \( u^i \) is not periodic.

The weak periodicity condition (4.2.60)a can be enforced using Lagrange multiplier, penalty or augmented Lagrange multiplier method. Here we will discuss how to approximately satisfy it independent of the specific unit cell. We will require (4.2.60)a to hold for arbitrary coarse-scale stress \( P^C_{ijk} \left( \bar{X}_i, \boldsymbol{X} \right) = P^\delta_{ik} \bar{X}_i + Q_{ijk} \bar{X}_i \chi_j \) which yields
\[
\int_{\partial \omega_{i,j}} u^i_j N^\alpha d\Gamma = 0
\]
\[
\int_{\partial \omega_{i,j}} u^i_j \chi_N N^\alpha d\Gamma = 0
\]  \hspace{1cm} (4.2.61)

Integrating (4.2.61) by parts and combining with (4.2.60)b for \( p = 0 \) leads to
\[
\int_{\partial \omega_{i,j}} \frac{\partial u^i_j}{\partial \chi_w} d\Theta = 0; \quad \int_{\partial \omega_{i,j}} \frac{\partial u^i_j}{\partial \chi_w} \chi_N d\Theta = 0
\]  \hspace{1cm} (4.2.62)

Integrating (4.2.60)b for \( p = 2 \) by parts twice and exploiting (4.2.60)b for \( p = 0 \) and (4.2.62) yields
\[
\int_{\partial \omega_{i,j}} \frac{\partial u^i_j}{\partial \chi_w} N^\alpha d\Gamma = 0
\]  \hspace{1cm} (4.2.63)

Further integrating by parts the above results in
\[
\int_{\partial \omega_{i,j}} \frac{\partial^2 u^i_j}{\partial \chi_w^2} d\Theta = 0
\]  \hspace{1cm} (4.2.64)

The upshot of (4.2.60)b for \( p = 0 \), (4.2.62) and (4.2.64) is that the perturbation \( u^i \) should not affect the overall displacement, the overall deformation gradient, and the overall gradient of the deformation gradient.

Furthermore, combining (4.2.61)a with (4.2.61)b for \( k = j \) yields homogeneous constraints on each of the six bounding surfaces \( \partial \Theta^i_j \) of the unit cell
\[
\int_{\omega_{i,j}} u^i_j d\Gamma = 0 \quad \forall j = 1, 2, \ldots, 6
\]  \hspace{1cm} (4.2.65)

where \( \bigcup_{j=1}^6 \partial \Theta^i_j = \partial \Theta^i_x \) and \( \partial \Theta^i_j \cap \partial \Theta^i_x = 0 \quad \forall i \neq j \). Equation (4.2.65) can be interpreted as a weak compatibility condition between adjacent unit cells. In [85,86] it has been shown that equation (4.2.65)a is necessary to pass the patch test in a mesh consisting of finite elements enriched with a fine-scale kinematics interfacing standard finite elements with homogenized material properties. Equation (4.2.65)a was also employed in [34,35,51,86] in conjunction with periodic boundary conditions.

So far we satisfied (4.2.60)b for bi-linear test functions in the computational unit cell \( \Theta^i_x \) rather than for arbitrary test functions in \( W_{\omega^i_x} \). To account for the relaxed constraint we will limit the value of perturbation \( u^i \) by inserting a thin pad region around the unit cell domain as shown in Figure 4.3.3. Furthermore, by introducing the pad region with
homogeneous boundary conditions on its external boundary, equation (4.2.63) is satisfied approximately due to (4.2.65).

**Figure 4.3.3:** Pad region around the unit cell domain

**Remark 5:** Most of the investigators [14,34,35,87] that considered higher order homogenization theories, enforced periodicity on $u^i$, but not on its gradient. The fact that periodicity (or rather weak periodicity) of $u^i$ gradients is not enforced has interesting implications even in the context of homogeneous materials. Consider a unit cell made of a homogeneous material subjected to coarse-scale displacements $u^c = X_1X_2X_3$. If we seek for a periodic correction $u^i$ without requiring periodicity of its gradients, then an equilibrated unit cell solution $u^c_i + u^i$ will switch from the prescribed hourglass mode to a pure bending mode. This is desirable when one wants to capture bending with a single solid element through the plate thickness. However, if an adjacent unit cell is subjected to uniform field than the deformation between the two cells will be incompatible. In general, compatibility between the adjacent cells cannot be enforced if the deformation of each unit cell is controlled by what happens in the interior.

### 4.3.4 Discretization of the coarse-scale problem

The coarse-scale displacement $u^c_i(X)$ is discretized using $C^0$ continuous coarse-scale shape functions $N^c_{ia}(X)$ on $\Omega_X$

$$u^c_i(X) = N^c_{ia}(X)d^c_a$$

where $d^c_a$ denotes nodal displacements; Greek subscripts are reserved for finite element degrees-of-freedom and summation convention over repeated degrees-of-freedom is employed.
We will consider Galerkin approximation where the test function \( w^C_i(X, \chi) \) is discretized using the same \( C^0 \) continuous interpolants expressed as a function of local unit cell coordinates \( \chi = X - X_i \)

\[
w^C_i(X, \chi) = N^C_{ia}(\tilde{X}_i, \chi) c^C_a
\]  

Inserting (4.2.67) into the coarse-scale weak form (4.2.56) yields the discrete coarse-scale problem, which states: Given \( r^C_{i+1} \) and \( u^C_{i+1} \), find \( d^C_{i+1} \) such that

\[
r^C_{i+1} = f^m_a - f^{ext}_a = 0
\]

\[
u^C_{i+1} = u_{i+1} \quad \text{on} \quad \partial \Omega^+_i;
\]

where \( r^C_{i+1} \) and \( u^C_{i+1} \) are the coarse-scale residual and displacement increment in the \((n+1)\)th load increment, respectively, and

\[
f^m_a = \sum_{i=1}^{N} \int_{\Omega_i} \omega(X) \left( \frac{\partial N^C_i(X, \chi)}{\partial \chi_j} \right) P_a^C(\tilde{X}_i, \chi) d\Omega
\]

\[
f^{ext}_a = \int_{\Omega_i} N^C_a B^T d\Omega + \int_{\partial \Omega_i} N^C_a T^C_{i,\alpha} d\Gamma
\]

where \( f^m_a \) and \( f^{ext}_a \) are the internal and external forces, respectively.

**Figure 4.3.4:** Mixed Nonlocal-Local Quadrature Scheme

The integral over the computational unit cell domain will be evaluated using local quadrature, which yields

\[
f^m_a = \sum_{l=1}^{k} \sum_{m=1}^{N} J^a(\tilde{X}_i, \tilde{X}_m) W_{lm} \left( \frac{\partial N^C_i(X, \chi)}{\partial \chi_j} \right) P_a^C(\tilde{X}_i, \tilde{X}_m) \bigg|_{\tilde{X}_m}
\]

where the pair of coordinates \((\tilde{X}_i, \tilde{X}_m)\) denotes position of local quadrature point \( \tilde{X}_m \) in the coordinate system of the computational unit cell positioned at \( \tilde{X}_i \), as shown in Figure 4.3.4;
\( J^* (\tilde{X}_j, \tilde{X}_u) \) and \( w_{nJ} \) denote the computational unit cell Jacobean and the corresponding weight, respectively.

### 4.3.5 Discretization of the computational unit cell problem

The unit cell displacements in the computational unit cell can be expressed as a sum of the coarse-scale displacements \( u^c_i (X) \) and the fine-scale perturbation \( u^e_i (\tilde{X}_j, \chi) \)

\[
u^e_i (\tilde{X}_j, \chi) = u^c_i (X) + u^e_i (\tilde{X}_j, \chi)
\]

where

\[
u^e_i (\tilde{X}_j, \chi) = N_{i\beta}^F (\chi) d_{\beta} (\tilde{X}_j)
\]

or by direct discretization

\[
u^e_i (\tilde{X}_j, \chi) = N_{i\beta}^F (\chi) d_{\beta} (\tilde{X}_j)
\]

where \( N_{i\beta}^F (\chi) \) is a fine-scale shape function; \( d_{\beta} (\tilde{X}_j) \) the total nodal displacement in the computational unit cell and \( d^1_{\beta} (\tilde{X}_j) \) the corresponding perturbation.

The unit cell problem can be either solved directly for the total displacement \( d_{\beta} (\tilde{X}_j) \) or for the perturbation \( d^1_{\beta} (\tilde{X}_j) \). The corresponding two approaches referred hereafter as the total [88,89,90]) and the correction-based [91] approach, respectively.

We consider Galerkin approximation of the fine-scale test function on \( \Theta_{\tilde{X}_j} \)

\[
w^e_i (\tilde{X}_j, \chi) = N_{i\beta}^F (\chi) c^i_{\beta} (\tilde{X}_j)
\]

which yields the discrete unit cell problem subjected to weak periodicity conditions. We will assume that \( d^1_{\beta} (\tilde{X}_j) \) and \( c^i_{\beta} (\tilde{X}_j) \) satisfy homogeneous linear constraints. Let \( \tilde{d}_{\eta} (\tilde{X}_j) \) and \( \tilde{c}_{\eta} (\tilde{X}_j) \) be the independent degrees-of-freedom, then linear transformation operator \( T_{\eta\beta} \) can be defined as

\[
d^1_{\beta} (\tilde{X}_j) = T_{\eta\beta} \tilde{d}_{\eta} (\tilde{X}_j), \quad c^i_{\beta} (\tilde{X}_j) = T_{\eta\beta} \tilde{c}_{\eta} (\tilde{X}_j)
\]

In summary, the discrete unit cell problem is formulated as follows. Given the coarse-scale deformation \( u^c_n (X) \) and prior solution \( d_n (\tilde{X}_j) \), find \( d^1_n (\tilde{X}_j) \) such that
subjected to weak periodicity conditions. The left superscript in (4.2.77) denotes the iteration count of the coarse-scale problem; \(d(\tilde{X}_i)\) denotes previously (at the load step \(n\)) converged solution in the computational unit cell positioned at \(\tilde{X}_i\).

For the correction-based approach, the leading order deformation gradient can be written as a sum of known coarse-scale deformation gradient \(F_{ik}^C(X)\) and the unknown perturbation

\[
F_{ik}^C(\tilde{X}_i, \tilde{X}) = F_{ik}^C(X) + \frac{\partial N_{\rho}^F(X)}{\partial X_k} d^i(\tilde{X}_i)
\]

Consequently, the discrete unit cell problem can be solved for the unknown perturbation \(d^i(\tilde{X}_i)\).

### 4.4. Numerical Examples

In this section, we consider several numerical examples to demonstrate the versatility of the computational continua (to be referred hereafter as \(C^2\)) formulation to resolve the coarse-scale behavior of interest for large CUCs subjected to considerable coarse-scale gradients. The results of the computational continua \(C^2\) are compared with the classical coarse-scale continua resulting from \(O(1)\) homogenization (to be referred here as \(O(1)\)) and the direct numerical simulation (DNS) capable of resolving fine-scale details. Here for simplicity, we restrict ourselves to two-dimensional problems. We first study a single coarse-scale element formulation consisting of multiple unit cells followed by the consideration of multiple coarse-scale element domains.

#### 4.4.1. A single coarse-scale element study

Here we consider a two-dimensional coarse-scale domain discretized with a single four-node quadrilateral element subjected to a hourglass deformation mode \(u_i^C = X_1X_2\), \(u_2^C = 0\). The coarse-scale quantities of interest are internal energy density and internal force vector and we report the normalized error in these quantities of interest as a function of the ratio between the size of coarse-scale domain \(L\) and the unit cell size \(l\). We consider different material models including elasticity, hyperelasticity, monotonic plasticity and
cyclic plasticity. Figure 4.4.1 depicts an example of the coarse-scale problem domain and the CUC.

**Figure 4.4.1.** Problem domain consisting of four unit cells (left), coarse-scale element domain (center) and a unit domain (right).

**Figure 4.4.2.** Von Mise stress distribution: (left) DNS in the left upper portion of the coarse-scale domain—the peak value of Mises stress is \(4.696 \times 10^8\); (center) C2 formulation—the peak value of Mises stress is \(4.177 \times 10^8\); (right) O(1) formulation—the peak value of Mises stress is \(1.82 \times 10^8\).

### 4.4.1.1. Linear elastic material.

We consider a unit cell made of linear isotropic elastic material with \(E = 4 \times 10^{10}\) and \(\nu = 0.3\), having a circular hole in the center. We consider a square coarse-scale domain with \(L = 288\) and subject its vertices to displacements \(d^{(1)} = [1, 0], \ d^{(2)} = [-1, 0], \ d^{(3)} = [1, 0], \ d^{(4)} = [-1, 0]\) with linear variation between the vertices.
Figure 4.4.2 compares the von Mises stress distributions obtained using DNS, $C^2$ and O(1) formulations. It is not surprising that O(1) theory shows substantially different stress distributions as it is subjected to constant deformation gradient. Note that $C^2$ formulation subjects the CUC to the boundary displacements similar to those obtained from DNS. Consequently, the peak stress values obtained by $C^2$ are much better than those obtained by the O(1) formulation.

Internal force vectors in the coarse-scale element denoted by $f_{C^2}^{int}$ and $f_{O(1)}^{int}$ were calculated for the $C^2$ and O(1) formulations, respectively, and were compared with the reaction force vector $r_{DNS}$ obtained by DNS. The normalized errors, defined as $\tilde{f}_{C^2}^{int} = \|r_{DNS} - f_{C^2}^{int}\|/\|r_{DNS}\|$ and $\tilde{f}_{O(1)}^{int} = \|r_{DNS} - f_{O(1)}^{int}\|/\|r_{DNS}\|$, respectively, are depicted in Figure 4.4.3 (left) for various ratios of $L/l$. Figure 4.4.3 (right) compares the relative error in the energy densities denoted by $e_{O(1)}$ and $e_{C^2}$ as a function of the unit cell size $L/l$. It can be seen that unlike $O(1)$ continua, $C^2$ formulation captures the size dependence of the internal energy density. Figure 4.4.3 also gives the results of the formulation (denoted by $C^*$) when local Gauss quadrature points are used instead of nonlocal quadrature points.

![Figure 4.4.3](image-url)  
*Figure 4.4.3. The normalized error in the internal force (left) and in the energy density (right) as a function of unit cell size $L/l$.*

It can be seen that for all CUC sizes considered, $C^2$ has less than 3% error in the two quantities of interest; yet O(1) results in errors as high as 18% in particular when the CUC size is large. As the unit cell size reduces, the difference between the classical
homogenization and computational continua becomes insignificant and in the limit the two solutions coincide.

4.4.1.2. Hyperelastic material.

A hyperelastic material with Young’s modulus \( E \) depending on equivalent strain 
\[
\varepsilon^{\text{eq}} = \varepsilon_{11}^1 + \varepsilon_{22}^2 - \varepsilon_{11} \varepsilon_{22} + 3 \varepsilon_{12}^1 \]
and \( \nu = 0.3 \) has been considered for the matrix phase as depicted in the following table:

<table>
<thead>
<tr>
<th>( \varepsilon^{\text{eq}} )</th>
<th>0</th>
<th>0.0025</th>
<th>0.005</th>
<th>0.0075</th>
<th>0.009</th>
<th>0.01</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E \times 10^{10} )</td>
<td>4</td>
<td>24</td>
<td>54</td>
<td>94</td>
<td>160</td>
<td>160</td>
</tr>
</tbody>
</table>

**Table 4.4.1.** Dependence of Young’s modulus on equivalent strain

The inclusion phase is assumed to be elastic with \( E=20\times10^{10}, \nu = 0.3 \).

The normalized error in the internal force vector as a function of time and the CUC size is depicted in Figure 4.4.4. The normalized error in the coarse-scale energy density as a function of time for the CUC sizes of \( L/l=2, L/l=3 \) and \( L/l=4 \) is depicted in Figure 4.4.5. Figure 4.4.6 summarizes the dependence of the energy density on \( L/l \) as obtained in the last load increment.

![Figure 4.4.4](image1)

**Figure 4.4.4.** The normalized error in the internal force for hyperelastic material as a function of load for unit cell sizes: \( L/l=2 \) (left), \( L/l=3 \) (center) and \( L/l=4 \) (right).
Figure 4.4.5. The normalized error in the energy density for hyperelastic material as a function of load for unit cell sizes of: \( L/l = 2 \) (left), \( L/l = 3 \) (center) and \( L/l = 4 \) (right).

Figure 4.4.6. Energy density in the final load increment as a function of unit cell size \( L/l \).

Figure 4.4.7. The normalized error in the internal force for plasticity as a function of load for unit cell sizes of: \( L/l = 2 \) (left), \( L/l = 3 \) (center) and \( L/l = 4 \) (right).
As in the elasticity case, the $C^2$ formulation gives rise to errors that do not exceed 4% in both quantities of interest throughout the entire loading history. The $O(1)$ formulation, on the other hand, results in errors that are up to four times higher.

### 4.4.1.3. Monotonic plasticity.

We consider von Mises plasticity for the matrix phase and linear elasticity for the inclusion phase with $E = 12 \times 10^{10}$, $\nu = 0.3$. The yield stress in the matrix phase is assumed to depend on the equivalent plastic strain as shown in the following table:

<table>
<thead>
<tr>
<th>$\varepsilon^{eq}$</th>
<th>0.0</th>
<th>0.001</th>
<th>0.002</th>
<th>0.003</th>
<th>0.004</th>
<th>0.005</th>
<th>0.006</th>
<th>0.007</th>
<th>0.008</th>
<th>0.009</th>
<th>0.01</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y, 10^7$</td>
<td>3</td>
<td>3.2</td>
<td>3.6</td>
<td>4.6</td>
<td>6.2</td>
<td>9.4</td>
<td>15.8</td>
<td>28.6</td>
<td>54.2</td>
<td>105.4</td>
<td>206.6</td>
</tr>
</tbody>
</table>

**Table 4.4.2.** Dependence of the yield stress on the equivalent strain

The normalized error in the internal force vector and in the energy density as a function of time and the CUC size are depicted in Figures 4.4.7 and 4.4.8, respectively.

#### 4.4.1.4. Cyclic plasticity

The cyclic load history prescribed by controlling nodal displacements is shown in Table 4.4.3.

The error in the internal force is depicted in Figure 4.4.9 for $L/l=2$. The error in the internal force was not normalized since the denominator might be close to zero due to force removal.
Table 4.4.3. Cyclic load history

<table>
<thead>
<tr>
<th>Node</th>
<th>Step 1</th>
<th>Step 2</th>
<th>Step 3</th>
<th>Step 4</th>
<th>Step 5</th>
<th>Step 6</th>
<th>Step 7</th>
<th>Step 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
</tr>
<tr>
<td>2</td>
<td>[−1, 0]</td>
<td>[0, 0]</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
<td>[−1, 0]</td>
<td>[0, 0]</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
</tr>
<tr>
<td>3</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
<td>[−1, 0]</td>
<td>[0, 0]</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
<td>[−1, 0]</td>
<td>[0, 0]</td>
</tr>
<tr>
<td>4</td>
<td>[−1, 0]</td>
<td>[0, 0]</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
<td>[−1, 0]</td>
<td>[0, 0]</td>
<td>[1, 0]</td>
<td>[0, 0]</td>
</tr>
</tbody>
</table>

Figure 4.4.9. Cyclic plasticity: the error in the internal force and the norm of the reaction force vector obtained by DNS as a function of time for $L/l=2$.

4.4.2. Cantilever beam problem

Consider a cantilever beam problem consisting of eight unit cells subjected to uniform pressure load as shown in Figure 4.4.10 (a). The left end of the cantilever is fixed. For the C2 and O(1) homogenization, the coarse-scale domain is modeled by 8 eight-node quadrilateral elements. Quadratic elements are required for the C2 formulation to resolve the linear coarse-scale stress field within the element. The CUC has a square domain with a very weak circular inclusion of a diameter equal to half of the unit cell size as shown in Figure 4.4.10 (c). We consider a CUC size equal to the coarse-scale element size. Linear elastic material properties are assumed. The nondimensional units are as follows: $E_{\text{matrix}}=4.0\times10^9$, $\nu_{\text{matrix}}=0.3$, $E_{\text{inclusion}}=4.0$, $\nu_{\text{inclusion}}=0.3$, pressure load equal to $1.5\times10^6$ and coarse-scale element size equal to 288.
Figure 4.4.10. (a) Geometry, load and boundary conditions; (b) coarse-scale finite element mesh consisting of 8 eight-node elements; and (c) a unit cell equal to the size of the coarse-scale element.

The reference solution is obtained by DNS using a very fine finite element mesh as shown on the Figure 4.4.11, which depicts the deformed mesh and the von Mises stress distribution.

Figure 4.4.11. Deformation and von Mises stress distribution as obtained by direct numerical simulation.

The maximum deflection (point A in Figure 4.4.10) as obtained by $C^2$ is compared with the reference solution (DNS) and the following three O(1) formulations:

- $O(1)-4$: Classical O(1) formulation where the CUC is subjected to constant deformation gradient and periodicity constraint; reduced integration (four quadrature points) is used to integrate the coarse-scale element.

- $O(1)-9$: Classical O(1) formulation where the CUC is subjected to constant deformation gradient and periodicity constraint; full integration (nine quadrature points) is used to integrate the coarse-scale element.
O(1)-4-Full: Modified O(1) formulation where the CUC is subjected to complete deformation field extracted from the coarse-scale element and periodicity constraint; reduced quadrature is used to integrate the coarse-scale element.

The results of the maximum displacements at point A are given in Table 4.4.4.

<table>
<thead>
<tr>
<th></th>
<th>DNS</th>
<th>C^2</th>
<th>O(1)-4</th>
<th>O(1)-4-Full</th>
<th>O(1)-9</th>
</tr>
</thead>
<tbody>
<tr>
<td>u_y(X_A)</td>
<td>-67.7839</td>
<td>-65.5284</td>
<td>-97.5683</td>
<td>-97.4983</td>
<td>-97.503</td>
</tr>
<tr>
<td>u_y(X_A)</td>
<td>-5.39595</td>
<td>-5.29128</td>
<td>-8.00685</td>
<td>-8.0064</td>
<td>-8.00444</td>
</tr>
</tbody>
</table>

**Table 4.4.4.** Maximum displacement (Point A in Figure 4.4.10) as obtained by DNS, C^2 and three O(1) formulations.

The error in the displacement norm at point A is 3.99% for the C^2 formulation and over 43% for the three O(1) formulations—more than a factor of 10 in error reduction. Obviously as the coarse-scale fields in the CUC become more uniform, improvements offered by C^2 become more modest and in the limit the two formulations coincide. For instance, for the same beam size but with two rows of unit cells, the C^2 provides reduction of error by a factor of 1.7.

**Figure 4.4.12.** von Mises stress distribution in the unit cell adjacent to the clamped end as obtained by direct numerical simulation (DNS), Computational Continua (C^2) and three variants of the O(1) homogenization.
Figure 4.4.12 compares the von Mises stress distribution in the unit cell adjacent to the clamped end. The maximum values are compared in Table 4.4.5. The stress distribution in the CUC is obtained in the post-processing stage by subjecting the CUC to the coarse-scale deformation.

<table>
<thead>
<tr>
<th></th>
<th>DNS</th>
<th>C²</th>
<th>O(1)-4</th>
<th>O(1)-4 Full</th>
<th>O(1)-9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum von Mises stress</td>
<td>3.186e+08</td>
<td>2.982e+08</td>
<td>4.280e+07</td>
<td>3.720e+08</td>
<td>4.296e+07</td>
</tr>
</tbody>
</table>

Table 4.4.5. Maximum von Mises stress in the unit cell adjacent to the clamped end as obtained by DNS, C² and three O(1) formulations.

4.5. Conclusions and discussion

Unlike the generalized continua, which assumes scale separation and is limited to infinitesimal unit cells, and the nonlocal continua for which construction of general purpose nonlocal kernels for heterogeneous media is questionable, the computational continua possess the generality and the versatility not found in the existing methods. The combination of nonlocal quadrature and the coarse-scale function reproduces the exact coarse-scale variational statement provided that the coarse-scale fields are smooth. The unit cell is permitted to be as large as a coarse-scale element and the resulting formulation requires C0 continuity only, involves no additional degrees-of-freedom and no higher-order boundary conditions. The versatility of the formulation was confirmed on limited numerical examples.

Several important characteristics of the method, such as
1. Can the method be applied to unit cell larger than coarse-scale elements?
2. Does the method serve as a localization limiter?
3. Can the method be used to propagate discontinuities?

have not been investigated. In the following, we will comment on the above issues, but in depth study is required.

The answer to the first question is ‘yes’. However, if the unit cell is larger than coarse-scale element, it is necessary to carry out the integration over the unit cell domain rather than over the elements. This of course complicates the integration as it requires additional triangulation or increasing number of quadrature points [52].
The answer to the second question is ‘no’. In other words, if the fine-scale equations are not well posed (strain softening, mesh dependence, etc.) the computational continua will inherit the same deficiencies. The nonlocal character of the computational continua formulation is intended to reproduce the overall fine-scale behavior rather than to modify it as is often the case in nonlocal theories. The responsibility of constructing a well-posed problem falls squarely on the governing equations on the fine scale rather than on the coarse graining process.

The answer to the third question is mixed. The discontinuities contained in the interior of the unit cell are computationally resolved and then transferred to the coarse-scale in the form of linear coarse-scale stress function. Larger discontinuities are reflected by directionally softer coarse-scale element behavior, but in the absence of coarse-scale kinematical enrichment (such as multiscale XFEM [45, 62]) or remeshing, computational continua without enrichment is not well equipped to propagate large discontinuities.

One of attractive use of these methods – to characterize various materials – engineering for imperfections, geotechnical materials to seek for mineral, oil, voids, various inclusions and layers etc, biomaterials for imaging, to seek for tumors.

References


