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FEUP FACULDADE DE ENGENHARIA
UNIVERSIDADE DO PORTO

Assignment 1

Professor:
José Manuel de Almeida César de Sá

Student:
José Luís Passos Vila-Chã

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Chapter 1

Introduction

Chapter 2

FFT-based methods for mechanical problems

In the following, an overview of the literature on FFT-based methods for the determination of the overall and local response of a composite material from actual images or morphological simulations of its microstructure is presented.

To establish some context, let the microstructure of the material be represented by a periodic cell Ω. The material response at a point $\boldsymbol{x} \in \Omega$ is specified by the constitutive relation $\boldsymbol{\sigma}(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{x}))$ assigning the stress response $\boldsymbol{\sigma}$ to a given strain $\boldsymbol{\varepsilon}$ locally at $\boldsymbol{x}$. Furthermore, the total strain $\boldsymbol{\varepsilon}$ is split into a homogeneous average strain tensor $\boldsymbol{E}$ and an Ω -periodic fluctuating strain field $\boldsymbol{\varepsilon}^*$, i.e.

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \boldsymbol{E} + \boldsymbol{\varepsilon}^*(\boldsymbol{x}) \text{ for } \boldsymbol{x} \in \Omega, \quad \int_\Omega \boldsymbol{\varepsilon}^*(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \boldsymbol{0}. \tag{2.1}$$

The average strain $\boldsymbol{E}$ represents a given macro-scale excitation, while the fluctuating micro-scale strain field $\boldsymbol{\varepsilon}^*$ is the primary unknown.

The fluctuating strain field $\boldsymbol{\varepsilon}^*$ is determined by the stress equilibrium and strain compatibility conditions, which under quasi-static assumptions and in small strains read as,

$$-\nabla \cdot \boldsymbol{\sigma}\left(\boldsymbol{x}, \boldsymbol{E} + \boldsymbol{\varepsilon}^*(\boldsymbol{x})\right) = 0 \text{ for } \boldsymbol{x} \in \Omega, \tag{2.2}$$

$$\boldsymbol{\varepsilon}^* \in \mathcal{E} = \left\{\nabla_s \boldsymbol{u}^*, \boldsymbol{u}^* \text{ is an } \Omega\text{-periodic displacement field}\right\}, \tag{2.3}$$

where $\nabla\cdot$ stands for the divergence operator and ∇_s stands for the symmetrized gradient operator. The goal of the methods presented in the following is to solve Equation (2.2) under the compatibility restriction expressed by Equation (2.3).

The FFT based methods, first introduced by Moulinec and Suquet (1994, 1995), enjoy wide usage across many domains. They have been integrated into efficient and robust two-scale FE-FFT-based computatinal approaches (Kochmann et al., 2018a) and now even figure in comercial software such as DAMASK (Roters et al., 2019) and FeelMath (Schwichow, 2020; FraunhoferITWM, 2020). Their application ranges from crystal plasticity (e.g. Lebensohn (2001); Shanthraj et al. (2015); Kochmann et al. (2018b); Lebensohn and Rollett (2020); Wicht et al. (2020b)), hypoelasticity (e.g. Ma and Truster (2019)), failure and damage (e.g. Ernesti et al. (2020); Ernesti and Schneider (2021); Geus (2016); Magri et al. (2021); Wang et al. (2018)) and

multi-physics simulations (e.g. Vinogradov and Milton (2008); Brenner (2010); Shanthraj et al. (2019); Göküzüm et al. (2019); Zhou and Bhattacharya (2020); Wicht et al. (2020a)). They have also been used in the contex of reduced order models (e.g. Kochmann et al. (2019); Gierden et al. (2021)).

Comparisons between the FEM and the FFT-based methods can be found in Michel et al. (1999) and Vondrejc and Geus (2020). The first focuses on the "basic scheme" and concludes that the FFT-based method is much faster than FEM when the contrast between phase properties is not too large. This advantage decreases as the contrast increases, in favor of the FEM. In the second contribution, Galerkin-based formulations are considered. The advantage of FEM for the case of rough data with jumps in material coefficients regarding both memory usage and speed is reasserted. The results for continuous material coefficients are inconclusive.

The main classification scheme adopted follows Zeman et al. (2017) and is based on the discretization approach. The first set of methods, which include the original contribution from Moulinec and Suquet (1994), are labeled as "Conventional FFT" and the second class as "Variational FFT". In the last section, a few methods not fitting this classification scheme are also presented.

2.1 Conventional FFT

Following Zeman et al. (2017), the "Conventional FFT" methods, based on the basic scheme by Moulinec and Suquet (1994), are derived from the following integral equation for the fluctuating strains $\boldsymbol{\varepsilon}^* \in \mathcal{E}$,

$$\int_\Omega \Gamma^{\text{ref}}(\boldsymbol{x}-\boldsymbol{y}) : \boldsymbol{\sigma}\left(\boldsymbol{y}, \boldsymbol{E}+\boldsymbol{\varepsilon}^*(\boldsymbol{y})\right) \mathrm{d}\boldsymbol{y} = \boldsymbol{0} \text{ for all } \boldsymbol{x} \in \Omega, \tag{2.4}$$

where Γ^{ref} is the Green function of the reference problem. This reference problem is an auxiliary local problem with the homogeneous constitutive relation

$$\sigma(\boldsymbol{x}, \varepsilon(\boldsymbol{x})) = C^{\text{ref}} : \boldsymbol{\varepsilon}(\boldsymbol{x}) \text{ for } \boldsymbol{x} \in \Omega. \tag{2.5}$$

In the seminal contribution by Moulinec and Suquet (1994, 1995), Equation (2.4) is solved using a fixed-point iteration scheme after discretizing it through a point collocation method, the basis function being trigonometric polynomials (Zeman et al., 2017). It is originally formulated for linear elasticity and small strains. In Michel et al. (2000, 2001), the authors extend this scheme to materials with non-linear mechanical behavior laws.

It has become very popular as a method used for the determination of local fields and effective properties since it does not require meshing. Thus, it allows the direct use of experimental images obtained by advanced imaging techniques such as micro-computed tomography. Besides, from a computational standpoint, it is also a very fast and memory-efficient method. It enjoys from current implementations of the Fast Fourier transform, which are extremely powerful. Moreover, the scheme supports matrix-free solvers, even for strongly non-linear materials. Lastly, the method is also simple to code and use.

Despite all these favorable characteristics, the method also has some drawbacks. It is not suitable for composites with infinite contrast between the phases and near interfaces between phases where large differences in the material properties are found, spurious features have also been reported (Ma et al., 2021). Furthermore, the convergence rate as a function of the material contrast is only linear.

As already mentioned, this class of methods uses a regular mesh, where the basis functions are trigonometric polynomials. Exceptions are Bonnet (2007), Monchiet and Bonnet (2012), Monchiet (2015) and Nguyen et al. (2021). In the first three, the exact Fourier transforms of the elasticity tensor are used. This can be achieved because the Fourier transforms of the characteristic functions of the inclusion phases are known, being limited to circles and ellipses. The last work uses the approximate Fourier transform of the elasticity tensor, but the phases are not limited to circles and ellipses. More complex phase domains are approximated through the union of polygon and polyhedra (e.g. flower-shaped inclusions in 2D and torus-shaped inclusion in 3D) for which the Fourier transforms of the characteristic functions are known.

A further classification of the "Conventional methods" can be introduced, according to Schneider (2019). For the first kind, each iterate satisfies the mechanical compatibility condition, whereas, for the second kind, compatibility is only ensured upon convergence. The polarization schemes and solvers based on the Hashin-Shtrikman principle constitute the former kind. The latter includes the conjugate gradient method, the Newton-scheme (coupled to different linear solvers), and the fast gradient methods.

Regarding the contributions based on polarization, the original work is due to Eyre and Milton (1999). It is developed in the context of electrical conductivity, hence the use of the term "polarization" in connection with these schemes. Accordingly, the procedure iterates on the polarization field, and not on the strain field, as per usual. Combined with the rewriting of the expression for the original scheme, this leads to faster convergence rates, superlinear, when compared with the "basic scheme", as a function of the material contrast. In Michel et al. (2001) this approach is extended to linear elasticity, and a related approach based on an augmented Lagrangian is also introduced. Convergence for infinite contrast is achieved for this last method. Lastly, in Monchiet and Bonnet (2012) a further extension is proposed, with the scheme suggested including both of the polarization-based works previously mentioned. Convergence for infinite contrast is likewise achieved. In Schneider et al. (2019) two flaws in these methods are pointed out in the non-linear context. Firstly, the optimal choice of algorithmic parameters is only known for the linear elastic case. Secondly, in its original version, each iteration of the polarization scheme requires solving a nonlinear system of equations for each voxel. The authors cast these methods into a simpler form using the Douglas-Rachford splitting, thus, avoiding the solution of non-linear equations in each iteration. In Moulinec and Silva (2014), Moulinec et al. (2014) and Schneider et al. (2019) comparisons between these methods and others can be found. Finally, the linear solvers of Brisard and Dormieux (2010, 2012) also belong to the class of polarization schemes, although they operate on a different polarization (Schneider, 2020b).

Beyond the "basic scheme" of Moulinec and Suquet (1994) further improvements within the same framework have been proposed. In the first place improvements still dealing with linear behavior at small strains are introduced. In the original approach, a fixed point iteration/Richardson iteration/Neumann series-based scheme is used (see Moulinec et al. (2018) for an in-depth convergence analysis). It is the most memory-efficient method available in its class and is also robust, but slow for highly contrasted problems. Moreover, the only role of the (material-dependent) reference problem is to ensure the convergence of the Richardson iteration scheme used to solve the resulting system of linear equations. As an alternative, Zeman et al. (2010) propose a conjugate gradient-based approach. It proceeds from the discretization of the governing integral

equation by the trigonometric collocation method to give a linear system that can be efficiently solved by conjugate gradient methods. The authors claim a significant increase of the convergence rate for problems with high-contrast coefficients at a low overhead per iteration. The scheme is also independent of the reference problem.

According to Kabel et al. (2014), regarding non-linear problems, be it concerning small or large strain, there are two solution strategies. Firstly, a fixed point iteration can be employed to solve the nonlinear equation introduced in Moulinec and Suquet (1998) for small deformations and extended to large deformations in Eisenlohr et al. (2013). Also for small deformations, Schneider et al. (2017) and Schneider (2020a) present the use of the fast gradient methods (Nesterov's method, heavy-ball method, and Fletcher-Reeves CG), which also forego the linearization of the nonlinear equations. The fast gradient methods combine fast convergence with a low memory footprint. However, they suffer from a delicate parameter selection (Schneider, 2020a).

Alternatively, one can use the Newton or quasi-Newton methods to tackle the nonlinear problem by solving a sequence of linear problems. In the context of small strains, Gélébart and Mondon-Cancel (2013) solve the linearized equations found through the Newton method using the conjugate gradient scheme. Low sensitivity to the reference material and an improved efficiency, for a soft or a stiff inclusion, when compared to the "basic scheme" is reported. In addition to prescribed macroscopic strain, the proposed method is extended to mixed loadings.

Concerning large strains, using Newton methods to linearize the nonlinear equations, Lahellec et al. (2003) present a scheme where a fixed-point approach is used to solve the linearized equations. In Kabel et al. (2014), fixed-point schemes are also considered, in addition to Newton-Raphson and Netwon-Krylov/conjugate gradient methods. In connection to the last method, a memory-efficient version is also presented.

Quasi-Newton methods are available in the literature, as well. In Wicht et al. (2019) two algorithms based on the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method, one of the most powerful Quasi-Newton schemes, are introduced. More specifically, the BFGS update formula is utilized to approximate the global Hessian or the local material tangent stiffness. Both for Newton and Quasi-Newton methods, a globalization technique is necessary to ensure global convergence. Specific to the FFT-based context, a Dong-type line search is promoted, avoiding function evaluations altogether. Another Quasi-Newton method, mentioned in Wicht et al. (2019) and extended to polarization methods in Wicht et al. (2021), is the Anderson acceleration method. It is a method for improving the convergence behavior of fixed-point iterations, where derivatives of the fixed-point mapping are not available. Based on a limited number (the so-called depth) of previous iterates, Anderson acceleration generates the next iterate based on a mixture of previous iterates, where the mixing coefficients solve an associated low-dimensional optimization problem. In Schneider (2019) the Barzilai-Borwein is applied to the problem at hand. It may be interpreted as the basic scheme with adaptive time-stepping (or, equivalently, adaptive reference material). Thus, it has a low memory footprint but is competitive in terms of convergence speed when compared to the solvers mentioned above. However, it is an intrinsically non-monotone method, ie, the residual is not monotonically decreasing from one iteration to the next. This behavior is unfamiliar and may limit the applicability for industrial applications.

Table 2.1 reproduces a Table found in Wicht et al. (2019) detailing the memory footprint and other characteristics regarding the different solvers available.

Table 2.1: Summary of the performance comparison between the investigated solution schemes (Wicht et al., 2019)

Solution scheme	Memory footprint (strain-like fields)	Summary and remarks
Basic scheme	1	• Gradient descent method • Lowest memory requirements • Slowest among the studied solvers
Anderson acceleration	$2m+2$	• Limited-memory Quasi-Newton method • Optimal depth m between 2 and 5 • Accelerates the basic scheme but slower than the remaining algorithms
L-BFGS	$2m+4$	• Limited-memory Quasi-Newton method • Optimal depth m between 2 and 5 • Outperformed by the more memory--efficient Barzilai-Borwein method
Barzilai-Borwein	2	• Gradient descent with step size based on Quasi-Newton methods • Nonmonotonic convergence behavior • Fastest choice for inexpensive material laws
Newton-CG	8.5	• Inexact Newton method • Highest efficiency in combination with Eisenstat and Walker's forcing-term choice 2 • Requires computing the material tangent • Fastest choice for expensive material laws
BFGS-CG	10.5	• Inexact Quasi-Newton method • Uses the BFGS update to approximate the material tangent • Matches performance of Newton-CG for small load steps, slightly slower otherwise

Abbreviations: BFGS, Broyden-Fletcher-Goldfarb-Shanno; CG, conjugate gradient.

2.2 Variational FFT

According to Zeman et al. (2017) the so-called "Variational FFT" schemes, are based on the weak form of the equilibrium equation

$$\int_{\Omega} \delta\boldsymbol{\varepsilon}^*(\boldsymbol{x}) : \boldsymbol{\sigma}\left(\boldsymbol{x}, \boldsymbol{E} + \boldsymbol{\varepsilon}^*(\boldsymbol{x})\right) \mathrm{d}\boldsymbol{x} = 0, \tag{2.6}$$

with the compatibility constraint enforced by

$$\delta\boldsymbol{\varepsilon}^*(\boldsymbol{x}) = [\boldsymbol{G} * \boldsymbol{\zeta}](\boldsymbol{x}) = \int_{\Omega} \boldsymbol{G}(\boldsymbol{x} - \boldsymbol{y}) : \boldsymbol{\zeta}(\boldsymbol{y}) \mathrm{d}\boldsymbol{y} \text{ for } \boldsymbol{x} \in \Omega, \tag{2.7}$$

where $\boldsymbol{G}$ is a projection operator, $\boldsymbol{\zeta}$ is a test function and $*$ stands for the convolution.

Vondřejc and co-workers first established the connection between FFT-based schemes and Finite Elements in the framework of conventional Galerkin methods with a specific choice of basis functions and numerical quadrature (Vondřejc et al., 2014) or exact integration (Vondřejc et al., 2015) for small strains. The main advantage of this approach is the fact that it does not rely on the notion of a reference problem. Such a feature is particularly attractive for non-linear problems, for which the concept of the Green functions cannot be used. From a conceptual standpoint, this framework has the benefit that discretization, quadrature, constitutive linearization, and the solution of a linear system can be properly distinguished and optimized individually (see e.g. Mishra et al. (2015), Mishra et al. (2016) and Vondrejc and Geus (2020)).

Zeman et al. (2017) offers a very clear presentation of this approach and supplies the demonstrations regarding robust convergence for several types of non-linear constitutive behavior in small strains. In De Geus et al. (2017) the extension to finite strain is achieved, and the corresponding Python code of only 59 lines (without comments) is also supplied for a linear hyperelastic material. A further extension is advanced in Lucarini and Segurado (2019a), where stress and mixed control of the macroscopic load history is achieved using a direct method based on a modified project operator and preserving the computational performance of the original method.

Having arrived at the set of non-linear equations found from the descritization of Equation (2.6), the methods used to solve them can, in principle, be the ones detailed above for the "Conventional FFT".

2.3 Other methods

This section collects together all the contributions that do not fit into the above categories of "Conventional FFT" and "Variational FFT".

Following Willot and co-workers (Willot and Pellegrini, 2008; Willot et al., 2014; Willot, 2015) the equilibrium equations are discretized using finite differences, and these discretized equations are solved using the "basic scheme". The only difference is found in the Green operator, nevertheless, it leads to much more accurate local fields, particularly in the very stiff or soft inclusions and in the vicinity of interfaces. The convergence rate is also found to be much faster compared with the different methods employing the original operator, in particular for highly-contrasted media. Different finite difference and finite element discretizations have also been introduced (Schneider et al., 2016, 2017; Djaka et al., 2017; Eloh et al., 2019). Brisard and Dormieux (2010, 2012) introduced a discretization by voxel-wise constant finite elements based

on the Hashin-Shtrikman variational principle (Hashin and Shtrikman, 1962). Also based on the same principle, Tu et al. (2020) discretizes the problem using splines instead.

In Yvonnet (2012), unlike other algorithms presented so far based on the Fourier transform, the scheme put forth strictly operates in the real-space domain and removes the numerical Fourier and inverse Fourier transforms at each iteration. For this purpose, the linear operator related to the Lippmann–Schwinger equation is constructed numerically employing transformation tensors in the real-space domain.

Concerning the approximate discretization of microstructure features, more precisely of the voxels which include the interface between phases, Mareau and Robert (2017) proposes the use of composite voxel methods. These methods use simple homogenization rules to calculate the effective behavior of heterogeneous voxels, capturing more accurately, the fact they contain material that belongs to different phases. Another example of similar techniques can be found in Kabel et al. (2017).

Lucarini and Segurado (2019b) present a method completely distinct from the ones presented so far in that the unknown field is not the strain field but the displacement field. It is shown that the algorithm does not require the definition of a reference medium and that the linear systems which arise in the method are fully ranked and therefore admit the use of preconditioners. Furthermore, in the iterative solution procedure, the convergence rate is higher than the FFT-based variational approach, and the memory usage lower.

In To and Bonnet (2020) an FFT-based numerical scheme to compute the effective conductivity of porous materials is developed. To avoid the convergence issues due to the nonuniqueness of the full field solution, the problem is reformulated using the temperature field in the skeleton as an unknown variable. Thus, in the derived governing equation, the internal temperature field can be computed from the value on the pore boundary.

Chapter 3

Variational formulation

3.1 Local problem and its weak form

In what follows, the microstructure of the material is to be represented by a periodic cell Ω_μ. In two dimensions, $\Omega_\mu = \left(-l_1/2, l_1/2\right) \times \left(-l_2/2, l_2/2\right)$ with area $v_{\mu,0} = l_1 l_2$. In three dimensions, $\Omega_\mu = \left(-l_1/2, l_1/2\right) \times \left(-l_2/2, l_2/2\right) \times \left(-l_3/2, l_3/2\right)$ with volume $v_{\mu,0} = l_1 l_2 l_3$. The material response at a point $\boldsymbol{Y} \in \Omega_{\mu,0}$ is specified by the constitutive relation $\boldsymbol{\sigma}_\mu(\boldsymbol{Y}, \boldsymbol{\varepsilon}_\mu(\boldsymbol{Y}))$ assigning the stress response $\boldsymbol{\sigma}_\mu$ to a given strain $\boldsymbol{\varepsilon}_\mu$ locally at $\boldsymbol{Y}$. Furthermore, the total strain $\boldsymbol{\varepsilon}_\mu$ is split into a homogeneous average strain tensor present at the macroscopic point $\boldsymbol{X}$, $\boldsymbol{\varepsilon}(\boldsymbol{X})$, and an Ω_μ-periodic fluctuating strain field $\tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y})$, i.e.

$$\boldsymbol{\varepsilon}_\mu(\boldsymbol{Y}) = \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y}) \text{ for } \boldsymbol{Y} \in \Omega_{\mu,0}, \quad \int_{\Omega_{\mu,0}} \tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y}) \mathrm{d}v = \boldsymbol{0}. \tag{3.1}$$

The average strain $\boldsymbol{\varepsilon}(\boldsymbol{X})$ represents a given macro-scale excitation, while the fluctuating micro-scale strain field $\tilde{\boldsymbol{\varepsilon}}_\mu$ is the primary unknown.

The fluctuating strain field $\tilde{\boldsymbol{\varepsilon}}_\mu$ is determined by the stress equilibrium and strain compatibility conditions, which under quasi-static assumptions and in small strains read as,

$$\operatorname{div}\left[\boldsymbol{\sigma}_\mu\left(\boldsymbol{Y}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y})\right)\right] = 0 \text{ for } \boldsymbol{Y} \in \Omega_{\mu,0}, \tag{3.2}$$

$$\tilde{\boldsymbol{\varepsilon}}_\mu \in \mathcal{E} = \left\{\nabla_0^{\mathrm{s}} \tilde{\boldsymbol{u}}_\mu \mid \tilde{\boldsymbol{u}}_\mu \text{ is an } \Omega_\mu\text{-periodic displacement field}\right\}, \tag{3.3}$$

where ∇_0^{s} stands for the symmetrized gradient operator. For the numerical treatment, the local problem (3.2) is recast into the weak form, which amounts to finding $\tilde{\boldsymbol{\varepsilon}}_\mu \in \mathcal{E}$ such that

$$\int_{\Omega_{\mu,0}} \delta\tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y}) : \boldsymbol{\sigma}_\mu\left(\boldsymbol{Y}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y})\right) \mathrm{d}v = 0, \tag{3.4}$$

holds for all $\delta\tilde{\boldsymbol{\varepsilon}}_\mu \in \mathcal{E}$ (where use has been made of the periodicity of the problem eliminate the boundary term).

3.2 Compatibility

The main difference in how one proceeds from the weak form (3.4) with respect to the conventional FE method is in the way in which the compatibility constraint,

Equation (3.3), is imposed for both the solution $\tilde{\boldsymbol{\varepsilon}}_\mu$ and the test fields $\delta\tilde{\boldsymbol{\varepsilon}}_\mu$. Commonly, these quantities are expressed with the help of Ω_μ-periodic displacement fields $\tilde{\boldsymbol{u}}_\mu$ and $\delta\tilde{\boldsymbol{u}}_\mu$. As $\tilde{\boldsymbol{\varepsilon}}_\mu = \nabla_0^{\mathrm{s}}\tilde{\boldsymbol{u}}_\mu$ and $\delta\tilde{\boldsymbol{\varepsilon}}_\mu = \nabla_0^{\mathrm{s}}\delta\tilde{\boldsymbol{u}}_\mu$, their compatibility follows directly by definition (3.3). Fourier-based methods, on the other hand, work directly with the strains and impose the compatibility of the solution and test fields by different means. For the test strains $\delta\tilde{\boldsymbol{\varepsilon}}_\mu$ the compatibility is imposed via a projection operator $\boldsymbol{G}$,

$$\delta\tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y}) = [\boldsymbol{G} * \boldsymbol{\xi}](\boldsymbol{Y}) = \int_{\Omega_{\mu,0}} \boldsymbol{G}(\boldsymbol{Y}-\boldsymbol{Y}') : \boldsymbol{\xi}(\boldsymbol{Y}')\mathrm{d}v' \quad \text{for } \boldsymbol{Y} \in \Omega_{\mu,0}, \tag{3.5}$$

where $*$ stands for the convolution. This operator maps an extended test function $\boldsymbol{\xi}$, taken from the space all of square-integrable symmetric tensor fields $\mathcal{H}$, to its compatible part, i.e. $\boldsymbol{G} * \boldsymbol{\xi} \in \mathcal{E}$ for all $\boldsymbol{\xi} \in \mathcal{H}$. The compatibility of the solution, $\tilde{\boldsymbol{\varepsilon}}_\mu \in \mathcal{E}$, will be enforced by different means later in Section 3.5.

The convolution format of Equation (3.5) suggests that it can be conveniently treated using the Fourier transform when the Fourier transform of the operator $\boldsymbol{G}$ is known analytically. Indeed, direct application of the convolution theorem[1] reveals that

$$[\boldsymbol{G} * \boldsymbol{\xi}](\boldsymbol{Y}) = \sum_{\boldsymbol{k}\in\mathbb{Z}^d} \check{\boldsymbol{G}}(\boldsymbol{k}) : \check{\boldsymbol{\xi}}(\boldsymbol{k})\varphi^{\boldsymbol{k}}(\boldsymbol{Y}) \quad \text{for } \boldsymbol{Y} \in \Omega_{\mu,0}, \tag{3.6}$$

where $\boldsymbol{k}$ is the discrete frequency vector in the two-dimensional Fourier domain $\mathbb{Z}^d$ with d equal to the dimension of the problem, and $\varphi^{\boldsymbol{k}}$ is the complex-valued Fourier basis function. These can be written as

$$\varphi^{\boldsymbol{k}}(\boldsymbol{Y}) = \exp\left(\mathrm{i}\boldsymbol{Y}\cdot\boldsymbol{\zeta}(\boldsymbol{k})\right) \text{ for } \boldsymbol{Y} \in \Omega_{\mu,0}, \tag{3.7}$$

where the scaled frequencies ζ_i account for the size of the unit cell through $\zeta_i(\boldsymbol{k}) = 2\pi k_i / l_i$, and $\check{\boldsymbol{\xi}}(\boldsymbol{k})$ stands for the complex-valued Fourier transform of $\boldsymbol{\xi}(\boldsymbol{Y})$,

$$\check{\boldsymbol{\xi}}(\boldsymbol{k}) = \frac{1}{v_{\mu,0}} \int_{\Omega_{\mu,0}} \boldsymbol{\xi}(\boldsymbol{Y})\varphi^{-\boldsymbol{k}}(\boldsymbol{Y})\mathrm{d}v \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d. \tag{3.8}$$

The closed-form expression for the Fourier transform of the projection operator $\check{\boldsymbol{G}}$ can be found in Equation (3.23), from which it follows that $\check{\boldsymbol{G}}$ is a self-adjoint operator[2]. Notice that no approximation is made in (3.6) because all quantities are Ω_μ-periodic and the sum is infinite.

Substituting (3.6) into the weak formulation in Equation (3.4) and employing the self-adjointedness of $\boldsymbol{G}$ provides an equivalent characterization of the unknown strain field $\tilde{\boldsymbol{\varepsilon}}_\mu \in \mathcal{E}$:

$$\int_{\Omega_{\mu,0}} [\boldsymbol{G} * \boldsymbol{\xi}](\boldsymbol{Y}) : \boldsymbol{\sigma}_\mu\Big(\boldsymbol{Y}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y})\Big)\mathrm{d}v = \int_{\Omega_{\mu,0}} \boldsymbol{\xi}(\boldsymbol{Y}) : [\boldsymbol{G} * \boldsymbol{\sigma}_\mu]\Big(\boldsymbol{Y}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y})\Big)\mathrm{d}v = 0, \tag{3.9}$$

for all $\boldsymbol{\xi} \in \mathcal{H}$. Because the extended test functions $\boldsymbol{\xi}$ are no longer constrained to be compatible, this form is better suited for the discretization than the original one in Equation (3.9).

[1] The convolutin theorem for Fourier Transforms reads: $\mathscr{F}(f * g) = \mathscr{F}(f)\mathscr{F}(g)$, for appropriate f and g.

[2] A self-adjoint operator A satisfies $(Af_1, f_2) = (f_1, Af_2)$.

3.3 Basis functions

The basis functions rely on an underlying regular grid of pixels $\boldsymbol{n}_\nu = [n_{\nu,1}, n_{\nu,2}]$ for 2D and of voxels $\boldsymbol{n}_\nu = [n_{\nu,1}, n_{\nu,2}, n_{\nu,3}]$ with $n_\nu = n_{\nu,1} \cdot n_{\nu,2}$ and $n_\nu = n_{\nu,1} \cdot n_{\nu,2} \cdot n_{\nu,3}$ nodes, respectively, along each coordinate, see Figure **??**.

$$\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu} = \sum_{i=1}^{d} \frac{k_i l_i}{n_{\nu,i}} \boldsymbol{e}_i \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}, \text{ with } d = 2 \text{ or } 3\ , \tag{3.10}$$

on which the microstructure is sampled, where $\boldsymbol{e}_i$, $i = 1,2,3$, are the unit basis vectors. As explained below, only grids with an odd number of nodes will be considered. The individual nodes are indexed by a parameter $\boldsymbol{k}$ from a reduced index set

$$\mathbb{Z}^d_{\boldsymbol{n}_\nu} = \left\{ \boldsymbol{k} \in \mathbb{Z}^d \mid \forall i \in [1,d] \cap \mathbb{Z} \left(-\frac{n_{\nu,i}}{2} < k_i < \frac{n_{\nu,i}}{2} \right) \right\} \quad \text{with } d = 2 \text{ or } 3, \tag{3.11}$$

it will become clear later that the indices $\boldsymbol{k}$ can be naturally identified with the discrete frequencies from (3.3). Finally, we assign the integration weight $w = v_{\mu,0}/n_\nu$, equal to the pixel/voxel size, to each node.

It is convenient to use the *fundamental trigonometric polynomials* defined on the grid $\mathbb{Z}^2_{\boldsymbol{n}_\nu}$,

$$\varphi^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}(\boldsymbol{Y}) = \frac{1}{n_\nu} \sum_{\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_\nu}} \omega^{-\boldsymbol{k}\boldsymbol{m}}_{\boldsymbol{n}_\nu} \varphi^{\boldsymbol{m}}(\boldsymbol{k}) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_\nu}, \tag{3.12}$$

as the basis functions to approximate the weak form in Equation (3.9). Here, $\varphi^{\boldsymbol{m}}$ stands for the Fourier basis function (Equation (3.7))) and $\omega^{\boldsymbol{k}\boldsymbol{m}}_{\boldsymbol{n}_\nu}$ are the complex-valued coefficients of the Discrete Fourier Transform (DFT),

$$\omega^{\boldsymbol{k}\boldsymbol{m}}_{\boldsymbol{n}_\nu} = \omega^{\boldsymbol{m}\boldsymbol{k}}_{\boldsymbol{n}_\nu} = \varphi^{\boldsymbol{k}}\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_\nu}\right) = \exp\left(\mathrm{i}\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu} \cdot \boldsymbol{\zeta}(\boldsymbol{m})\right) \text{ for } \boldsymbol{k}, \boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_\nu}. \tag{3.13}$$

The solution $\tilde{\boldsymbol{\varepsilon}}_\mu$ and the test functions $\boldsymbol{\xi}$ in Equation (3.6) will be approximated as a linear combination of the basis functions $\varphi^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}$; the corresponding approximation space of the tensor-valued trigonometric polynomials will be referred to as $\mathcal{T}_{\boldsymbol{n}_\nu}$. These approximations are conforming, i.e., $\mathcal{T}_{\boldsymbol{n}_\nu} \subset \mathcal{H}$, as long as the number of nodes n_ν is odd. This conformity is lost when n_ν is even, resulting in a much more elaborate treatment.

The computational convenience of trigonometric polynomials follows from the fact that they can be efficiently manipulated using the Fast Fourier Transform (FFT), because of (i) the involvement of the DFT coefficients $\omega^{\boldsymbol{k}\boldsymbol{m}}_{\boldsymbol{n}_\nu}$ in Equation (3.12) and (ii) the ability to work with quantities defined in the Fourier space, because they incorporate the Fourier basis functions $\varphi^{\boldsymbol{m}}$.

In what follows, the most important steps needed to discretize the weak form in Equation (3.4) are collected.

As can be seen from Figure **??**, in the real space the fundamental trigonometric polynomials are not locally supported, unlike the conventional Finite Element shape functions, however they are still interpolatory and form the partition-of-unity, because they satisfy

$$\varphi^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_\nu}\right) = \delta^{\boldsymbol{k}\boldsymbol{m}} \text{ for } \boldsymbol{k}, \boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_\nu}, \quad \sum_{\boldsymbol{k} \in \mathbb{Z}^2_{\boldsymbol{n}_\nu}} \varphi^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}(\boldsymbol{Y}) = 1 \text{ for } \boldsymbol{Y} \in \Omega_{\mu,0}, \tag{3.14}$$

where δ^{km} is the Kronecker delta. In the Fourier domain, they are locally supported on $\mathbb{Z}^d_{n_v}$,

$$\check{\varphi}^{k}_{n_v}(m) = 0 \quad \text{for } k \in \mathbb{Z}^d_{n_v}, m \in \mathbb{Z}^d \setminus \mathbb{Z}^d_{n_v}, \tag{3.15}$$

because their definition (Equation (3.12)) contains only the Fourier basis functions φ^m associated with the frequencies from the grid $\mathbb{Z}^d_{n_v}$.

As a consequence, every trigonometric polynomial $\tau \in \mathcal{T}_{n_v}$ admits two equivalent representations on the same grid $\mathbb{Z}^d_{n_v}$ that involve its nodal values $\tau\left(Y^k_{n_v}\right)$, and the Fourier coefficients $\check{\tau}(k)$. Their mutual relation is established by the forward and inverse DFTs,

$$\check{\tau}(k) = \mathcal{DFT}\left(\tau\right)(k) = \frac{1}{n_v} \sum_{m \in \mathbb{Z}^d_{n_v}} \omega^{-km}_{n_v} \tau\left(Y^m_{n_v}\right) \quad \text{for } k \in \mathbb{Z}^d_{n_v}, \tag{3.16}$$

$$\tau\left(Y^k_{n_v}\right) = \mathcal{DFT}^{-1}\left(\check{\tau}\right)(Y^k_{n_v}) = \sum_{m \in \mathbb{Z}^d_{n_v}} \omega^{km}_{n_v} \check{\tau}(m) \quad \text{for } k \in \mathbb{Z}^d_{n_v}. \tag{3.17}$$

3.3.1 Numerical integration

The scalar product of two trigonometric polynomials $\tau \in \mathcal{T}_{n_v}$ and $\theta \in \mathcal{T}_{n_v}$ can be evaluated exactly by the trapezoidal rule,

$$\int_{\Omega_{\mu,0}} \tau(Y) : \theta(Y) \mathrm{d}v = w \sum_{k \in \mathbb{Z}^d_{n_v}} \tau\left(Y^k_{n_v}\right) : \theta\left(Y^k_{n_v}\right), \tag{3.18}$$

which assigns the same integration weight, equal to the pixel area w, to each grid node.

3.3.2 Convolution

Convolution. of a trigonometric polynomial $\tau \in \mathcal{T}_{n_v}$ with the projection operator G from (3.5) can be evaluated efficiently at the grid nodes $Y^k_{n_v}$ by DFT. Accordingly, from Equation (3.6) one finds

$$[G * \tau]\left(Y^k_{n_v}\right) = \sum_{m \in \mathbb{Z}^d} \check{G}(m) : \left[\check{\tau}(m) \varphi^m\left(Y^k_{n_v}\right)\right]. \tag{3.19}$$

Noting that in the frequency domain the basis functions have compact support (Equation (3.15)) and applying the definition for the coefficients of the DFT (Equation (3.13)), yields

$$\sum_{m \in \mathbb{Z}^d} \check{G}(m) : \left[\check{\tau}(m) \varphi^m\left(Y^k_{n_v}\right)\right] = \sum_{m \in \mathbb{Z}^d_{n_v}} \check{G}(m) : \left[\check{\tau}(m) \omega^{km}_{n_v}\right]. \tag{3.20}$$

Thus, from the definition of the Discrete Fourier Transform in Equation (3.16), the desired result is achieved

$$[G * \tau]\left(Y^k_{n_v}\right) = \sum_{m \in \mathbb{Z}^d_{n_v}} \omega^{km}_{n_v} \check{G}(m) : \left[\frac{1}{n_v} \sum_{n \in \mathbb{Z}^d_{n_v}} \omega^{-mn}_{n_v} \tau\left(Y^n_{n_v}\right)\right], \tag{3.21}$$

which can be written in a more compact form as

$$[G * \tau]\left(Y^k_{n_v}\right) = \mathcal{DFT}^{-1}\left(\check{G} : \mathcal{DFT}\left(\tau\right)\right)\left(Y^k_{n_v}\right). \tag{3.22}$$

For the non-zero frequency $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v} \setminus \{\boldsymbol{0}\}$, the Fourier transform of the fourth-order projection operator $\check{\boldsymbol{G}}$ is provided by

$$\begin{aligned}\check{\boldsymbol{G}}_{ijlm}(\boldsymbol{k}) = &\frac{1}{2}\frac{\zeta_i(\boldsymbol{k})\delta_{jl}\zeta_m(\boldsymbol{k}) + \zeta_i(\boldsymbol{k})\delta_{jm}\zeta_l(\boldsymbol{k}) + \zeta_j(\boldsymbol{k})\delta_{il}\zeta_m(\boldsymbol{k}) + \zeta_j(\boldsymbol{k})\delta_{im}\zeta_l(\boldsymbol{k})}{\|\boldsymbol{\zeta}(\boldsymbol{k})\|^2} \\ &- \frac{\zeta_i(\boldsymbol{k})\zeta_j(\boldsymbol{k})\zeta_l(\boldsymbol{k})\zeta_m(\boldsymbol{k})}{\|\boldsymbol{\zeta}(\boldsymbol{k})\|^4},\end{aligned} \tag{3.23}$$

where ζ_i are the scaled frequencies and δ_{ij} stands for the Kronecker delta. For $\boldsymbol{k} = \boldsymbol{0}$, $\check{\boldsymbol{G}}_{ijlm}(\boldsymbol{0}) = 0$ because of the zero-mean property. See Appendix (**??**) for the proof that $\boldsymbol{G}$ is the operator with the desired properties described above.

3.4 Discretization

One is now in a position to discretize the weak form of Equation (3.4) with trigonometric polynomials. Following the standard Galerkin procedure, the unknown field $\tilde{\boldsymbol{\varepsilon}}_\mu$ and the test field $\boldsymbol{\xi}$ are approximated in the same way

$$\tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y}) \approx \sum_{\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y}) \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}\right), \tag{3.24}$$

$$\boldsymbol{\xi}(\boldsymbol{Y}) \approx \sum_{\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y}) \boldsymbol{\xi}\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}\right). \tag{3.25}$$

The nodal strains, $\tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}\right)$ for $\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$, and the nodal values of test fields, $\boldsymbol{\xi}\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}\right)$ for $\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$, are respectively located in the corresponding finite-dimensional spaces $\mathbb{E}_{\boldsymbol{n}_v} \subset \mathbb{T}_{\boldsymbol{n}_v}$. The (constrained) space $\mathbb{E}_{\boldsymbol{n}_v}$ thus collects the nodal values of compatible trigonometric polynomials from $\mathcal{T}_{\boldsymbol{n}_v} \cap \mathcal{E}$, whereas (unconstrained) $\mathbb{T}_{\boldsymbol{n}_v}$ collects nodal values of all trigonometric polynomials from $\mathcal{T}_{\boldsymbol{n}_v}$.

Introducing these expansions into Equation (3.9) yields

$$\int_{\Omega_{\mu,0}} \Big(\sum_{\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y}) \boldsymbol{\xi}\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}\right) \Big) : [\boldsymbol{G} * \boldsymbol{\sigma}_\mu]\Big(\boldsymbol{Y}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \sum_{\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y}) \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}\right)\Big) \mathrm{d}v = 0, \tag{3.26}$$

to be satisfied for arbitrary $\boldsymbol{\xi}\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}\right)$ from $\mathbb{T}_{n_v}$, $\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$. Application of the trapezoidal quadrature rule (Equation (3.18)) provides

$$w \sum_{\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}} \Big(\sum_{\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}) \boldsymbol{\xi}\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}\right) \Big) : [\boldsymbol{G} * \boldsymbol{\sigma}_\mu]\Big(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \sum_{\boldsymbol{m} \in \mathbb{Z}^d_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}\right)\Big) \approx 0, \tag{3.27}$$

note that this step introduces an approximation error because the constitutive relation $\boldsymbol{\sigma}_\mu$ does not necessarily map trigonometric polynomials to trigonometric polynomials. By exploring the Kronecker delta property of the basis functions (Equation (3.14)), the previous relation further simplifies to

$$\sum_{\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}} \boldsymbol{\xi}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) : [\boldsymbol{G} * \boldsymbol{\sigma}_\mu]\Big(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\Big) = 0. \tag{3.28}$$

Because the test strains $\boldsymbol{\xi}(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v})$, for $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$, are arbitrary, one finally obtains from (3.28) that the nodal strain values, $\tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}) \in \mathbb{E}_{\boldsymbol{n}_v}$, for $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$, follow from the system of

non-linear nodal equilibrium conditions,

$$[\boldsymbol{G} * \boldsymbol{\sigma}_\mu]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right) = \boldsymbol{0} \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}, \tag{3.29}$$

which can be also be written as

$$\mathscr{D}\mathscr{F}\mathscr{T}^{-1}\left(\tilde{\boldsymbol{G}} : \mathscr{D}\mathscr{F}\mathscr{T}\left(\boldsymbol{\sigma}_\mu\right)\right)\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right) = \boldsymbol{0} \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}. \tag{3.30}$$

where the non-linearity originates solely from the constitutive relation, because the projection operator $\boldsymbol{G}$ is independent of $\tilde{\boldsymbol{\varepsilon}}_\mu$.

Therefore, apart from enforcing the strain compatibility, the symmetric matrix $\boldsymbol{G}$ also enforces the nodal equilibrium conditions. Also notice that, in analogy to Section 3.2, the constraint $\tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}) \in \mathbb{E}_{\boldsymbol{n}_v}$, for $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$, still needs to be accounted for.

3.5 Linearization

The conventional Newton scheme is used to find the solution to the system (3.30) iteratively. For this purpose, we express the nodal unknowns in the $(i+1)$-th iteration as

$$\tilde{\boldsymbol{\varepsilon}}^{(i+1)}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) = \tilde{\boldsymbol{\varepsilon}}^{(i)}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) + \delta\tilde{\boldsymbol{\varepsilon}}^{(i+1)}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}. \tag{3.31}$$

Equation (3.30) is then linearized around $\tilde{\boldsymbol{\varepsilon}}^{(i)}_\mu$, with $\tilde{\boldsymbol{\varepsilon}}^{(0)}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) \in \mathbb{E}_{\boldsymbol{n}_v}$, for $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$. As a result, one obtains the linear system for the nodal strain increment $\delta\tilde{\boldsymbol{\varepsilon}}^{(i+1)}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) \in \mathbb{E}_{\boldsymbol{n}_v}$, for $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$,

$$\begin{aligned}[\boldsymbol{G} * \boldsymbol{K}^{(i)}]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right)\delta\tilde{\boldsymbol{\varepsilon}}^{(i+1)}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) \\ = -[\boldsymbol{G} * \boldsymbol{\sigma}_\mu]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v},\end{aligned} \tag{3.32}$$

where the local tangent matrix $\boldsymbol{K}^{(i)}$ is given by

$$\boldsymbol{K}^{(i)}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right) = \frac{\partial \boldsymbol{\sigma}_\mu}{\partial \boldsymbol{\varepsilon}_\mu}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right) \text{ for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}. \tag{3.33}$$

Three considerations must be taken into account when solving the linearized system (Equation (3.32)): (i) the corresponding system matrix is dense, singular, and very costly to assemble for large grids, (ii) the multiplication with the system matrix is cheap and does not require the matrix assembly, because it involves the multiplication with structurally sparse matrices (recall that the convolution with $\boldsymbol{G}$ can be performed efficiently by FFT (Equation (3.22)), and (iii) the solver must enforce the compatibility constraint $\tilde{\boldsymbol{\varepsilon}}^{(i+1)}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) \in \mathbb{E}_{\boldsymbol{n}_v}$, for $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$.

All these aspects invite the application of (projected) iterative solvers involving only matrix-vector products, such as specific-purpose solvers [29], or selected general-purpose iterative algorithms for symmetric positive systems [16], because the operator $\boldsymbol{G}$ enforces the compatibility and equilibrium conditions simultaneously. Specifically, we will use the conventional Conjugate Gradient algorithm [30], which enforces the compatibility constraint at every iteration and outperforms alternative solvers in terms of convergence rate, as demonstrated recently in [16].

3.6 Algorithm

To summarize, the incremental-iterative Newton-Conjugate Gradient solver is outlined as a pseudo-algorithm in Box 3.1. For later reference, it is emphasized that the algorithm implements two termination criteria for the Newton and the Conjugate Gradient solvers that involve the two tolerances η^{NW} and η^{CG}, respectively. Finally, note that the same procedure applies to history- and rate-dependent material laws, once the time-incremental stress-strain laws and consistent constitutive tangents are adopted, replacing $\boldsymbol{\sigma}_{\mu}^{(i)}$ and $\boldsymbol{K}^{(i)}$ in Equation (3.32).

Box 3.1: Pseudo-code for the Newton-CG algorithm solving the equilibrium problem for non-linear behavior.

(i) Set the initial conditions: $t = t_0$

(ii) Set strain fluctuations to zero: $\tilde{\boldsymbol{\varepsilon}}_{\mu}^{(0)}(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}) = \boldsymbol{0}$ for $\boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^{d}$

(iii) Initialize other history variables (material dependent)

(iv) Enter increment loop

(1) Set Newton counter to zero: $i = 0$

(2) Initialize, indicating no convergence yet: $\delta\tilde{\boldsymbol{\varepsilon}}_{\mu}^{(i)}(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}) = \infty$ for $\boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^{d}$

(3) Enter Newton loop

(a) Compute the constitutive response (material dependent):

$$\boldsymbol{\sigma}_{\mu}^{(i)}(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}) = \boldsymbol{\sigma}_{\mu}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_{\mu}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right)\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^{d}$$

(b) Compute the consistent tangent (material dependent):

$$\boldsymbol{K}^{(i)}(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}) = \frac{\partial \boldsymbol{\sigma}_{\mu}}{\partial \boldsymbol{\varepsilon}_{\mu}}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}, \boldsymbol{\varepsilon}(\boldsymbol{X}) + \tilde{\boldsymbol{\varepsilon}}_{\mu}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right)\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^{d}$$

(c) Use the standard Conjugate Gradient method to solve

$$[\boldsymbol{G} * \boldsymbol{K}^{(i)}]\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right)\delta\tilde{\boldsymbol{\varepsilon}}_{\mu}^{(i+1)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) = -[\boldsymbol{G} * \boldsymbol{\sigma}_{\mu}^{(i)}]\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^{d}$$

until the desired accuracy η^{CG} is reached.

(d) Update the strain: $\tilde{\boldsymbol{\varepsilon}}_{\mu}^{(i+1)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) = \tilde{\boldsymbol{\varepsilon}}_{\mu}^{(i)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) + \delta\tilde{\boldsymbol{\varepsilon}}_{\mu}^{(i+1)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right)$

(e) If the desired accuracy η^{NW} has not been reached, update $i = i+1$ and go to step (a).

(4) Set the "intial guess" for the next increment: $\tilde{\boldsymbol{\varepsilon}}_{\mu}^{(t+\Delta t)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) = \tilde{\boldsymbol{\varepsilon}}_{\mu}^{(i)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right)$

(5) Update other history variables (material dependent)

(6) If $t \leq T_0$, proceed to next increment $t = t + \Delta t$ and go to step (1).

3.7 Extension to finite strain

This section presents the adaptations needed to extend the scheme introduced above to finite strains.

3.7.1 Problem statement

The goal is again to solve for static mechanical equilibrium in the periodic cell for a given applied overall deformation. The balance of linear momentum, pulled-back to the (undeformed) reference configuration, reads

$$\operatorname{div}_0 \boldsymbol{P}_\mu = \boldsymbol{0} \tag{3.34}$$

involving the divergence with respect to the reference configuration of the transposed first Piola-Kirchhoff stress tensor $\boldsymbol{P}_\mu$. The stress $\boldsymbol{P}_\mu$ depends non-linearly on the deformation gradient $\boldsymbol{F}_\mu$

$$\boldsymbol{P}_\mu = \boldsymbol{P}_\mu(\boldsymbol{F}_\mu). \tag{3.35}$$

3.7.2 Weak form

The integral form is obtained by multiplying (3.34) with test functions $\delta\boldsymbol{y}$ and integrating over the reference domain $\Omega_{\mu,0}$

$$\int_{\Omega_{\mu,0}} \delta\boldsymbol{y} \cdot \left(\operatorname{div}_0 \boldsymbol{P}_\mu\right) \mathrm{d}v = 0, \tag{3.36}$$

which must hold for all periodic $\delta\boldsymbol{y}$. Subsequently, integration by parts is applied in conjunction with Gauss' divergence theorem. The boundary term that arises vanishes because of periodicity. The result reads

$$\int_{\Omega_{\mu,0}} \boldsymbol{P}_\mu : \left(\operatorname{div}_0 \delta\boldsymbol{y}\right) \mathrm{d}v = 0, \tag{3.37}$$

where : denotes a double tensor contraction. To make use of the FFT-based methods, the weak form of Equation (3.37) is accordingly reformulated using the deformation gradient $\boldsymbol{F}_\mu$ as

$$\int_{\Omega_{\mu,0}} \boldsymbol{P}_\mu : \delta\boldsymbol{F}_\mu \, \mathrm{d}v = 0, \tag{3.38}$$

in which the test functions $\delta\boldsymbol{F}_\mu$ are periodic and compatible. Note that compatibility is guaranteed when $\delta\boldsymbol{F}_\mu$ is the gradient of a virtual position vector, as in Finite Elements, but now must be enforced as a constraint in conjunction with Equation (3.38).

3.7.3 Projection to a compatible solution space

As in the case of small strains, the compatibility of the test functions $\delta\boldsymbol{F}_\mu$ is imposed employing a projection operator $\boldsymbol{G}$ (different from the previous one). It maps an arbitrary field $\bar{\boldsymbol{A}}$ to its compatible part $\boldsymbol{A}$ through

$$\boldsymbol{G} * \overline{\boldsymbol{A}} = \boldsymbol{A}, \tag{3.39}$$

wherein $*$ is the convolution operator. The convolution can be evaluated in Fourier space as a simple, local, double tensor contraction. Furthermore, $\boldsymbol{G}$ has a simple closed-form expression in Fourier space,

$$\check{\boldsymbol{G}}_{ijlm}(\boldsymbol{k}) = \begin{cases} 0 & \text{for } \boldsymbol{k} = \boldsymbol{0} \\ \dfrac{\delta_{im}\zeta_j(\boldsymbol{k})\zeta_l(\boldsymbol{k})}{\|\boldsymbol{\zeta}\|^2} & \text{otherwise} \end{cases}, \tag{3.40}$$

wherein $\boldsymbol{k}$ is the (spatial) frequency vector and ζ_i are the scaled frequencies that account for the size of the cell through $\zeta_i(\boldsymbol{k}) = k_i/L_i$ (with L_i the size of the periodic cell in direction i). Its background and interpretation are discussed in Appendix **??**.

Application of Equation 3.39 to the weak form of Equation 3.38 results in

$$\int_{\Omega_{\mu,0}} (\boldsymbol{G} * \delta\bar{\boldsymbol{F}}_\mu) : \boldsymbol{P}_\mu^T \mathrm{d}v = \int_{\Omega_{\mu,0}} \delta\bar{\boldsymbol{F}}_\mu : (\boldsymbol{G} * \boldsymbol{P}_\mu) \mathrm{d}v = 0, \tag{3.41}$$

whereby the symmetry of $\boldsymbol{G}$ has been used. Equation (3.41) should now hold for arbitrary, i.e. not necessarily compatible, periodic test functions $\delta\bar{\boldsymbol{F}}_\mu$. Please note that the deformation gradient $\boldsymbol{F}_\mu$, hidden in the stress $\boldsymbol{P}_\mu$ through Equation (3.35), should still satisfy the compatibility constraint.

3.7.4 Discretization

Adopting a Galerkin scheme, the unknown field $\boldsymbol{F}_\mu$ and the test functions $\delta\bar{\boldsymbol{F}}_\mu$ are discretized in the same way. Like in Finite Elements, the continuous fields $\boldsymbol{F}_\mu$ and $\delta\bar{\boldsymbol{F}}_\mu$ are approximated by a finite number of n nodal values that are multiplied with shape functions associated with each node, i.e.

$$\boldsymbol{F}_\mu(\boldsymbol{Y}) \approx \sum_{\boldsymbol{m}\in\mathbb{Z}^2_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y})\boldsymbol{F}_\mu(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}), \tag{3.42}$$

$$\delta\bar{\boldsymbol{F}}_\mu(\boldsymbol{Y}) \approx \sum_{\boldsymbol{m}\in\mathbb{Z}^2_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y})\bar{\boldsymbol{F}}_\mu(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}). \tag{3.43}$$

Just as before, the Fundamental trigonometric polynomials are used as shape functions.

The discretization is applied to the weak form (Equation (3.41)) which therefore becomes

$$\int_{\Omega_{\mu,0}} \Big(\sum_{\boldsymbol{m}\in\mathbb{Z}^2_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y})\bar{\boldsymbol{F}}_\mu(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}) \Big) : [\boldsymbol{G} * \boldsymbol{P}_\mu]\Big(\boldsymbol{Y}^{\boldsymbol{k}}_{n_v}, \sum_{\boldsymbol{m}\in\mathbb{Z}^2_{\boldsymbol{n}_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y})\boldsymbol{F}_\mu(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v})\Big) \mathrm{d}v = 0. \tag{3.44}$$

3.7.5 Quadrature

The integration is again performed using the trapezoidal rule, which applied to Equation (3.44) yields

$$w \sum_{\boldsymbol{k}\in\mathbb{Z}^2_{n_v}} \Big(\sum_{\boldsymbol{m}\in\mathbb{Z}^2_{n_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y}^{\boldsymbol{k}}_{n_v})\bar{\boldsymbol{F}}_\mu(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v}) \Big) : [\boldsymbol{G} * \boldsymbol{P}_\mu]\Big(\boldsymbol{Y}^{\boldsymbol{k}}_{n_v}, \sum_{\boldsymbol{m}\in\mathbb{Z}^2_{n_v}} \varphi^{\boldsymbol{m}}_{\boldsymbol{n}_v}(\boldsymbol{Y}^{\boldsymbol{k}}_{n_v})\boldsymbol{F}_\mu(\boldsymbol{Y}^{\boldsymbol{m}}_{\boldsymbol{n}_v})\Big) \mathrm{d}v \approx 0. \tag{3.45}$$

The fact that the shape functions can be expressed in terms of the discrete Fourier coefficients is now exploited; and the delta property of the shape functions (Equation (3.14)), writing

$$\sum_{\boldsymbol{k}\in\mathbb{Z}^d_{\boldsymbol{n}_v}} \bar{\boldsymbol{F}}_\mu(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}) : [\boldsymbol{G} * \boldsymbol{P}_\mu]\Big(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{F}_\mu(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v})\Big) = 0. \tag{3.46}$$

Because the test functions $\bar{\boldsymbol{F}}_\mu(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v})$, for $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$, are arbitrary, one finally obtains from (3.46) that the nodal strain values, $\boldsymbol{F}_\mu(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v})$, for $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$, follow from the system of non-linear nodal equilibrium conditions,

$$[\boldsymbol{G} * \boldsymbol{P}_\mu]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{F}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right) = \boldsymbol{0} \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}, \tag{3.47}$$

which can be also be written as

$$\mathscr{DFT}^{-1}\left(\tilde{\boldsymbol{G}} : \mathscr{DFT}\left(\boldsymbol{P}_\mu\right)\right)\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{F}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right) = \boldsymbol{0} \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}. \tag{3.48}$$

where the non-linearity originates solely from the constitutive relation, because the projection operator $\boldsymbol{G}$ is independent of $\boldsymbol{F}_\mu$.

Therefore, apart from enforcing the strain compatibility, the symmetric matrix $\boldsymbol{G}$ also enforces the nodal equilibrium conditions. Also notice, that once more, the constraint regarding the compatibility of $\boldsymbol{F}_\mu$, still needs to be accounted for.

The weak form in Equation (3.48) is a non-linear equation, as the material model involves a non-linear relation between the first Piola-Kirchhoff stress and the deformation gradient. Newton iterations are employed to solve the nodal equilibrium equations (3.48). To this end the nodal unknowns at iteration $i+1$ are expressed as

$$\boldsymbol{F}_\mu{}^{(i+1)}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) = \boldsymbol{F}_\mu{}^{(i)}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) + \delta\boldsymbol{F}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}, \tag{3.49}$$

where $\boldsymbol{F}_\mu{}^{(i)}$ are the last known iterative values of the deformation gradients and $\delta\boldsymbol{F}_\mu$ are their iterative updates. Note that δ is now used to indicate a small variation. The stresses are linearized around $\boldsymbol{F}_\mu{}^{(i)}$. In a material point this corresponds to

$$\delta\boldsymbol{P}_\mu = \boldsymbol{K}^{(i)} : \delta\boldsymbol{F}_\mu. \tag{3.50}$$

Combined with the discretized weak form in Equation (3.47), the iterative update $\delta\boldsymbol{F}_\mu$ is found by solving the following linearized system

$$[\boldsymbol{G} * \boldsymbol{K}^{(i)}]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{F}^{(i)}_\mu\left(Y^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right) : \delta\boldsymbol{F}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right) = -[\boldsymbol{G} * \boldsymbol{P}_\mu]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v}, \boldsymbol{F}^{(i)}_\mu\left(Y^{\boldsymbol{k}}_{\boldsymbol{n}_v}\right)\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}. \tag{3.51}$$

Note that the compatibility of the deformation gradient field still needs to be enforced. This is done by solving the linear system of Equation (3.51) using an iterative solver which delivers a compatible solution in each iteration [18 – 21, 24]. To satisfy compatibility during the entire iterative process, projection-based iterative methods such as e.g. the conjugate gradient (CG) method and the generalized minimal residual method (GMRES), Chebyshev iterations, or Richardson iterations (used in the original Moulinec-Suquet algorithm [5, 6]) can be used [19, 20]. Alternatively, compatibility is satisfied only at convergence using the accelerated method of Ref. [25].

3.7.6 Implementation

The numerical algorithm requires the solution of (3.48) in an incremental-iterative fashion. Each increment thereby consists of Newton iterations updating the nodal deformation gradients $\boldsymbol{F}^{(i+1)}_\mu(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_v})$, for $\boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_v}$ using (3.49)-(3.51) until equilibrium is satisfied up to an accuracy η^{NW}, by employing the linearized constitutive response. The linear system in Equation (3.51) is solved up to an accuracy η^{CG} using the conjugate gradient iterative solver.

Boundary conditions With the periodic micro-fluctuations of $\boldsymbol{F}_\mu$ following from equilibrium and compatibility, only the macroscopic deformation or stress needs to be prescribed. Here only a fully prescribed macroscopic deformation gradient is considered $\bar{\boldsymbol{F}}_\mu$, as this is the easiest and the most efficient choice.

The starting point is an equilibrium state given by $\boldsymbol{F}_\mu^{(0)}$, to which a macroscopic deformation gradient $\bar{\boldsymbol{F}}_\mu$ is applied. More specifically, we apply the difference of $\boldsymbol{F}$ and to the mean of $\boldsymbol{F}_\mu^{(0)}$

$$\Delta\bar{\boldsymbol{F}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) = \bar{\boldsymbol{F}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) - \int_{\Omega_{\mu,0}} \boldsymbol{F}_\mu^{(0)}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) \mathrm{d}\nu \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_\nu}. \tag{3.52}$$

For the first Newton iteration, equilibrium reads

$$[\boldsymbol{G} * \boldsymbol{P}_\mu]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}, \boldsymbol{F}_\mu^{(0)}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) + \Delta\bar{\boldsymbol{F}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) + \delta\boldsymbol{F}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right)\right) = \boldsymbol{0} \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_\nu}. \tag{3.53}$$

Linearization of (3.53) results in

$$\begin{aligned}[\boldsymbol{G} * \boldsymbol{K}^{(0)}]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}, \boldsymbol{F}_\mu^{(0)}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right)\right) : \delta\boldsymbol{F}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) = \\ - [\boldsymbol{G} * \boldsymbol{K}^{(0)}]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}, \boldsymbol{F}_\mu^{(0)}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right)\right) : \Delta\bar{\boldsymbol{F}}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_\nu},\end{aligned} \tag{3.54}$$

where $\boldsymbol{K}^{(0)}$ is the constitutive tangent about $\boldsymbol{F}_\mu^{(0)}$. Note that use has been made of the fact that $\boldsymbol{F}_\mu^{(0)}$ is in equilibrium, i.e. that $[\boldsymbol{G} * \boldsymbol{P}_\mu]\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}, \boldsymbol{F}_\mu^{(0)}\right) = \boldsymbol{0}$. After solving the system in Equation (3.54) one sets

$$\boldsymbol{F}_\mu^{(1)}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) = \boldsymbol{F}_\mu^{(0)}\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) + \Delta\bar{\boldsymbol{F}}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) + \delta\boldsymbol{F}_\mu\left(\boldsymbol{Y}^{\boldsymbol{k}}_{\boldsymbol{n}_\nu}\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}^d_{\boldsymbol{n}_\nu}, \tag{3.55}$$

and proceed normally. It is thereby important to point out that the definition of $\mathbb{G}$ ensures that the mean

$$\int_{\Omega_{\mu,0}} \delta\boldsymbol{F} \mathrm{d}\nu = \boldsymbol{0}. \tag{3.56}$$

All iterations thus satisfy the prescribed $\bar{\boldsymbol{F}}$ exactly. The interpretation of Equation (3.54) is that, by solving the linear system, the macroscopic deformation, $\Delta\bar{\boldsymbol{F}}$, is distributed over this microstructure using the tangent $\boldsymbol{K}^{(0)}$, which contains the microstructural heterogeneity. Equation (3.54) therefore has strong similarities with the application of essential (Dirichlet) boundary conditions in the Finite Element Method.

Box 3.2 presents the pseudo-code for the Newton-CG scheme used to solve the non-linear equilibrium equations at finite strains.

Box 3.2: Pseudo-code for the Newton-CG algorithm solving the equilibrium problem for non-linear behavior at finite strains.

(i) Initialize $\boldsymbol{F}_\mu^{(0)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{(k)}\right) = \boldsymbol{I}$ for $\boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^d$ and history variables

(ii) Enter increment loop

(1) Set Newton counter to zero: $i = 0$

(2) Enter Newton loop

(a) Compute the constitutive response (material dependent): $\boldsymbol{F}_\mu^{(i)} \rightarrow \boldsymbol{K}^{(i)}, \boldsymbol{P}_\mu^{(i)}$

(b) According to

- If $i = 0$ then enforce the boundary condition:
  Solve

$$[\boldsymbol{G} * \boldsymbol{K}^{(0)}]\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}, \boldsymbol{F}_\mu^{(0)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right)\right) : \delta \boldsymbol{F}_\mu\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) = -[\boldsymbol{G} * \boldsymbol{K}^{(0)}]\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}, \boldsymbol{F}_\mu^{(0)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right)\right) : \Delta \bar{\boldsymbol{F}}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^d,$$

$$\boldsymbol{F}_\mu^{(1)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) = \boldsymbol{F}_\mu^{(0)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) + \Delta \bar{\boldsymbol{F}}_\mu\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) + \delta \boldsymbol{F}_\mu\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^d,$$

- else, enforce the equilibrium iteration

$$[\boldsymbol{G} * \boldsymbol{K}^{(i)}]\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}, \boldsymbol{F}_\mu^{(i)}\left(Y_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right)\right) : \delta \boldsymbol{F}_\mu\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) = -[\boldsymbol{G} * \boldsymbol{P}_\mu^{(i)}]\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}, \boldsymbol{F}_\mu^{(i)}\left(Y_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right)\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^d.$$

$$\boldsymbol{F}_\mu{}^{(i+1)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) = \boldsymbol{F}_\mu{}^{(i)}\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) + \delta \boldsymbol{F}_\mu\left(\boldsymbol{Y}_{\boldsymbol{n}_v}^{\boldsymbol{k}}\right) \quad \text{for } \boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{n}_v}^d,$$

(c) If the desired accuracy η^{NW} has not been reached, update index $i = i + 1$ and go to (a)

(3) Store the converged state $\boldsymbol{F}^{(i+1)}$ and the history variables, set $\boldsymbol{F}_\mu^{(0)} = \boldsymbol{F}_\mu^{(i+1)}$, and go to (1)

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