

Model order reduction for FE-FFT-based multiscale material modeling

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Summary

The material behavior of a structural component is determined by the underlying microstructure and its associated features and local interactions. Therefore, multiscale simulations can provide valuable information on the overall constitutive response of the material and thus on its use in practical applications. Since these simulations are generally computationally expensive, the application of suitable multiscale methods is a challenging task. In order to reduce the numerical costs, various model order reduction techniques have been developed and applied. The goal, and at the same time the challenge, of model order reduction techniques is to decrease the computational complexity and effort of the numerical simulations while maintaining high accuracy of the numerical results.

The given cumulative dissertation presents a collection of journal articles and conference proceedings contributing to this research field. It aims to generalize a framework for an efficient and accurate two-scale FE-FFT-based method, which is based on a coarsely discretized microstructure. Additionally, the thesis intends to significantly improve the accuracy of a reduced FFT-based microscale simulation, in which the computations in Fourier space are performed using a reduced set of Fourier modes.

Starting by addressing the motivation and research relevant questions of this dissertation, next a comprehensive literature review on the current trends in computational multiscale modeling as well as the latest developments in FFT-based microscale and FE-FFT-based two-scale methods is presented. Earlier works in this field are discussed in the first journal article, which provides an overview of several FFT-based algorithms and solvers including their applications, methods to reduce the effect of Gibbs oscillations, specific model order reduction techniques, and the FFT-based method in the context of FE-FFT-based two-scale simulations.

Subsequently, two papers deal with an efficient FE-FFT-based two-scale simulation framework applied to model the material behavior of viscoplastic polycrystals. Within this framework a coarsely discretized microstructure is used for the two-scale simulations, where the minimum number of grid points, which is required to generate accurate macroscopic results, is defined in a pre-processing step. Highly resolved microstructural results can be generated in a post-processing step. The papers focus on generalizing this framework to the finite strain regime and to the thermomechanically coupled case.

The following five works focus on a reduced FFT-based microscale simulation utilizing a decreased number of Fourier modes for the computations in Fourier space, wherein the accuracy of the obtained results directly depends on the choice of the considered Fourier modes. First, for the investigation of two-phase microstructures, a geometrically adapted sampling pattern

is introduced, which consists of the Fourier modes with the highest amplitudes resulting from a Fourier transformation of the characteristic function of the given microstructure. The characteristic function captures the representation of phases within the microstructure. Thereafter a strain-based sampling pattern is suggested, where the aforementioned characteristic function is replaced by the microstructural strain field. Compared to the results obtained with the geometrically adapted sampling pattern, this strain-based sampling pattern leads to even more accurate results. Furthermore, since the definition of a characteristic function is no longer required, it can be used to investigate complex polycrystalline microstructures with challenging microstructural effects, e.g., considering crystal plasticity or solid-solid phase transformations. Finally, to demonstrate the universality of the model order reduction technique, its application is shown in the context of various improvements for the FFT-based method. It is implemented, for example, in combination with finite-difference-based operator approximations to reduce the effect of Gibbs oscillations, or with fast gradient solvers to reduce the number of iterations required to reach a converged solution.

Zusammenfassung

Das Materialverhalten eines Bauteils wird durch seine zugrundeliegende Mikrostruktur und von ihren Merkmalen sowie lokalen Wechselwirkungen bestimmt. Mehrskalige Simulationen können daher wertvolle Informationen über das Gesamtverhalten des Werkstoffs und damit über seine Verwendungsmöglichkeiten in praktischen Anwendungen liefern. Da derartige Simulationen in der Regel sehr rechenintensiv sind, stellt die Anwendung geeigneter Multiskalenmethoden eine große Herausforderung dar. Um diesen numerischen Aufwand zu verringern, wurden verschiedene Modellreduktionstechniken entwickelt und angewendet. Das Ziel und zugleich die Herausforderung von Modellreduktionstechniken besteht darin, die Komplexität und den Aufwand numerischer Simulationen zu reduzieren und gleichzeitig eine hohe Genauigkeit der Ergebnisse zu gewährleisten.

Die vorliegende kumulative Dissertation setzt sich aus verschiedenen wissenschaftlichen Artikeln und Konferenzbeiträgen zusammen, die einen Beitrag zu diesem Forschungsgebiet leisten. Das Ziel der Dissertation liegt zum einen in der Verallgemeinerung eines Frameworks, welches für effiziente und genaue zweiskalige FE-FFT-basierte Simulation geeignet ist und für die zweiskalige Simulation nur eine grob diskretisierte Mikrostruktur berücksichtigt. Zum anderen soll die Genauigkeit einer reduzierten FFT-basierten Mikrostruktursimulation, bei der die Berechnungen im Fourierraum mit einer reduzierten Anzahl an Fourier-Modi durchgeführt werden, signifikant verbessert werden.

Zunächst werden die Motivation und die forschungsrelevanten Fragen dieser Dissertation dargelegt. Anschließend wird ein umfassender Literaturüberblick über die aktuellen Trends in der computergestützten mehrskaligen Materialmodellierung sowie über die neuesten Entwicklungen im Bereich der FFT-basierten Mikrostruktursimulation und der FE-FFT-basierten zweiskaligen Simulation gegeben. Frühere Veröffentlichungen auf diesem Gebiet werden im ersten Journalartikel diskutiert, der den aktuellen Stand der Technik der verschiedenen FFT-basierten Algorithmen und Solver sowie deren Anwendungen, der Methoden zur Minimierung der Auswirkungen von Gibbs-Oszillationen, der Techniken zur Modellreduktion und den aktuellen Stand der Technik für die Anwendung der FFT-basierten Methode im Rahmen zweiskaliger FE-FFT-basierter Simulationen übersichtlich darstellt.

Anschließend befassen sich zwei Publikationen mit einem effizienten Framework für zweiskalige FE-FFT-basierte Simulationen, mithilfe dessen das Materialverhalten von viskoplastischen Polykristallen modelliert wird. Hierbei wird für die zweiskalige Simulation eine grob diskretisierte Mikrostruktur verwendet, wobei die minimale Anzahl an Gitterpunkten, die für die Erzeugung genauer makroskopischer Ergebnisse erforderlich ist, in einem Pre-Processing-

Schritt definiert wird. Hochaufgelöste mikrostrukturelle Ergebnisse können in einem Post-Processing-Schritt erzeugt werden. Die Fachbeiträge befassen sich mit der Verallgemeinerung dieses Frameworks für den Bereich großer Deformationen und für den thermomechanisch gekoppelten Fall.

Die nachfolgenden fünf Artikel beschäftigen sich mit einer reduzierten FFT-basierten Mikrostruktursimulation, bei der eine reduzierte Anzahl an Fourier-Modi für die Berechnungen im Fourier-Raum verwendet wird. Dabei ist die Genauigkeit der numerischen Ergebnisse direkt von der Auswahl der verwendeten Fourier-Modi abhängig. Zunächst wird für die Untersuchung zweiphasiger Mikrostrukturen ein geometrisch angepasstes Auswahlmuster eingeführt, das sich aus den Fourier-Modi mit den höchsten Amplituden, welche sich aus der Fourier-Transformation der charakteristischen Funktion der jeweiligen Mikrostruktur ergeben, zusammensetzt. Die charakteristische Funktion erfasst die Phasenverteilung innerhalb der Mikrostruktur. Im Anschluss wird ein dehnungsbasiertes Auswahlmuster vorgeschlagen, welches zur Auswahl der Fourier-Modi anstelle der zuvor genannten charakteristischen Funktion das mikrostrukturelle Dehnungsfeld berücksichtigt. Diese Strategie führt, verglichen zu dem geometrisch angepassten Auswahlverfahren, zu noch genaueren Ergebnissen. Da darüber hinaus die Definition der charakteristischen Funktion entfällt, können auch komplexe polykristalline Mikrostrukturen mit anspruchsvollen mikrostrukturellen Effekten, wie z.B. Kristallplastizität oder Phasenumwandlungen, untersucht werden. Um die Allgemeingültigkeit der Modellreduktionstechnik zu demonstrieren, wird sie schließlich mit verschiedenen Modifikationen für die FFT-basierte Mikrostruktursimulation kombiniert. Beispielsweise wird sie mit der auf finiten Differenzen basierenden Operator-Approximation kombiniert, um den Effekt der Gibbs-Oszillationen zu verringern, oder mit Fast-Gradient-Solvern, um die Anzahl der erforderlichen Iterationen zur Erreichung einer konvergierten Lösung zu reduzieren.

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1 Introduction

1.1 Motivation

In general, material properties such as density, stiffness, or heat capacity observed at the engineering component level - the so-called macroscale - are effective properties that depend on the microstructure of the considered material. These properties result from the interaction of various features and mechanisms at smaller scales, from the atomic configuration of the material to its microscopic structure. Therefore, modeling complex engineering problems that involve specific microscopic characteristics, necessitates the use of multiscale modeling techniques instead of single scale methods. If the length scale of a particular scale is considered to be much larger than the length scale of the next smaller scale, scale separation may be assumed and the governing equations can be solved independently on each scale.

Nowadays, powerful computational modeling techniques are available to capture the individual features at the respective scales. Among several other methods, molecular dynamics at the atomic scale, phase field and Fast Fourier Transform-based techniques at the microscale, or finite and virtual element techniques at the macroscale are representative placeholders. More recently, methods based on the application of neural networks or direct data-driven methods have also been introduced and applied in this regard.

The connection of the aforementioned scales leads to multiscale simulation techniques. While generally several scales may be involved, this work considers only two-scale problems, where the macroscale is homogeneous and represents the engineering component level, and the microscale reveals microscopic features such as the polycrystalline microstructure of a metal component or the fibers embedded in a matrix material in fiber-reinforced composites (see Figure 1.1). Furthermore, the material is assumed to be statistically homogeneous and the macroscopic quantities are defined by the volume average of their corresponding microscopic counterparts.

The conventional approach to perform a two-scale simulation in continuum mechanics is to apply the finite element (FE) method on both scales to solve the individual boundary value problems, leading to the well-known FE² method. As the FE method is a well-established sim-

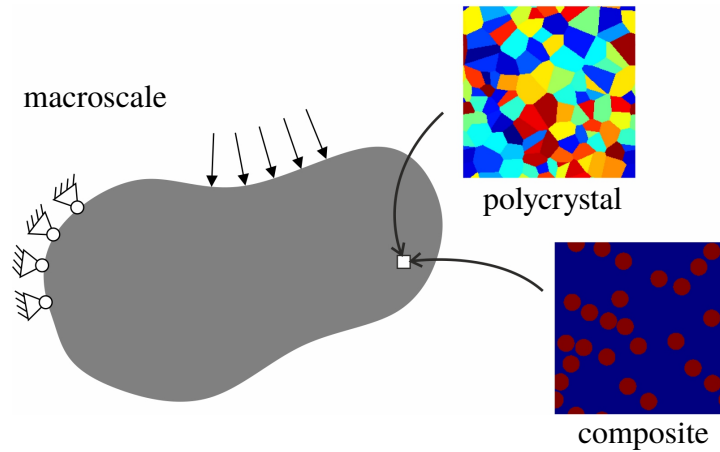


Figure 1.1: Representation of the macro- and microscale. The microscale is depicted here for either a polycrystalline metal or a fiber-reinforced composite.

ulation technique, numerous extensions and optimizations have been introduced over the years. To increase the efficiency and robustness of the method, a reduced integration with hourglass stabilization [1, 2] or a finite element discretization based on mixed variational principles [3, 4] have for example been proposed. Additionally, model order reduction techniques, such as the proper orthogonal decomposition (POD) [5, 6] or the further combination with the discrete empirical interpolation method [7], have been developed and applied to reduce the computational effort of solving the governing equations. Despite these optimizations, performing this type of multiscale simulation still requires significant computational resources.

Within the framework of the FE^2 method, the FE simulation at the microscale can also be replaced by other simulation methods. The focus here is on the Fast Fourier Transform (FFT)-based method leading to an FE-FFT-based method in the sense of a two-scale simulation. Compared to the FE method, the FFT-based method has several advantages for the simulation of periodic microstructures. In particular, periodic meshing of complex microstructures can be avoided (images such as EBSD data of polycrystalline microstructures can be used directly without meshing), periodic boundary conditions are implicitly part of the FFT-based method, and the related simulation is in general more efficient and requires less memory than an FE simulation (see e.g. [8, 9, 10]).

The FFT-based method was introduced by Moulinec and Suquet [11, 12] and first used in a concurrent two-scale simulation by Spahn et al. [13]. It is based on the reformulation of the microscopic boundary value problem in terms of the Lippmann-Schwinger equation which is then solved in Fourier space. There are also several approaches to increase the efficiency and robustness of the FFT-based method, such as the use of fast or conjugate gradient solvers or finite-difference-based operator approximations in order to reduce the effect of Gibbs os-

cillations (see e.g. [10, 14, 15] for state-of-the-art reviews). Besides these optimizations, the application of model order reduction techniques to FFT-based microscale simulations or FE-FFT-based two-scale simulations is rather new and hardly investigated, which motivates the main goals of this dissertation.

This dissertation aims to develop a generalized efficient and accurate solution strategy for FE-FFT-based two-scale simulations as well as to significantly increase the accuracy of the simulation results obtained by a reduced FFT-based microscale simulation. The idea of the efficient two-scale solution strategy is based on using a coarsely discretized microstructure for the actual two-scale simulation, which leads to accurate macroscopic results, while highly resolved microstructural results are generated for any integration point of particular interest in a post-processing step. This method was introduced in [16] predicting the mechanical behavior of polycrystalline materials at small strains. In this work, a generalization to the finite strain regime and to the thermomechanically coupled case is presented. Furthermore, the thesis deals with a model order reduction technique for the FFT-based microscale simulation, which is based on using only a reduced set of Fourier modes for the required computations in Fourier space [17]. Since the required Fourier modes can be defined on-the-fly, the method does not require any pre-computations, which is a huge advantage compared to other model order reduction techniques, such as the proper orthogonal decomposition, which for example requires a numerically costly generation of snapshots. In this thesis it is shown that, depending on the choice of the strategy used to define the reduced set of Fourier modes, the accuracy of the results obtained from the reduced simulation can be significantly increased. Moreover, the application of this model order reduction technique is discussed in the context of the aforementioned optimizations, i.e. in combination with finite-difference-based operator approximations and fast gradient solvers, for the FFT-based method.

1.2 State-of-the-art in multiscale material modeling

The present dissertation focuses on the FFT-based method for the simulation of periodic microstructures [11, 12] and the related two-scale FE-FFT-based method [13, 18]. As the first journal article of this thesis (Chapter 2; Gierden et al., 2022 [15]) already provides a comprehensive literature review in this respect, in Subsection 1.2.1, only the latest developments, which have not yet been included in the review article, will be discussed. Next to the FE-FFT-based method, there are several other methods for modeling heterogeneous materials at different length scales. Therefore, also the current trends in computational multiscale modeling, focusing here on data-driven multiscale methods, are addressed in 1.2.2. In this context, a

reliable data generation is often performed by highly resolved microscale simulations, where the FFT-based microstructure simulation with the model order reduction techniques presented in this thesis can also be used to ensure an efficient overall multiscale method.

1.2.1 FFT-based microscale and FE-FFT-based two-scale methods

The Fast Fourier Transform-based simulation method was introduced by Moulinec and Suquet [11, 12] and serves as an efficient and accurate method for the highly resolved simulation of periodic microstructures. Therefore, it is perfectly suited for a two-scale simulation technique. Using the FE method to describe the macroscopic boundary value problem, Spahn et al. were the first to propose a concurrent two-scale FE-FFT-based method [13]. While the aforementioned authors focused on composite materials, Kochmann et al. [18] were the first authors predicting the macroscopic and microscopic fields in polycrystalline materials by applying the two-scale FE-FFT-based method.

After the FFT-based microscale simulation was introduced in the late 1990s, several spectral algorithms and solvers have been proposed to increase the efficiency and robustness of the method. In addition, methods to reduce the effect of Gibbs oscillations [19] and the first specific model order reduction techniques for the FFT-based method have been developed. These improvements have made the method well suited for the microscale simulation of composites and polycrystalline materials. A comprehensive literature review of the aforementioned developments can be found in [10, 14], while in [15] (Chapter 2) the further application of the FFT-based microscale method to two-scale FE-FFT-based simulations is additionally reviewed.

Regarding the latest developments in the research field of spectral algorithms for the FFT-based microscale simulation, the class of polarization-based schemes, firstly introduced by Eyre and Milton [20], provides an efficient solution method. However, the performance of the polarization-based schemes strongly depends on the choice of the required reference material. In this context, an Anderson-accelerated polarization scheme was introduced in [21] and a scheme based on an adaptive selection of the reference material behavior was investigated in [22]. While both methods show a robust and fast convergence behavior, the scheme based on an adaptive selection of the reference material behavior has a lower memory demand [22].

Another spectral algorithm is the FFT-Galerkin approach [23], in which the weak form of the microscopic boundary value problem is discretized using trigonometric polynomials. In order to use this approach to model the material behavior of incompressible media, a mixed FFT-Galerkin approach has recently been introduced, where the hydrostatic pressure is used as an additional unknown next to the deformation gradient [24]. In addition, this variational

framework has been adapted to solve thermomechanically coupled boundary value problems in [25] to predict the material behavior of shape memory alloys. Moreover, also a finite element discretization on a regular grid has been integrated into the FFT-based framework [26, 27]. In this context, an optimal preconditioner was proposed in [28].

Besides these improvements for the spectral algorithms, the FFT-based method is known to suffer from spurious oscillations that occur at sharp contrasts in the local properties of the microstructure, which are referred to as Gibbs oscillations [19]. Therefore, reducing the effect of these oscillations is of great interest and a constantly relevant research topic. In this regard, a widely used method is based on finite-difference-based operator approximations in the context of solving the microscopic balance equations [29, 30]. In [31] it was shown that using the basic scheme of Moulinec and Suquet [11, 12] or the optimized discretization based on the finite-difference-based operator approximation of Willot [30] both converge to the theoretical solution. Another common method to reduce the effect of Gibbs oscillations relies on composite voxels [32], which result from homogenizing the properties of voxels crossed by an interface. This leads to smoother interfaces and thus reduces the effect of Gibbs oscillations. Current improvements of this method concern the use of a level-set technique to compute the volume fractions of the individual phases in a composite voxel [33], the application to the modeling of interface fracture in composite materials [34] and the use of composite boxels [35], which are not restricted to equidistant side lengths, in contrast to composite voxels. Furthermore, by using the aforementioned finite element discretization integrated into the FFT-based solver, a reduced integration with hourglass stabilization [36] or a compatibility projection for linear finite elements [37] can be used to reduce the effect of the spurious oscillations.

In order to minimize the computational effort of FFT-based microscale simulations in general, the development and application of specific model order reduction techniques is also of great interest and relevance. In this context, the model order reduction technique based on solving the convolution integral in Fourier space using a reduced set of Fourier modes [17] is modified by selecting the respective set of Fourier modes according to a strain-based sampling pattern [38]. Using this modification of the aforementioned model order reduction technique, the microstructural fields in elasto-viscoplastic polycrystals [39] and polycrystals undergoing solid-solid phase transformations [40] can now be captured. Recently, a method based on a wavelet analysis has also been proposed. Here the computational costs of the FFT-based microscale simulation in real space are reduced by minimizing the number of constitutive model evaluations [41]. Another possibility to circumvent the constitutive model evaluation at each grid point is given by the local defect correction method, coupling an overall coarse discretization with several locally refined discretizations [42].

Next to the described improvements and developments of the FFT-based simulation technique, the application of the method itself to compute the microstructural and overall fields in periodic microstructures is also still a rapidly growing area of research. A major application is the simulation of polycrystalline microstructures. Thus, the method has been used to study additive manufactured metals [43, 44, 45], to predict slip and kink bands e.g. by considering a strain gradient crystal plasticity material model [46, 47, 48, 49], or to analyze the effect of irradiation on the mechanical behavior of metals used in nuclear reactors [50, 51]. Other works also deal with the anisotropic martensitic phase transformation in dual-phase steels [52], with ductile fracture in polycrystalline materials [53], with lattice based microstructures [54, 55] or even with the study of the propagation of acoustic waves in elastic polycrystals [56].

In addition, the spectral solver is frequently used for the simulation of composites. For example, different strategies for the generation of statistically representative unit cells [57], the particle size effect in ductile composites [58] and the effective viscosity of short fiber reinforced thermoplastics [59] have been investigated. Moreover, the microstructural and overall behavior of concrete [60, 61, 62] and braided composites [63] have been studied using the FFT-based simulation method.

Next to using the FFT-based method to solve the mechanical boundary value problem, in [64] the thermal conductivity of thermal interface materials has been estimated. Furthermore, coupled mechanisms such as thermomechanically coupled [25, 65] or chemo-mechanically coupled processes [66] have been investigated.

Finally, and as mentioned at the beginning, the FFT-based microscale simulation can be perfectly integrated into any concurrent two-scale simulation approach, such as the FE-FFT-based simulation method. In [67], for example, this approach has been used to study the damage behavior in woven composite structures. Furthermore, the thermomechanically coupled material behavior of polycrystals [68, 69] and solid-solid phase transformations in polycrystals [70] has been investigated in the context of an efficient solution strategy for FE-FFT-based two-scale methods.

Besides these concurrent two-scale simulations, the FFT-based microscale simulation can also be used to train the effective material response in a pre-processing step, which is then used within the macroscale simulation. In this context, the overall stiffness of 3D printed carbon fiber reinforced composites has been estimated by a dual-scale FFT-based method operating on two different microscopic length scales [71]. In addition, a reduced-order model based on pre-computed POD modes obtained from FFT-based microscale simulations has been used to study the stiffness degradation in thermoplastic composites [72, 73]. More recent methods also involve data-driven methods, such as machine learning surrogate models, for example

based on artificial neural networks trained by FFT-based microscale simulations, to study the effect of fillers and voids on the fracture behavior of adhesives [74] and to study the material behavior of polycrystalline microstructures [75]. Alternatively the machine learning surrogate models may be based on deep material networks, which are trained by FFT-based microscale simulations and subsequently used to study the mechanical [76, 77] and thermomechanically coupled [78] behavior of fiber-reinforced thermoplastics.

1.2.2 Current trends in computational multiscale modeling

As described in the previous subsection, besides model order reduction techniques, also data-driven approaches can be used in two-scale simulations to reduce the high computational costs. Considering data-driven methods, model-based data-driven methods (machine learning-based approaches), e.g., based on the aforementioned artificial neural networks or deep material networks, as well as approaches based on model-free data-driven methods have recently been applied in the field of computational multiscale modeling (see [79] for a state-of-the-art review). However, the reliable applicability of these approaches often requires highly resolved microscale simulations. These simulations can be efficiently performed by applying the FFT-based simulation method with the model order reduction techniques presented in this thesis. Therefore, a brief overview of different methods for data-driven multiscale material modeling is given in the following.

The idea of using artificial neural networks to replace a classical constitutive model was introduced in [80]. Here, the neural network was trained with experimental data to predict the stress for a given strain state. However, such a training procedure requires an extremely large amount of experimental data. This led to the idea of generating the necessary macroscopic data through highly resolved and detailed microscale simulations. Such a non-concurrent data-driven two-scale simulation was first introduced in [81, 82]. Here, the artificial neural network was trained by microscale simulations of concrete microstructures to predict the relation between the macroscopic stress and a resulting crack opening. Then, the trained neural network can be used as a constitutive model within the finite element simulation of the macroscopic material behavior. In [83], a further approach is introduced that utilizes the neural networks to define the macroscopic constitutive law in terms of an effective potential. This simulation approach has been applied to study several nonlinear elastic composites. In addition, a combination of neural networks which are trained by microscale simulations with classical material models is introduced in [84]. For the investigation of history dependent material behavior, e.g. elasto-plasticity, different artificial neural network-based multiscale approaches have been proposed in [85, 86, 87]. Moreover, in [75, 88] an artificial neural network has also been

trained to predict the material behavior of polycrystalline materials. In [89], the combination of neural networks with model order reduction techniques is introduced and applied to model the material behavior of three-phase microstructures.

The deep material network was introduced in [90, 91] in the context of multiscale material modeling. Its structure is analogous to the structure of a neural network. However, in contrast to the previously mentioned methods, this approach uses the stiffness tensors of the individual phases as inputs and provides the overall homogenized stiffness tensor of the microstructure as output, rather than using the strain as input and the stress as output. Thus, the homogenized stiffness tensor of a two-phase laminate is assigned to each node of the network, resulting in a hierarchically structured laminate. The idea of using such hierarchical laminates is based on the availability of the analytical solution for the homogenized stiffness tensor of two-phase laminates, which depends only on the orientation of the laminate and the individual volume fractions of the phases. These parameters can be trained in an offline step based on highly resolved microscale simulations. Although the deep material network is trained using only linear elastic data, it can still be used in a finite strain setting and, as proved in [92], to predict inelastic material behavior, as the effective inelastic behavior of composites is determined only by linear elastic localization. Furthermore, the inherent thermodynamic consistency of the deep material network and a rotation-free variant with arbitrary directions of the laminate were established in this work. This method was used to study the mechanical [76], the thermomechanically coupled [78] and the viscoplastic [77, 93] behavior of fiber-reinforced thermoplastics in a two-scale simulation, respectively. In addition, in [94] the two-scale simulation of strain localization is addressed, while in [95] the investigation of porous microstructures using an interaction-based material network is discussed. Moreover, in [96] a transfer learning approach is proposed for modeling microstructures with different volume fractions of the individual phases, and in [97] the deep material network is extended by considering cohesive zones. Finally, also an uncertainty quantification can be performed by using deep material networks [98, 99].

Besides the aforementioned model-based data-driven methods, a model-free data-driven method was introduced in [100]. While it was originally restricted to elastic material behavior, it was extended to inelastic material behavior in [101]. Instead of fitting a material model or training an artificial neural network, this model-free data-driven approach is based directly on the available stress and strain data. While still relying on the basic physical principles, i.e., the balance equations and kinematic relations, which define a constraint set in this approach, the constitutive behavior is modeled by minimizing the distance between the points in the constraint set and the admissible material states characterized by the available stress-strain data. Similar to the training of neural networks, the amount of data required for this type of modeling

is very large, and thus, the data generation through experiments is difficult. This again led to the idea of generating the necessary macroscopic data by means of highly resolved microscale simulations, either in an offline pre-processing step [102], or even on-the-fly [103, 104] leading to a non-concurrent or concurrent two-scale approach, respectively. The non-concurrent model-free data-driven two-scale approach has been used to study microstructures with non-local effects [105] and to account for microscopic uncertainties [106]. Furthermore, in [107] it has been combined with model-based methods to study architected metamaterials. The concurrent model-free data-driven two-scale method was used to analyze open-cell foams [108] and granular materials [109], while different goal-oriented strategies for a data set enrichment have been proposed.

In any case, since a large number of microscale simulations is necessary to generate the required data for these data-driven methods, advanced microscale methods are required to provide an efficient overall solution strategy. In this context, the FFT-based simulation technique in combination with the different model order reduction techniques presented in this thesis provides a valuable solution method to ensure efficient microscale simulations and thus an efficient data generation.

1.3 Outline of the dissertation

The present cumulative dissertation consists of several journal articles and contributions to conference proceedings, which are presented in the individual chapters. It is organized as follows: Chapter 2 presents a comprehensive review of the two-scale FE-FFT-based method and the FFT-based microscale method for the simulation of heterogeneous materials. Thereafter, Chapters 3 and 4 deal with the generalization of an efficient two-scale FE-FFT-based method for the simulation of polycrystalline materials. Regarding the FFT-based microscale simulation, Chapters 5 to 9 focus on improving a model order reduction technique specifically adapted to the spectral solver. Finally, Chapter 10 summarizes the fundamental results and provides an outlook on possible further extensions and improvements regarding multiscale material modeling. The outline of the individual articles is given below:

Article 1 (Chapter 2) provides a comprehensive literature review of FFT-based microscale methods and of the two-scale FE-FFT-based method. The paper includes the improvements and general trends until 2022. The review article focuses on different FFT-based algorithms and solvers as well as their application to the simulation of composites and polycrystalline materials. In addition, different methods to reduce the effect of Gibbs oscillations and model order reduction techniques for the FFT-based microscale simulation are discussed. Focusing on the

FE-FFT-based two-scale method, a distinction is made between concurrent and non-concurrent methods. With respect to the concurrent methods the computation of the macroscopic tangent operator is discussed in detail. Finally, efficient two-scale solution strategies are presented and an overview of the application of the FE-FFT-based two-scale method to the simulation of composites and polycrystalline materials is given.

Article 2 (Chapter 3) deals with the efficient two-scale FE-FFT-based simulation of elasto-viscoplastic polycrystals at finite strains. Here, a solution technique introduced by Kochmann et al. [16, 110] restricted to simulations in the small strain regime is adapted to the finite strain regime and applied to the mechanical simulation of a deep rolling process. The idea of the model order reduction technique is based on using a coarsely discretized microstructure for the two-scale simulation. The minimum number of grid points needed to generate accurate macroscopic results is determined within a pre-processing step. By storing the macroscopic deformation gradient of any integration point of particular interest, highly resolved results can be computed in a post-processing step using a finely discretized microstructure.

Article 3 (Chapter 4) presents a condensed version of an article in preparation. It extends the aforementioned purely mechanical two-scale FE-FFT-based simulation framework to the thermomechanically coupled case. The general settings of the simulation, i.e. the consideration of elasto-viscoplastic polycrystals at finite strains as well as the use of the previously introduced model order reduction technique, are maintained. In addition to solving the balance of linear momentum, considering the thermomechanically coupled case also requires solving the balance of internal energy on both scales. The results illustrate the performance of the model order reduction technique for the simulation of thermomechanically coupled processes.

Article 4 (Chapter 5) discusses a model order reduction technique for the FFT-based solver. The basic idea of this model order reduction technique, first introduced in [17], is to use only a reduced set of Fourier modes for computations in Fourier space. The accuracy of this technique is highly sensitive to the choice of the Fourier modes considered. Article 4 introduces a geometrically adapted sampling scheme. In this context, the two phases of a two-phase microstructure are captured by a characteristic function which is then transferred into Fourier space. Approximating this characteristic function using only a reduced set of Fourier modes, the most accurate results are obtained by choosing the Fourier modes with the highest amplitudes. These Fourier modes then define the sampling pattern used for the reduced FFT-based microscale simulation. Compared to the previously proposed fixed sampling pattern, this geometrically adapted sampling pattern leads to significantly more accurate results.

Article 5 (Chapter 6) also deals with the optimization of the choice of Fourier modes used for the reduced FFT-based microscale simulation. Instead of the geometrically adapted sampling

pattern, Article 5 introduces a strain-based sampling strategy. Hence, the norm of the microscopic strain is transferred into Fourier space after each converged local iteration. Similar to the strategy presented in Article 5, the Fourier modes with the highest amplitudes, resulting from this Fourier transformation, should be chosen in order to obtain accurate results. Comparing the results of a microscale simulation of a two-phase microstructure with elasto-plastic constitutive behavior the accuracy of the solution is significantly increased using a strain-based instead of a geometrically adapted sampling pattern. This is the case for both the elastic and the plastic regime. Especially in the plastic regime, the strain-based sampling strategy leads to significantly more accurate results, since the relation between the characteristic function used for the geometrically adapted sampling pattern and the microscopic strains is less pronounced. Moreover, while the geometrically adapted sampling pattern is defined once at the beginning of the simulation, the strain-based sampling pattern can be adjusted after each load step leading to higher flexibility and accuracy.

Article 6 (Chapter 7) is a condensed version of Article 5 (Chapter 6). It considers the strain-based sampling pattern for the reduced spectral solver and focuses on the calculation of the mechanical fields in a polycrystalline microstructure. Since the strain-based sampling pattern is computed directly from the microstructural strain field and does not require the definition of a characteristic function (compared to the geometrically adapted sampling pattern), the application of the strain-based sampling strategy is straightforward even for the complex microstructure of a polycrystal.

Article 7 (Chapter 8) also represents a more specified version of Article 5 (Chapter 6). In this article, the developed FFT-based model order reduction technique has been applied to an even more complex material behavior. Namely, a polycrystalline microstructure characterized by solid-solid phase transformations between austenite and martensite is investigated. Since the strain-based sampling pattern can be updated after each load step, accurate results can be generated even accounting for such a complex microstructural material behavior.

Article 8 (Chapter 9) deals with the general applicability of the reduced FFT-based microstructure simulation. The presented model order reduction technique, where a reduced set of Fourier modes is used for the FFT-based microstructure simulation, was initially introduced for the FFT-based basic fixed-point scheme. Having discussed the optimization of the sampling strategy to define the reduced set of Fourier modes in the previous articles, this article presents the application of the reduced spectral solver in combination with different general improvements for the FFT-based microstructure simulation. The article focuses on finite-difference-based operator approximations used to reduce the effect of Gibbs oscillations and on fast gradient solvers which improve the convergence behavior of the algorithm compared to the basic fixed-

point scheme. Considering the finite-difference-based operator approximation, it was shown that the model order reduction technique works best for microstructures with small phase contrast. Regarding the different fast gradient solvers, the presented model order reduction technique can be universally integrated into any solver, resulting in similar relative CPU time reductions.

2 | Article 1:

A review of FE-FFT-based two-scale methods for computational modeling of microstructure evolution and macroscopic material behavior

This article was published as:

Gierden, C., Kochmann, J., Waimann, J., Svendsen, B. and Reese, S. [2022], ‘A review of FE-FFT-based two-scale methods for computational modeling of microstructure evolution and macroscopic material behavior’, *Archives of Computational Methods in Engineering* **29** (6), 4115 – 4135.

Disclosure of the individual authors’ contributions to the article:

C. Gierden reviewed the relevant existing literature and wrote the article. J. Kochmann, J. Waimann, B. Svendsen and S. Reese provided conceptual advice, proofread the article, and made valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

2.1 Abstract

The overall, macroscopic constitutive behavior of most materials of technological importance such as fiber-reinforced composites or polycrystals is very much influenced by the underlying microstructure. The latter is usually complex and heterogeneous in nature, where each phase constituent is governed by non-linear constitutive relations. In order to capture such microstructural characteristics, numerical two-scale methods are often used. The purpose of the current work is to provide an overview of state-of-the-art finite element (FE) and FFT-based two-scale computational modeling of microstructure evolution and macroscopic material behavior. Spahn et al. [13] were the first to introduce this kind of FE-FFT-based methodology, which has emerged as an efficient and accurate tool to model complex materials across the scales in the recent years.

2.2 Introduction

At small length scales, most materials are heterogeneous, such as composites, porous media, or polycrystalline aggregates. Accordingly, e.g. polycrystals are composed of several grains which might vary in spatial distribution, size, morphology and crystallographic orientation. In addition, one grain could also consist of a phase mixture. The related heterogeneous structure has a great impact on the microstructural effects and thus results in more complex non-linear constitutive relations. Examples are grain-wise elasto-viscoplastic material behavior or ductile damage behavior related to the grain boundaries. The material behavior's complexity is increased by microstructural changes which influence the grain's structure, such as martensitic phase transformations and dynamic recrystallization; see Figure 2.1. These effects make it even more difficult to establish appropriate overall constitutive relations to describe the material behavior. Instead of finding such a phenomenological expression, a multiscale approach enables to separately examine the different scales. Within a two-scale simulation approach, the macroscale is used to capture the overall boundary value problem including the external boundary conditions. Meanwhile, the material behavior at the macroscale is determined by the mean response of the smaller scale (microscale). Various methods have been developed to capture the structure, properties and physical behavior of the microstructure and its overall constitutive response. These so-called multiscale schemes may be classified in three major groups: (semi-)analytical methods (e.g. [111, 112]), computational methods (e.g. [13, 113]) and hybrid methods (e.g. [114, 115]).

The focus of the present paper is on one particular computational two-scale technique, namely

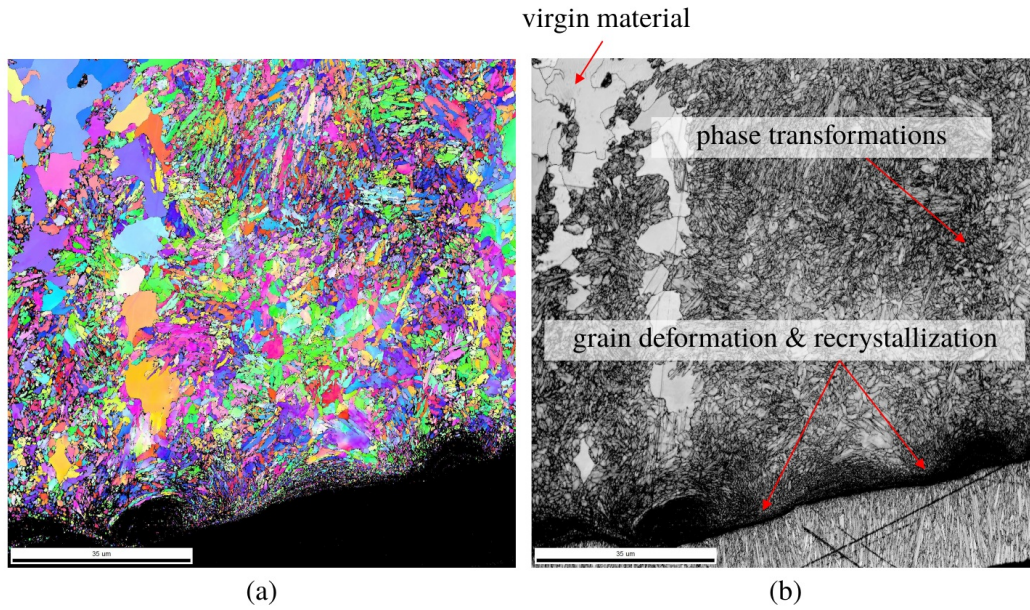


Figure 2.1: Ferrite/pearlite-annealed 42CrMo4 steel microstructure: (a) inverse pole figure illustrating the grain orientations and (b) image quality map obtained from EBSD measurements illustrating microstructural grain changes, such as phase transformations and recrystallization [116].

the FE-FFT-based method. This methodology was first proposed by Spahn et al. (2014) [13] and serves as an efficient and powerful alternative compared to the classical computational homogenization method, the FE^2 method [8, 9, 117]. The FE-FFT-based method includes a finite element (FE) approach for the macroscale simulation and an evaluation of the behavior at the microscale based on fast Fourier transforms (FFT). The macroscopic material behavior is then defined as volume average of its microscopic counterpart. While the FE approach is widely used in terms of computational mechanics, the FFT-based method is rather new and was introduced by Moulinec and Suquet (1994, 1998) [11, 12]. It serves as alternative to the classical FE-based simulation of periodic microstructures and is based on solving a global integral equation known as the Lippmann-Schwinger equation [118, 119], which is defined by Green's function and a polarization stress.

The review paper is structured as follows: After a brief review of the three groups of multiscale techniques (Section 2.3), a review of the FFT-based microstructure simulation is given in Section 2.4. This includes a brief summary of FFT-based algorithms (Sections 2.4.2 and 2.4.3), FFT-based model-order reduction techniques (Section 2.4.4), as well as the applications of the FFT-based simulation (Section 2.4.5). In addition a brief comparison of the FFT-based method to the FE-based method is given in Section 2.4.6. Finally, in Section 2.5, the FE-FFT-based

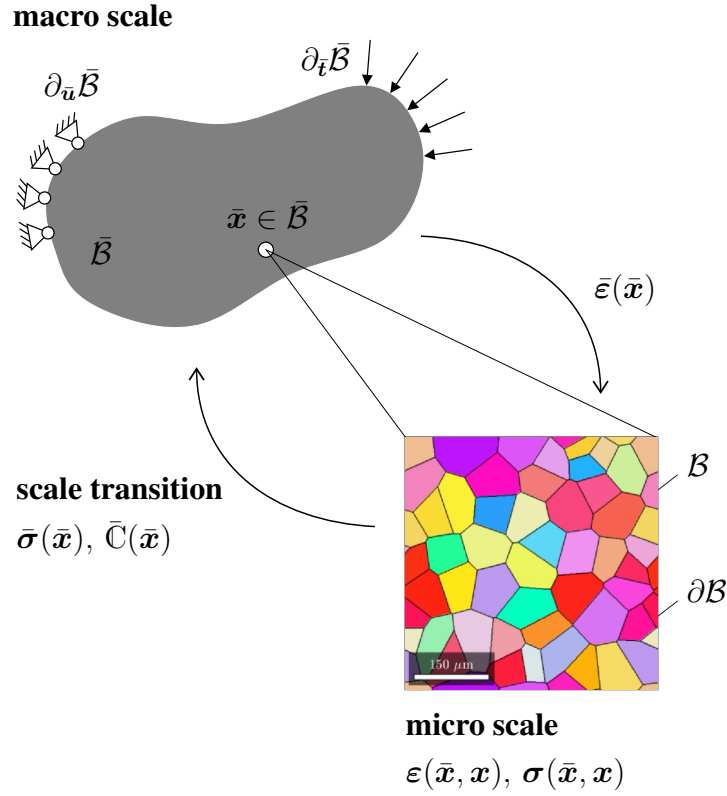


Figure 2.2: Schematic of the two-scale simulation approach incorporating a polycrystalline microstructure.

two-scale method is discussed for different applications. The paper ends with a conclusion in Section 2.6.

2.3 Overview of multiscale methods

Figure 2.2 presents the key idea of a multiscale approach in terms of a mechanical boundary value problem considering small strain kinematics. On the macroscale the macroscopic strain $\bar{\boldsymbol{\varepsilon}}(\bar{\mathbf{x}})$ at the macroscopic position $\bar{\mathbf{x}}$ is computed. This macroscopic strain is used on the microscale to compute the overall strain $\boldsymbol{\varepsilon}(\bar{\mathbf{x}}, \mathbf{x})$ and stress $\boldsymbol{\sigma}(\bar{\mathbf{x}}, \mathbf{x})$ response. In terms of a spatially resolved microstructure simulation, $\mathbf{x}$ represents the microscopic position. Vice versa, the resulting macroscopic stress $\bar{\boldsymbol{\sigma}}(\bar{\mathbf{x}})$ and macroscopic tangent operator $\bar{\mathbb{C}}(\bar{\mathbf{x}})$ are defined as volume averages of their overall counterparts.

Besides this two-scale method, also multiscale methods incorporating more than two scales (for example all the way down to the atomistic level, e.g. [120]) exist. Nevertheless we restrict ourselves exclusively to the two-scale method. Doing that, Table 2.1 and the following three

Table 2.1: Classification of the three major different two-scale methods

(Semi-)analytical methods	Hybrid methods	Computational methods
Arithmetic and harmonic mean e.g. [111, 112]	TFA / NTFA e.g. [114]; [121]; [122]	FE ² method e.g. [113, 123, 124]
Eshelby solution e.g. [125]; [126]; [127]	Clustering analysis e.g. [115, 128]	FE-FFT method e.g. [13, 18, 129]
Variational approach e.g. [130, 131, 132]		

Subsections briefly summarize the three different classifications of two-scale methods, the (semi-)analytical, the computational and the hybrid method.

2.3.1 (Semi-)analytical methods

In analytical methods, a deterministic or statistical representation of the microstructure is used. Often, closed form solutions of reference problems serve to compute the overall response of microscopic heterogeneous materials. If an explicit solution for the material behavior is not available but approximated by implicit equations, the method is called a semi-analytical method. In both cases, a spatially resolved visualization of the results on the microscale is not possible.

First attempts to compute the overall macroscopic material behavior of microscopic heterogeneous materials in terms of an analytical homogenization were established by Voigt [111] and Reuss [112]. Whereby Voigt assumes that the strain is constant within the microstructure, resulting in an overall stiffness tensor computed by using the arithmetic mean of the phase-wise stiffness tensor weighted by the corresponding volume fraction, Reuss considers a constant stress in the individual phases. This ansatz results in the computation of the arithmetic mean of the phase-wise compliance tensors again weighted by the corresponding volume fractions. These basic analytical homogenization methods are called “mean field methods”. In the context of statistical methods, the volume fractions of the different phases can be interpreted as

first order correlation functions. Since these basic approximations are only related to the volume fractions of certain phases, they are not very accurate in general, but still serve as upper and lower bounds of the averaged material response in terms of homogenization methods. Regarding polycrystalline materials, these bounds are often referred to as the Taylor [133] and Sachs [134] bounds. To generate more accurate homogenized results, the use of a two-point or higher-order correlation function enables the consideration of additional microstructural details [135, 136].

The work of Eshelby (1957) [125] deals with an ellipsoidal elastic inclusion embedded in a homogeneous infinite matrix. The present analytic solution for the so-called Eshelby's inclusion serves as the basis for different more precise mean field approaches [137], such as the Mori-Tanaka model [126] or the double inclusion method introduced in [138]. Furthermore, a self-consistent approximation was introduced in [127, 139, 140, 141] for the simulation of elastic composites and polycrystals. Within this self-consistent approach it is assumed that the material properties of the homogeneous infinite matrix coincide with the overall properties of the composite. An extension of this approach to the computation of the overall properties of non-linear composites is given in [142, 143] and of non-linear polycrystals in [144, 145, 146, 147, 148, 149].

A variational approach for the estimation of the behavior of linear composites with an isotropic microstructure was introduced by Hashin and Shtrikman [130, 131, 132, 150]. This approach is still based on the assumption of phase-wise constant fields, but in addition the stress state consists of two parts. One part is related to a homogenous reference material and the other part is related to a polarization stress which characterizes the fluctuation within the microstructure. The resulting inhomogeneous partial differential equation is solved by use of Green's function [151, 152] and hence, yields an integral formulation known as Lippmann-Schwinger equation [118, 119]. For homogeneous and isotropic reference materials which behave elastically, closed-form solutions for the Lippmann-Schwinger equation are available. Compared to the Voigt and Reuss bounds, which do not consider the fluctuation of the stress on the microscale, this variational approach leads to stricter bounds in terms of the overall response of the microstructural material behavior. An extension of the ansatz to anisotropic composites is given in [153] and to non-linear composites in [119, 154, 155, 156]. To further improve the accuracy of the application of the analytical homogenization on microstructures with large variations in their local properties, also second-order homogenization techniques based on incorporating field fluctuations have been proposed in [157, 158, 159, 160].

2.3.2 Computational methods

In contrast to (semi-)analytical methods, a computational multiscale method deals with a spatially resolved representation of the microstructure. In this context, the microstructure might be seen as a representative volume element (RVE) and/or unit cell, e.g. [154, 161, 162, 163], or a statistically similar RVE, e.g. [164, 165]. The macroscopic kinematics serve as an input for the RVE and thus influence the deformation of the microstructure. The macroscopic influence can be prescribed by different possible boundary conditions, such as linear displacements, constant tractions, or combined periodic displacements and anti periodic tractions, e.g. [166, 167, 168]. The most common method to solve the related microscopic boundary value problem (BVP) is the finite element method (e.g. [169, 170]). The performed computational simulation leads to spatially resolved representations of the microstructural fields, like the stress and the strain fields. Accordingly, the volume average of the local microscopic fields determines the required overall macroscopic response, see [161, 171]. Two-scale approaches which use the finite element method to calculate the BVPs on the micro-level as well as on the macro-level are called FE^2 methods [113, 123]. To calculate the required overall algorithmic tangent operator closed form expressions were derived in [172, 173]. An overview of recent developments, applications and challenges concerning the FE^2 method can be found in [124, 174].

Other microstructural methods in terms of a two-scale full field simulation are for example finite differences (FD)-based [175], Voronoi FE-based [176], virtual element-based [177, 178] and FFT-based solvers [13]. Among these methods, the FFT-based method has proven to be a fast and accurate tool in terms of a computational simulation of periodic microstructures in the recent years. An overview of recent developments, applications and challenges concerning the FFT-based microstructure simulation [11, 12] and the related FE-FFT-based two-scale method [13, 18] is given in Section 2.4 and 2.5, respectively.

A comparison of the aforementioned analytical and numerical methods is presented in [179, 180]. Concerning the computational methods, Section 2.4.6 gives a brief comparison of the FE- and FFT-based microstructure simulation.

2.3.3 Hybrid methods

Hybrid multiscale methods finally combine both, computationally efficient numerical methodologies and theoretical knowledge. In particular, numerical experiments, such as deforming a highly resolved microstructure incorporating different loading conditions, are performed in a pre-processing step to generate microstructural data, such as the point-wise material behavior related to the external loading. Then, the obtained information about the microstructural ma-

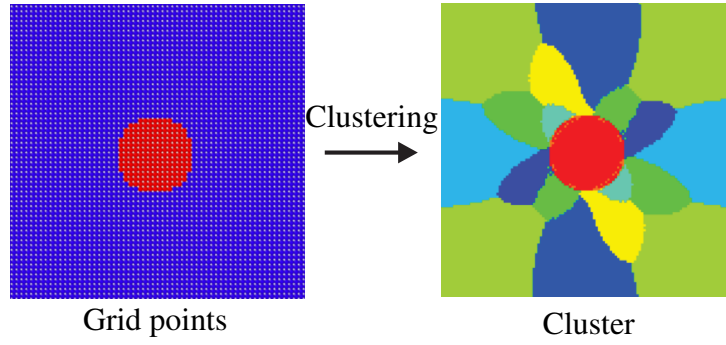


Figure 2.3: Highly resolved two-phase microstructure with a point-wise material behavior, while the inclusion is colored red and matrix is colored blue (*left*) and clustered microstructure with a cluster-wise constant material behavior, while each color represents one cluster (*right*).

terial behavior is used for the actual micromechanical modeling.

In this context, one methodology is the uniform transformation field analysis (TFA) [114, 181]. It is based on the assumption of piece-wise uniform plastic strain fields to reduce the degrees of freedom during the simulation. Therefore a significant reduction of computational time is gained. A generalization of this method in terms of the non-uniform TFA (NTFA) is given in [121, 122, 182, 183, 184]. Instead of considering uniform plastic strain fields, the latter quantities are decomposed into a set of plastic modes, which leads to nonuniform plastic strain fields. These modes have to be computed within a pre-processing step. Nevertheless, also the NTFA leads to a highly reduced set of constitutive equations, which again results in a significant reduction of the computational costs.

Another recently developed hybrid multiscale method is the self-consistent clustering analysis (SCA) [115, 128, 185, 186, 187]. This method is derived from the Lippmann-Schwinger equation [118, 119] and based on a clustered microstructure with cluster-wise constant micromechanical fields. A pre-processing step is used to group the highly resolved material behavior into these clusters, see Figure 2.3. Under the assumption of constant stress and strain fields during the actual simulation, a significant reduction of degrees of freedom and also a significant reduction of computational times compared to a full field computational two-scale simulation is gained. A generalization of the SCA to finite strain kinematics is given in [188].

2.4 FFT-based microstructure simulation

The FFT-based microstructure simulation is used in terms of a spatially resolved microstructure simulation. Initially, it was introduced by Moulinec and Suquet based on fixed-point iterations [11, 12]. This basic fixed-point scheme is reviewed in Section 2.4.1. It is followed

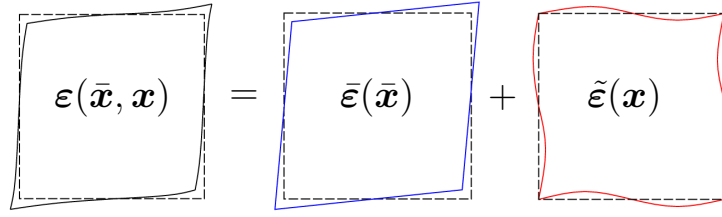


Figure 2.4: Additive split of the total strain into the constant macroscopic part and the fluctuating microscopic part.

by an overview of several more efficient FFT-based algorithms and solution methods (Section 2.4.2) and Section 2.4.3, discussing problems related to the Gibbs phenomenon. In addition, recently introduced model order reduction techniques for the FFT-based method are reviewed in Section 2.4.4. Subsequently, Section 2.4.5 provides an overview of different applications of the FFT-based method for the simulation of composite (Section 2.4.5.1) and polycrystalline (Section 2.4.5.2) microstructures, respectively. Finally, a brief comparison to the FE-based microstructure simulation is given in Section 2.4.6. A recapitulation of the FFT-based algorithms, solvers and their applications is also given in Table 2.2.

2.4.1 Basic fixed-point scheme

In terms of a spatially resolved microstructure simulation of a mechanical boundary value problem considering small strain kinematics, the overall strain $\varepsilon(\bar{x}, \mathbf{x})$ is additively split into the macroscopic part $\bar{\varepsilon}(\bar{x})$ (see Figure 2.2) and a microscopic fluctuating part $\tilde{\varepsilon}(\mathbf{x})$, see Figure 2.4. Since the balance of linear momentum holds for the macroscopic as well as for the microscopic scale, the microstructural mechanical boundary value problem is captured by

$$\begin{aligned} \operatorname{div} \boldsymbol{\sigma}(\bar{x}, \mathbf{x}) &= \mathbf{0} \\ \boldsymbol{\sigma}(\bar{x}, \mathbf{x}) &= \boldsymbol{\sigma}(\bar{x}, \mathbf{x}, \varepsilon(\bar{x}, \mathbf{x}), \boldsymbol{\alpha}(\bar{x}, \mathbf{x})) \\ \varepsilon(\bar{x}, \mathbf{x}) &= \bar{\varepsilon}(\bar{x}) + \tilde{\varepsilon}(\mathbf{x}). \end{aligned} \tag{2.1}$$

Thereby, $\operatorname{div}(\cdot)$ represents the divergence operator and the total stress field $\boldsymbol{\sigma}(\bar{x}, \mathbf{x})$ depends on the macroscopic position $\bar{x}$, the microscopic position $\mathbf{x}$, the related total strain field $\varepsilon(\bar{x}, \mathbf{x})$ as well as – related to the observed problem – on some internal variables $\boldsymbol{\alpha}(\bar{x}, \mathbf{x})$, e.g. the plastic strain and/or a grain orientation. Body forces are neglected within the microscopic BVP since they are already considered within the macroscopic BVP.

Considering periodic fields and boundary conditions, the microscopic boundary value problem may be solved using spectral methods [137, 151, 189]. Therefore, the inhomogeneous BVP with

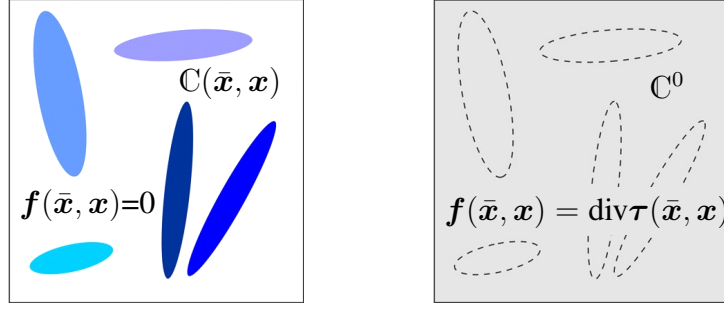


Figure 2.5: *Left*: Inhomogeneous microstructure with spatially varying material properties, such as a spatially depending stiffness tensor $\mathbb{C}(\bar{\mathbf{x}}, \mathbf{x})$, while body forces are neglected. *Right*: Homogeneous reference microstructure with a constant reference material behavior $\mathbb{C}^0$, while the inhomogeneities are described in terms of the body force $\mathbf{f}(\bar{\mathbf{x}}, \mathbf{x}) = \text{div} \boldsymbol{\tau}(\bar{\mathbf{x}}, \mathbf{x})$.

varying material properties, see Figure 2.5 (*left*), is reformulated as equivalent homogeneous BVP by introducing a microstructure with a homogeneous reference material behavior $\mathbb{C}^0$, see Figure 2.5 (*right*). Doing this, the equivalent homogeneous BVP reads

$$\begin{aligned} \text{div}[\mathbb{C}^0 : \boldsymbol{\varepsilon}(\bar{\mathbf{x}}, \mathbf{x})] &= -\text{div}[\boldsymbol{\tau}(\bar{\mathbf{x}}, \mathbf{x})] \\ \boldsymbol{\tau}(\bar{\mathbf{x}}, \mathbf{x}) &:= \boldsymbol{\sigma}(\bar{\mathbf{x}}, \mathbf{x}) - \mathbb{C}^0 : \boldsymbol{\varepsilon}(\bar{\mathbf{x}}, \mathbf{x}) \\ \boldsymbol{\varepsilon}(\bar{\mathbf{x}}, \mathbf{x}) &= \bar{\boldsymbol{\varepsilon}}(\bar{\mathbf{x}}) + \tilde{\boldsymbol{\varepsilon}}(\mathbf{x}), \end{aligned} \quad (2.2)$$

where $\boldsymbol{\tau}(\bar{\mathbf{x}}, \mathbf{x})$ is the so-called polarization stress, which represents the material inhomogeneities within the homogeneous reference material behavior.

Equation (2.2) may be solved by using Green's function $\mathbf{G}^0(\mathbf{x} - \mathbf{x}')$ or the Lippmann-Schwinger operator $\mathbb{I}^0(\mathbf{x} - \mathbf{x}')$ [151, 152], respectively, which yields to an integral form known as the Lippmann-Schwinger equation [118, 119]:

$$\boldsymbol{\varepsilon}(\bar{\mathbf{x}}, \mathbf{x}) = \bar{\boldsymbol{\varepsilon}}(\bar{\mathbf{x}}) - \int_{\Omega} \mathbb{I}^0(\mathbf{x} - \mathbf{x}') : \boldsymbol{\tau}(\mathbf{x}') \, d\mathbf{x}' \quad (2.3)$$

or in a compact notation:

$$\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \mathbb{I}^0 * \boldsymbol{\tau}. \quad (2.4)$$

Within Equation (2.3) $\mathbf{x}$ and $\mathbf{x}'$ represent different positions within the microstructural domain Ω with the side length L , while $*$ represents the convolution integral in Equation (2.4).

The Lippmann-Schwinger equation is solved by transferring it into Fourier space yielding:

$$\hat{\varepsilon}(\boldsymbol{\xi}) = \begin{cases} -\hat{\Gamma}^0(\boldsymbol{\xi}) \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) & \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\varepsilon}(\bar{\boldsymbol{x}}) & \forall \boldsymbol{\xi} = \mathbf{0} \end{cases}, \quad (2.5)$$

while $(\hat{\cdot})$ refers to the Fourier representation of the corresponding field depending on the wave vector $\boldsymbol{\xi}$, which gathers all the considered Fourier modes. The components $\xi_j (j = 1, 2, 3)$ of this wave vector are defined as

$$\xi_j(i) = \frac{2\pi}{L}i \quad \text{with} \quad i = -\frac{N}{2}, \dots, \frac{N}{2} - 1 \quad (2.6)$$

for a discretized microstructure with an even number of grid points N and

$$\xi_j(i) = \frac{2\pi}{L}i \quad \text{with} \quad i = -\frac{N-1}{2}, \dots, \frac{N-1}{2} \quad (2.7)$$

for a discretized microstructure with an odd number of grid points N .

In Fourier space, Green's function $\hat{\mathbf{G}}^0(\boldsymbol{\xi})$ and the Lippmann-Schwinger operator $\hat{\Gamma}^0(\boldsymbol{\xi})$ are explicitly known and just depending on this wave vector and the homogeneous reference material behavior $\mathbb{C}^0$:

$$\hat{G}_{ki}^0(\boldsymbol{\xi}) = (\mathbb{C}_{kji}^0 \xi_l \xi_j)^{-1} \quad (2.8)$$

and

$$\hat{\Gamma}_{ijkl}^0(\boldsymbol{\xi}) = \frac{1}{4} \left(\hat{G}_{jk,li}^0(\boldsymbol{\xi}) + \hat{G}_{ik,lj}^0(\boldsymbol{\xi}) + \hat{G}_{jl,ki}^0(\boldsymbol{\xi}) + \hat{G}_{il,kj}^0(\boldsymbol{\xi}) \right). \quad (2.9)$$

The basic fixed-point iteration scheme for the FFT-based microstructure simulation, which makes use of the Fourier representation of the Lippmann-Schwinger equation (Equation (2.5)) and the computation of the polarization stress $\boldsymbol{\tau}(\bar{\boldsymbol{x}}, \boldsymbol{x})$ in real space (Equation (2.2)) was introduced by Moulinec and Suquet [11, 12].

2.4.2 Overview and efficiency of FFT-based algorithms and solution methods

Recently, two review papers on FFT-based algorithms, solution methods and their applications were published by Schneider (2021) [14] and Lucarini et al. (2021) [10]. Nevertheless, this subsection briefly sums up the most important developments in this context.

Table 2.2: FFT-based numerical solution methods and applications.

Algorithms, solvers, and applications	Key references
FFT-based algorithms: - basic and related schemes - polarization-based scheme - scheme based on augmented Lagrangians - scheme based on discrete Green's operator - Fourier-Galerkin approach	Moulinec and Suquet [11], Moulinec and Suquet [12], Dreyer and Müller [190], Lebensohn [191], Lahellec et al. [192], Moulinec and Suquet [193], Eisenlohr et al. [194], Kabel et al. [195] Eyre and Milton [20], Michel et al. [196], Moulinec and Suquet [193], Vinogradov and Milton [197], Monchiet and Bonnet [198], Moulinec and Silva [199], Schneider et al. [200] Michel et al. [201], Michel et al. [196], Moulinec and Suquet [193], Lebensohn et al. [202], Moulinec and Silva [199] Jacques [203], Eloh et al. [204], Eloh et al. [205], Berbenni et al. [206], Khorrami et al. [207] Bonnet [208], Brisard and Dormieux [209], Brisard and Dormieux [210], Vondřejc et al. [23], Vondřejc et al. [211], Vondřejc [212], Zeman et al. [213], Geus et al. [214]
Solution methods: - fixed-point scheme - conjugate and fast gradient solver - quasi-Newton method - using high performance computing	Moulinec and Suquet [11], Moulinec and Suquet [12], Eisenlohr et al. [194], Eyre and Milton [20], Michel et al. [196], Schneider et al. [200], Michel et al. [201], Lebensohn et al. [202] Zeman et al. [215], Brisard and Dormieux [209], Brisard and Dormieux [210], Vondřejc et al. [23], Gélébart and Mondon-Cancel [216], Kabel et al. [195], Schneider [217] Shanthraj et al. [218], Schneider [219], Chen et al. [220], Chen et al. [221], Wicht et al. [222] Egghesad et al. [223], Grimm-Strele and Kabel [224], Egghesad and Knezevic [225], Egghesad et al. [226]

Methods to reduce the effect of Gibbs oscillations on convergence behavior	Willot et al. [227], Berbenni et al. [228], Willot [30], Lebensohn and Needleman [229], Schneider et al. [26], Schneider et al. [230], Vidyasagar et al. [231], Vidyasagar et al. [232], Anglin et al. [233], Kabel et al. [32], Elohe et al. [205], Khorrami et al. [207], Leute et al. [37]
Incorporating MOR techniques	Garcia-Cardona et al. [234], Kochmann et al. [17], Gierden et al. [235], Vondřejc et al. [236], Gierden et al. [237], Gierden et al. [38]
Simulation of composite microstructures - composites with finite phase contrast - composites with infinite phase contrast - damage, fracture and fatigue behavior	Moulinec and Suquet [11], Moulinec and Suquet [12], Eyre and Milton [20], Lahellec et al. [192], Vinogradov and Milton [197], Šmilauer and Bažant [238], Zeman et al. [215], Lavergne et al. [239], Ostrowski et al. [240] Michel et al. [201], Bilger et al. [241], Bilger et al. [242], Brisard and Dormieux [209], Monchiet and Bonnet [198], Ghosseinr and Lévesque [243], Vondřejc et al. [23], Gélébart and Mondon-Cancel [216], Kabel et al. [195], Schneider [217], Schneider [219], Wicht et al. [222], Charière et al. [244], Görthofer et al. [245] Spahn et al. [13], Sliseris et al. [246], Boeff et all [247], Wang et al. [248], Li et al. [249], Chen et al. [220], Ernesti et al. [250], Chen et al. [221], Cao et al. [251], Ma and Sun [252], Magri et al. [253], Köbler [254]

Simulation of polycrystalline microstructures	
- rigid-viscoplastic polycrystals	Lebensohn [191], Lebensohn et al. [255], Rollett et al. [256], Lee et al. [257]
- elasto-viscoplastic polycrystals (EVP)	Lebensohn et al. [202], Eisenlohr et al. [194], Kanjarla et al. [258], Roters et al. [259], Diehl et al. [260], Ozturk and Rollett [261], Cantara et al. [262], Niezgoda et al. [263], Kumar et al. [264], Kumar et al. [265], Lebensohn et al. [266], Cunningham et al. [267], Roters et al. [268]
- EVP coupled with a phase field model	Chen et al. [269], Zhao et al. [270], Kochmann et al. [18], Roters et al. [268], Ma and Sun [252]
- EVP coupled with dislocation dynamics	Berbenni et al. [228], Berbenni et al. [206], Djaka et al. [271], Bertin et al. [272], Santos et al. [273], Bertin and Capolungo [274]
- damage, fracture and fatigue behavior	Rovinelli et al. [275], Rovinelli et al. [276], Sharma et al. [277], Roters et al. [268], Sharma et al. [278], Ma and Sun [252], Lucarini et al. [279], Mareau [280]
Comparison to FE-based simulations	Michel et al. [117], Prakash and Lebensohn [8], Liu et al. [9], El Shawish et al. [281], Vondřejc and Geus [282]

The works presented in [11, 12, 190, 191] deal with the FFT-based basic fixed point scheme for small strain kinematics, reviewed in Section 2.4.1. The generalization of this method to finite strain kinematics is presented in [192, 194]. The rate of convergence of the basic fixed point scheme depends on the contrast between the phases, the choice for the homogeneous reference material behavior, and the material behavior itself (linear or non-linear). While different choices for the homogeneous reference material behavior are generally possible, the best convergence behavior for the fixed point scheme is gained by the arithmetic averages of the phase-dependent Lamé coefficients λ^0 and μ^0 [12, 195].

Independent of the choice for the reference material behavior, the convergence for the simulation of materials with high phase contrast is very slow and not even ensured for an infinite phase contrast. Improvements concerning the convergence behavior in this context are achieved by a polarization-based solution scheme [20, 196, 197] and a solution scheme based on augmented Lagrangians [196, 201, 202]. These methods are also called accelerated methods. While the polarization-based scheme relies on a reformulation of the Lippmann-Schwinger equation, the scheme based on augmented Lagrangians yields a reformulation of the microscopic BVP in terms of a minimization problem. A comparison of both methods with each other and to the basic fixed point scheme is given in [193]: For a low phase contrast the CPU time of the basic scheme is the shortest. For higher differences between the constituents, the accelerated schemes, are comparable, while the polarization-based scheme suffers at infinite phase contrast. A generalization of the polarization-based solution scheme for the simulation of composites with infinite phase contrast is given in [198]. A comparison of this general scheme to the initially proposed polarization-based scheme and to the solution scheme based on augmented Lagrangians shows, that the initially proposed polarization-based scheme and the solution scheme based on augmented Lagrangians are particular cases of this general polarization-based scheme [199]. Recently, a review of the polarization based schemes including an extension to the simulation of non-linear material behavior was given in [200].

A further accelerated solution strategy based on a conjugate gradient solver was introduced in [215] with a similar convergence behavior as the previous accelerated methods. This solution strategy is based on a linearized Lippmann-Schwinger equation (Equation (2.3)). Solving the resulting system of linear equations, the gradient decent method may be used. Using conjugate gradients in this context yields an Krylov subspace method, which is an efficient solution strategy of solving the system of linear equations. This first attempt on FFT-based conjugate gradient solvers suffers at infinite phase contrasts but has the advantage that it is independent of the choice for the reference material behavior. Another solution strategy incorporating the conjugate gradient solver [209], is based on a variational framework which minimizes the

energy of Hashin and Shtrikman [131]. This solution scheme also leads to convergence in the case of infinite phase contrast and is compared to the basic fixed point scheme in [210]. A further variational framework, based on a Galerkin discretization of the weak form of the microscopic boundary value problem with trigonometric polynomials, is given in [23]. The extension of the conjugate gradient based solver to capture non-linear material behavior is introduced in [216] and to finite strain kinematics in [195]. In addition, the equivalence of the basic fixed point scheme and a gradient descent method is shown in [195].

For complex material behavior, such as plasticity or damage, the conjugacy of the decent directions might get destroyed, so that the conjugate gradient solver will not converge anymore. Due to that, more stable solution strategies based on the non-linear generalized minimal residual method (GMRES) [218] or the fast gradient method of Nesterov [217] were developed. Recently, also a Barzilai-Borwein basic scheme [219] considering the Barzilai-Borwein step size selection technique for the gradient descent and a FFT-based solution scheme based on the heavy-ball method [250] were introduced. Furthermore, a Quasi-Newton method for a tangent-free FFT-based simulation of a complex non-linear material behavior is presented in [222]. Besides the investigations of these algorithms in the primal formulation of the unit cell problem, the effects of these solvers in a dual formulation [283] are investigated in [284].

Supplementary to the focus on computational efficiency, all these current developments also focus on a memory efficient implementation.

In addition, recent developments deal with the parallel implementation of these solvers using Message Passing Interface (MPI) and OpenMP [223, 224], or high-performance computational platforms integrating a graphics processing unit (GPU) [225, 226].

2.4.3 Methods to reduce the effect of Gibbs oscillations on convergence behavior

Concerning the FFT-based simulations, well known numerical artifacts are oscillations around discontinuities, known as the Gibbs phenomenon [19]. Approaches to tackle this problem use for example a modified Lippmann-Schwinger operator which approximates the differential operator in Equation (2.9) with first-order finite difference approximations [30, 227, 228, 229] as introduced by Willot [227]. Investigations by [26] show the equivalence of this modified scheme to a FFT-based finite element discretization which includes linear hexahedral elements with reduced integration. The modified FFT-based scheme may be further improved by using a finite difference discretization on a staggered grid, as shown in [230]. In addition, the artificial oscillations may also be treated by using higher-order finite difference approximations as

shown in [231, 232].

Other strategies of smoothing the results around discontinuities are based on regularization strategies [233] or composite voxels [32].

In Khorrami et al. [207], spectral algorithms are developed and compared for the numerical solution of periodic (quasi-static) elastic mechanical boundary-value problems. To this end, they employ two different approximations / discretizations of (truncated) Fourier series for periodic fields: (i) piecewise-constant approximation of the integrand of the Fourier mode integral, and (ii) trapezoidal approximation of this integral. Given these, a number of algorithms are formulated in the context of (I) Green-function preconditioning of stress divergence, and (II) finite-difference discretization of differential operators (i.e., the basis of the so-called "accelerated schemes": e.g., Moulinec and Silva [199]). These algorithms solve for displacement (i.e., rather than strain: e.g., Moulinec and Suquet [11]; Suquet [152]; Moulinec and Silva [199]; Willot [30]) via iteration (e.g., fixed-point in the linear, or Newton-Krylov in the non-linear, case). Differential operator discretization is based for example on central-differencing (CD), averaged CD (ACD), and averaged-forward-backward-differencing (AFB). As it turns out, AFB is equivalent to the "rotated scheme" (R) of Willot [30] in the context of trapezoidal discretization. Computational comparisons of these and related algorithms are carried out with the help of the (classic) benchmark case of a cubic-inclusion-matrix composite (e.g., Suquet [152]; Willot [30]) with discontinuous phase contrast at the matrix-inclusion interface. Related algorithms compared include that of Eloh et al. [205] based on the so-called "discrete Green operator", which employs piecewise-constant discretization, and Green-function preconditioning in Lippmann-Schwinger form, but not finite-difference discretization. For more information, the interested reader is referred to Khorrami et al. [207].

2.4.4 Model order reduction techniques for FFT-based solvers

Even though the FFT-based simulation of heterogeneous microstructures is already an efficient solution scheme, the computational costs for the simulation of highly resolved complex microstructures is still very intensive. Due to that, a recent research topic is the combination of the FFT-based solvers with model order reduction techniques.

A first FFT-based solver incorporating a model order reduction technique is given in [234] based on a proper orthogonal decomposition (POD), e.g. [285]. The POD projects the system equations onto a subspace spanned by a reduced basis of 'small' dimension. Doing that, so-called 'snapshots' need to be generated in a pre-processing step considering for example different loadings and loading directions. Subsequently, a snapshot matrix is computed, containing the corresponding strain solutions $\hat{\varepsilon}$ in Fourier space, followed by a singular value

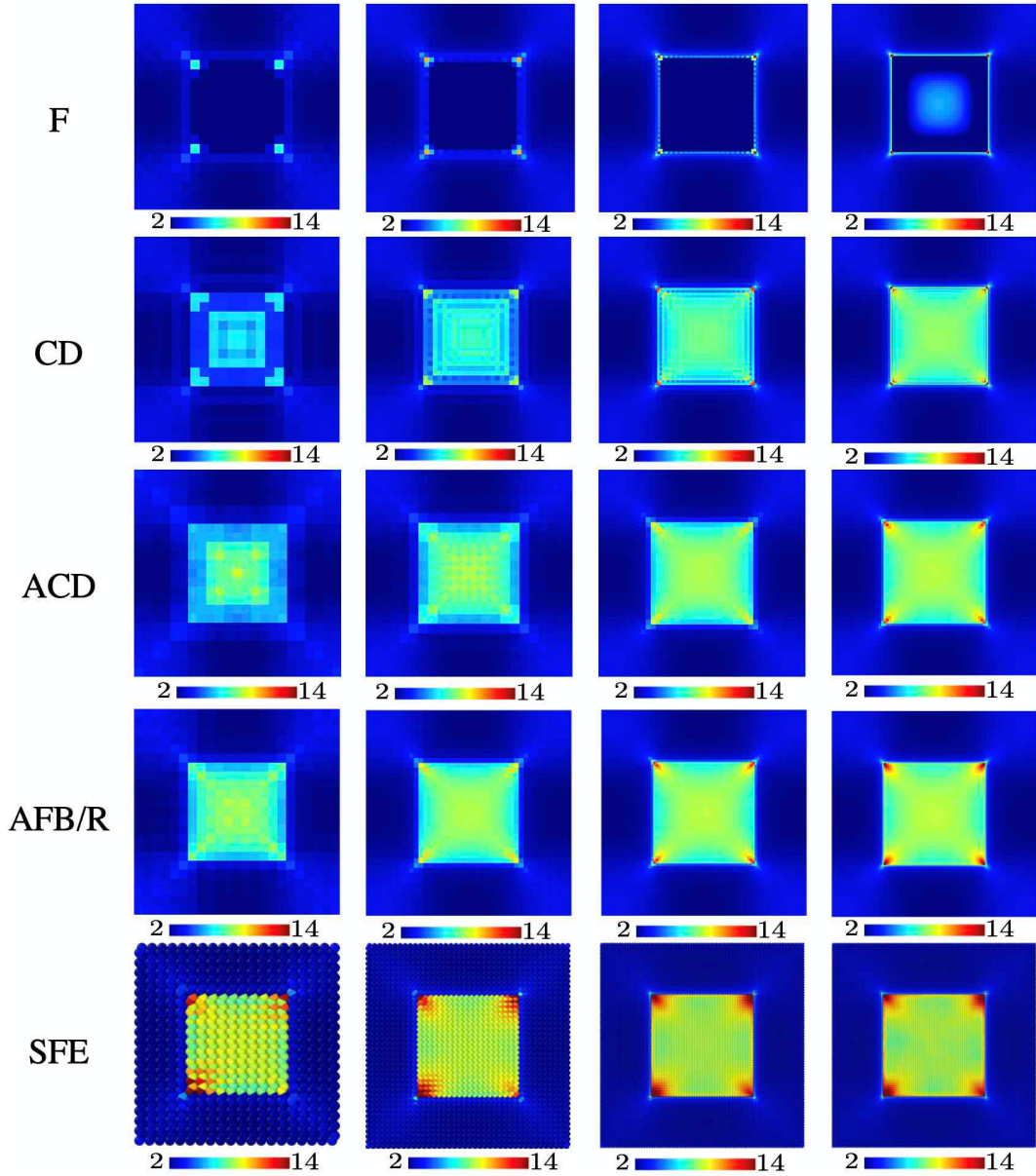


Figure 2.6: Results for the isotropic linear elastic 3D shear stress field σ_{12}/μ_M (x_1 horizontal, x_2 vertical, μ_M matrix shear modulus) obtained from different algorithms at a matrix-inclusion interface with discontinuous elastic stiffness phase contrast of 1000 for different spectral algorithms and different 3D numerical resolutions n^3 with $n = 22$ (left), $n = 42$ (middle left), $n = 82$ (middle right), and $n = 162$ (right). Compared here are algorithms employing finite-difference discretization based on central-differencing (CD), averaged CD (ACD), and averaged-forward-backward-differencing (AFB), which is equivalent to "rotated scheme" (R) of Willot [30]. Displayed for comparison as well are direct Fourier (F; no finite-difference discretization) and standard finite-element (SFE) solutions at the same resolution [207].

decomposition of this matrix and the computation of a projector operator for a given amount of the largest eigenvalues. This leads to a significant reduction of the computational time, with the drawback of a time consuming pre-processing step for the snapshot generation (but which must be only performed once for a given set of parameters).

Another model order reduction technique for the FFT-based microstructure simulation adapted to the intrinsic character of the spectral solver is based on solving the Lippmann-Schwinger equation in Fourier space (Equation (2.5)) by considering only a reduced set of Fourier modes. For this purpose, all Fourier modes are arranged on a grid with the lowest Fourier modes in the center. The first idea was to use a fixed, radial sampling pattern on this grid to determine the reduced set of Fourier modes [17]. After solving the Lippmann-Schwinger equation with this reduced set of Fourier modes, a reconstruction algorithm based on the TV_1 -algorithm [286] and a compatibility step was used to generate highly resolved microstructural fields. Since a fixed sampling pattern is used for all computations, no time consuming pre-processing step is necessary. An extension of this algorithm to finite strain kinematics is given in [235]. The accuracy of this model order reduction technique depends on the one hand on the number of considered Fourier modes and on the other hand on the choice of the considered Fourier modes. Due to that, an improved technique for the generation of a reduced set of wave vectors based on a geometrically adapted sampling pattern is proposed in [237]. Considering the same amount of Fourier modes, the solution based on such an adapted reduced set of Fourier modes leads to more accurate microstructural fields even without the reconstruction. A comparison of the stress fields generated by both techniques without the reconstruction and compatibility step is given in Figure 2.7. In [237] also a three dimensional extension of this model order reduction technique is given.

Yet another model order reduction technique is proposed in [236] based on low-rank tensor approximations. Within low-rank approximations, tensors are expressed by a smaller set of parameters (e.g. the representation of a second order tensor in terms of a generalized singular value) [287]. The utilization and investigation of different low-rank tensor approximations in terms of the Fourier-Galerkin method [23] again leads to an efficient FFT-based method.

2.4.5 Application of FFT-based simulations

The FFT-based simulation approach was introduced first in the context of computing the micromechanical fields within periodic microstructures of composite materials [11, 12]. The utilization of this method in terms of polycrystalline microstructures is given in [191]. In the past, numerous investigations and improvements for these simulations followed. An overview of microscale simulations of composites or polycrystalline materials in terms of the FFT-based

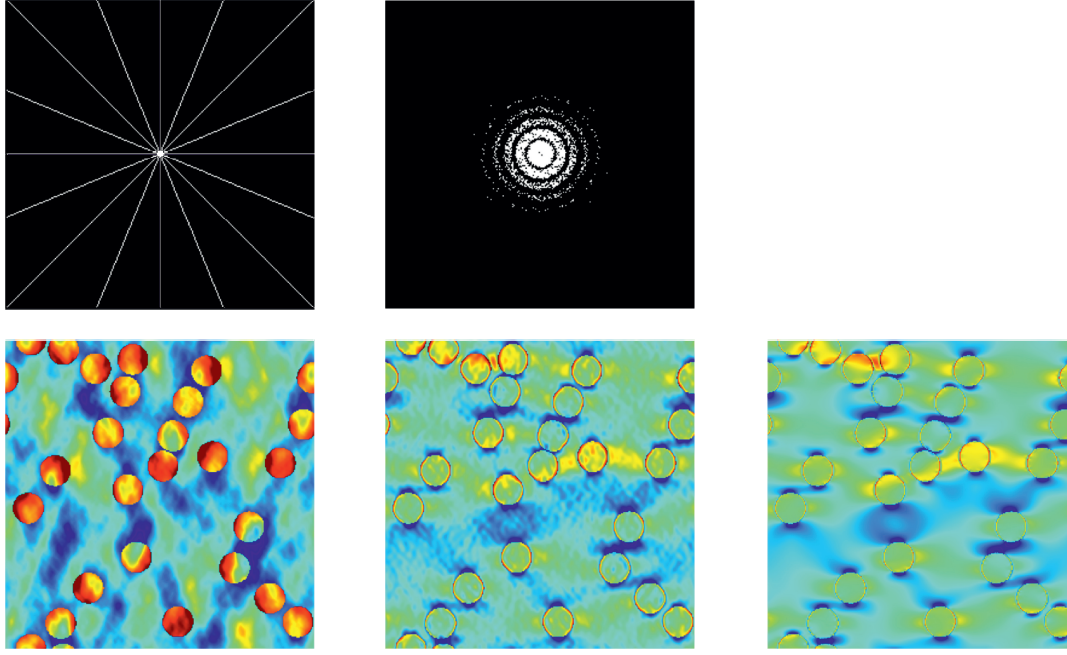


Figure 2.7: Fixed radial and geometrically adapted set of Fourier modes (*top*) and corresponding and reference stress distribution in a periodic composite microstructure (*bottom*).

simulation is presented in the following Subsections 2.4.5.1 and 2.4.5.2, respectively.

2.4.5.1 FFT-based simulation of composite microstructures

Considering linear or nonlinear mechanical composites with finite phase contrast, such as fiber reinforced materials, the FFT-based method was introduced in [11, 12] as alternative to the common FE-based microstructure simulation. Using the FFT-based method spatially resolved microstructural fields such as the microstructural strain field in a glass fiber reinforced plastic microstructure may be computed, see Figure 2.8.

To model composites with infinite phase contrast, such as microstructures with voids or rigid inclusions, an extension of the basic fixed-point scheme based on augmented Lagrangians was introduced in [201]. This method is applied in [241, 242] to investigate the effect of the microstructural distribution of voids in composite materials on the plastic overall response. In [288] also a comparison of similar results with the results from analytical homogenization is given. In addition, the effective properties of two-phase composites reinforced by randomly distributed spherical particles are investigated and compared to analytical homogenization methods in [243]. Both studies showed that the analytical models do not provide accurate results for a wide range of phase contrasts and volume fractions. Furthermore, in [289] the FFT-based method is used to predict the material properties in additively manufactured structures and in

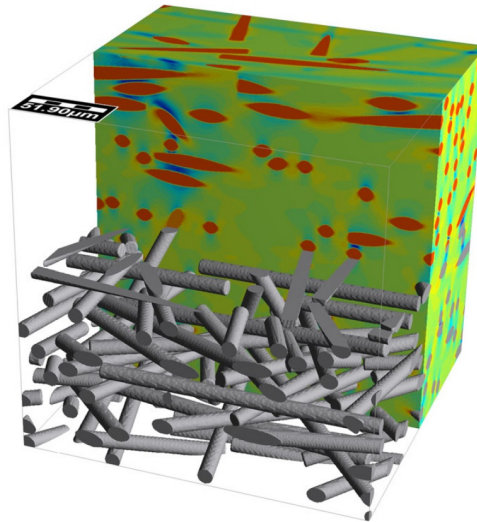


Figure 2.8: Strain distribution in a periodic glass fiber reinforced plastic microstructure [195].

[244] to display the mechanical fields in thermoplastic polymer composites filled with hollow glass microspheres. Also the effective properties of sheet molding compound composites may be computed in terms of a FFT-based simulation [245].

Besides the investigation on classical composites, the FFT-based method was also used to investigate the behavior of calcium silicate hydrates (C-S-H) in hardened cement paste [238]. The influence of size, distribution and shape of inclusions on the concrete creep properties was shown in [239] and the effect of regular and irregular coarse aggregates in self-compacting high-performance concrete was investigated in [240].

An additional field of the mechanical microstructure simulation is the prediction of the micromechanical damage behavior. In [13] the FFT-based method is combined with continuum damage mechanics to model the failure and progressive damage in composite materials. A similar simulation approach is used to compute the stiffness and strength of medium density fiberboards [246], to capture the progressive damage in 3D braided composites [248] and to capture the damage evolution in porous media, such as sandstone [249]. Instead of the continuum damage approach, the FFT-based method may also be combined with a phase-field approach (e.g. [290, 291]) to model the damage evolution. This approach was used to investigate the brittle fracture in an idealized continuous fiber composite [220, 250] and to analyze the damage initiation in a Silicon carbide (SiC/SiC) composite tube [221].

The FFT-based method furthermore enables to compute the microscopic responses of composite microstructures in different, non-mechanical contexts. This is for example necessary to investigate the behavior of thermoelastic composites [197], the thermal properties of liq-

uid metal elastomeric composites [292], the electrical conduction in periodic composites [215, 227], the electro-mechanically coupled material behavior [293] or the elastic wave propagation in heterogeneous media [294].

2.4.5.2 FFT-based simulation of polycrystalline microstructures

A general overview describing anisotropic heterogeneous crystalline materials is given in [295], discussing constitutive laws, kinematics, multiscale techniques and comparisons to experimental results. Considering computational homogenization of polycrystalline microstructures a detailed review is given in [296]. Lebensohn (2001) [191] was the first to utilize the FFT-based method in this context incorporating a rigid-viscoplastic material behavior. This full-field simulation approach was for example used to validate analytical methods for the prediction of the effective microstructural response in [233, 297, 298].

To generate polycrystalline microstructures, one possibility is to use a Voronoi tessellation as shown in [299, 300, 301]. An advantage of the FFT-based method is the possibility of computing the microstructural fields directly from an image of their microstructure. Therefore, modelling the subgrain texture evolution directly based on polycrystalline microstructures from electron back-scattering diffraction (EBSD)-based orientation imaging microscopy (OIM) was proposed in [255]. Using such polycrystalline microstructures, numerical experiments have been performed to show for example that stress hot spots occur close to grain boundaries [256]. In addition, the influence of the volume fraction and the contiguity of isotropic particles embedded in a polycrystalline matrix phase on the stress and strain-rate fields is investigated in [257]. It showed that the first and second moments of the stress and strain-rate are differently affected by these properties.

A generalization of the rigid-viscoplastic material behavior to an elasto-viscoplastic formulation in terms of a FFT-based microstructure simulation (EVP-FFT) is given by Lebensohn et al. (2012) [202] considering the small strain regime and by Eisenlohr et al. (2013) [194] considering the finite strain regime. Using this EVP-FFT-based method, further studies modelled the internal lattice strain distributions in stainless steel [258] or in dual phase steel microstructures [260, 261, 262]. Some exemplary results of using this EVP-FFT model are shown in Figure 2.9. A modification to include the shear transformation strain associated with deformation twinning is presented in [263, 264, 265]. Another extension of this model is based on augmented Lagrangians [201] for the simulation of void growth in polycrystalline materials [266]. This modified simulation approach is used to investigate the mechanical behavior of metal additive manufactured microstructures [267]. It showed that pores, which result from the additive manufacturing process itself, lead to significant stress hotspots.

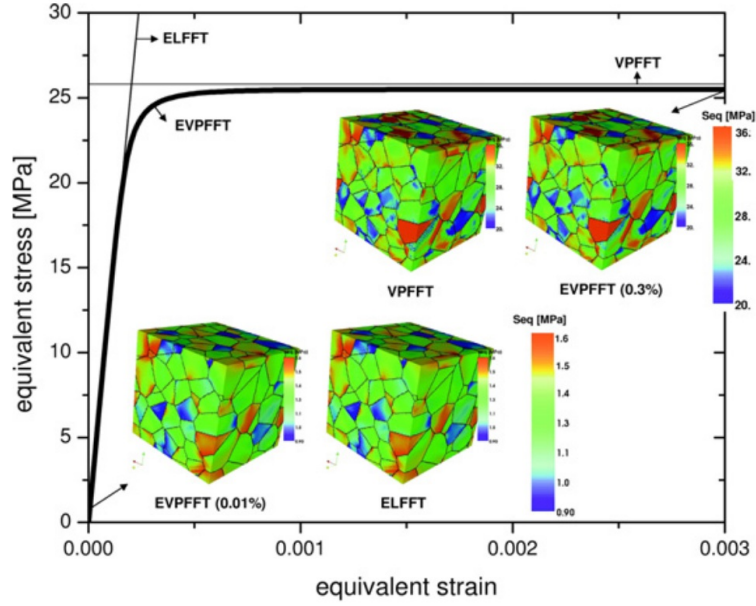


Figure 2.9: Effective equivalent stress—strain curve and microstructural equivalent stress fields S_{eq} predicted by the EVP—FFT model. For comparison, the results of a FFT-based simulation of a purely elastic (EL-FFT) and a purely viscoplastic (VP-FFT) material model with the same material parameters are shown [202].

Coupling the EVP-FFT-based method with a phase-field model (e.g. [290, 291]) enables the simulation of different additional physical processes. Examples are simulations to capture the recrystallization of polycrystals [269, 270], phase transformations [18] and fracture within polycrystalline microstructures [252], respectively. Further extensions concern the modelling of fatigue crack growth [275, 276], modelling interface decohesion in terms of a nonlocal interphase [277] or a gradient damage approach [278]. Incorporating crystallographic defects in terms of dislocations, introduced in [302], the EVP-FFT-based method was coupled with field dislocation dynamics (FDM) in [206, 228, 271] and discrete dislocation dynamics in [272, 273, 274]. To investigate the grain size on the flow stress of polycrystals, known as the Hall-Petch effect [303, 304], also an intrinsic material length scale associated with the plastic strain gradients may be introduced resulting in a strain gradient crystal plasticity approach [229, 305].

A comparison of the computed micromechanical fields to experimental mechanical fields is given in [306, 307, 308], with the microstructure model directly gained from EBSD measurements. The study confirmed a good correlation between the averaged results obtained from experiments and the results from simulations, while the local microstructural results do agree qualitatively. In addition, a virtual laboratory approach is introduced in [309] to determine the

initial yield surface for sheet metal forming operations based on highly resolved microstructural FFT-based simulations and to compare the results to experimental investigations.

An earlier overview of FFT-based simulation of polycrystalline microstructures is given in [310, 311] and the free simulation software DAMASK for the simulation of polycrystalline microstructures based on finite elements or fast Fourier transforms is introduced in [259, 268]. Besides the investigations on polycrystalline metallic microstructures, also the simulation of the micromechanical fields within polycrystalline ice was performed by using a FFT-based method [312, 313, 314].

2.4.6 Comparison between FE- and FFT-based computational methods

Compared to finite element simulations one major advantage of FFT-based simulations is the image processing-like character and the associated possibility of directly using images of a real microstructure for the numerical simulation [11, 12, 255]. Therefore, in contrast to the finite element method, it avoids possible difficulties due to meshing of complex microstructures. In addition, several studies, e.g. [8, 9, 117] showed, that the FFT-based method is more efficient than a classical FE-based microstructure simulation under the condition of periodicity.

A major disadvantage of FFT-based microstructure simulations is the restriction to periodic microstructures. This results from the intrinsic periodic ansatz functions. Nevertheless, considering a multiscale simulation these periodic microstructures are usually desired. In this case no additional effort is needed to prescribe the periodic boundary conditions.

Other disadvantages of the FFT-based basic fixed-point scheme are related to resolution errors due to the Gibbs phenomenon and numerical problems treating composites with high or infinite phase contrasts. These problems were addressed and solved in several works. Solutions concerning the resolution errors are for example elaborated in [30, 32, 227, 231, 233] by using finite difference approximations of the differential operator in Equation (2.9) or using composite voxels. Solutions concerning the treatment of microstructures with infinite phase contrast are addressed in [196, 198, 200, 201, 202] using polarization based schemes, solution schemes based on augmented Lagrangians or conjugate gradient solvers.

Based on the Galerkin discretization, introduced in [23, 209, 210] and improved in [211, 212], the analogy of the FFT-based solver to finite element based simulations is finally shown in [213, 214, 217]. This is done by constructing the FFT-based solver using a similar variational basis as for conventional FE methods. Due to that, the constitutive routines of the FE methods may directly be used within the FFT-based framework, while still profiting from the computational efficiency of the FFT-based solver.

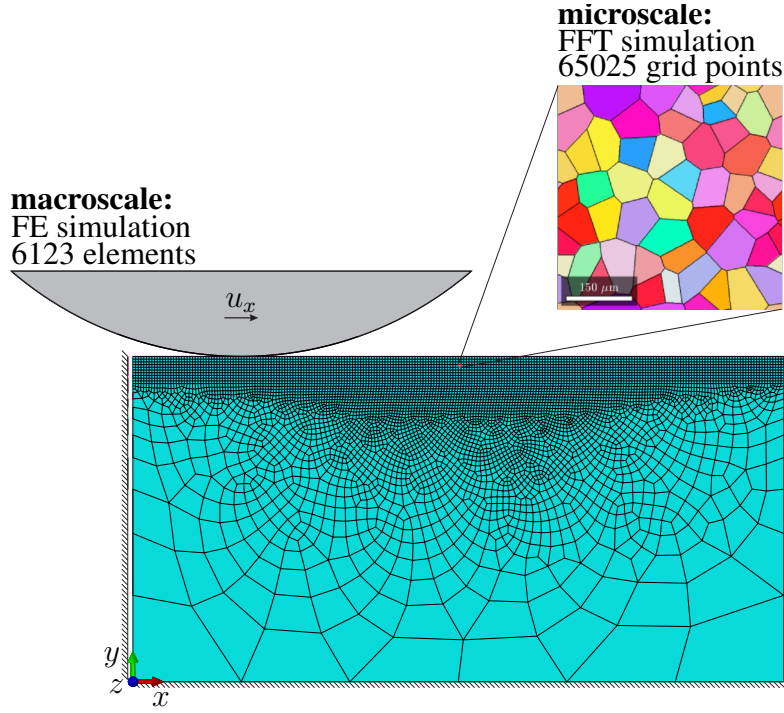


Figure 2.10: Example of a two-scale FE-FFT-based simulation. The FE simulation is used on the macroscale, while the FFT-based simulation is used on the periodic microscale.

2.5 FE-FFT-based two-scale simulation

The voxel like character of Fourier spectral solvers results in simple discretization of the underlying microstructure and periodic global ansatz functions intrinsically imply periodic boundary conditions. For this reason, the FFT-based method is a well-suited and efficient solver for the microscopic BVP in terms of a two-scale FE-FFT-based simulation. In this context, the macroscopic BVP is discretized into finite elements while the microscopic BVP is defined by a distinct number of grid points, see Figure 2.10. The overall macroscopic material behavior is then defined as volume average of its microscopic counterpart, which yields

$$\bar{\varepsilon}(\bar{x}) := \frac{1}{\Omega} \int_{\Omega} \varepsilon(\bar{x}, \mathbf{x}) \, d\Omega \quad (2.10)$$

$$\bar{\sigma}(\bar{x}) := \frac{1}{\Omega} \int_{\Omega} \sigma(\bar{x}, \mathbf{x}) \, d\Omega \quad (2.11)$$

in terms of small strain kinematics.

The novel FE-FFT-based two-scale simulation approach was first introduced for modeling

progressive damage within fiber-reinforced composites in [13]. As a first approach, the latter authors utilized the basic fixed-point scheme [11, 12] for the FFT-based microstructure simulation within a small strain regime. A more efficient FE-FFT-based two-scale method was proposed in [18] based on augmented Lagrangians [202] for the FFT-based simulation of polycrystalline materials incorporating phase-field-based simulations of microstructural phase transformations.

Considering a two-scale simulation, the computation of the macroscopic tangent operator is essential, but computationally very expensive. One way of computing the macroscopic tangent operator is based on a numerical approximation [13, 16, 18]. Therefore, the linearized stress increment

$$\Delta \bar{\sigma} = \frac{\partial \bar{\sigma}}{\partial \bar{\epsilon}} : \Delta \bar{\epsilon} \quad (2.12)$$

and the perturbed strain field

$$\bar{\epsilon}_{\Delta}^{kl} = \bar{\epsilon} + \frac{\Delta \bar{\epsilon}}{2} (\mathbf{e}_k \otimes \mathbf{e}_l + \mathbf{e}_l \otimes \mathbf{e}_k) = \bar{\epsilon} + \Delta \bar{\epsilon}^{kl} \quad (2.13)$$

with the perturbation strain $\Delta \bar{\epsilon}$ need to be taken into account. Performing a forward difference approximation of the stress increment and considering the definition of the perturbed strain field, the numerical tangent operator yields

$$\bar{\mathbb{C}}_{ijkl} = \frac{\partial \bar{\sigma}_{ij}}{\partial \bar{\epsilon}_{kl}} \approx \frac{\bar{\sigma}_{ij}(\bar{\epsilon}_{\Delta}^{kl}) - \bar{\sigma}_{ij}(\bar{\epsilon})}{\Delta \bar{\epsilon}}. \quad (2.14)$$

Consequently, in the three-dimensional case, six perturbations are necessary to compute the numerical tangent operator. These perturbations must be as small as possible in order to obtain an accurate approximation of the analytical tangent operator, while numerical problems due to too small perturbations need to be avoided, which leads to values between $\Delta \bar{\epsilon} = 10^{-8}$ and $\Delta \bar{\epsilon} = 10^{-6}$ for the perturbation.

Considering finite strain kinematics, with the macroscopic first Piola–Kirchhoff stress tensor $\bar{\mathbf{P}}$ and the macroscopic deformation gradient $\bar{\mathbf{F}}$, nine perturbations are needed in general to compute the numerical tangent operator, since $\bar{\mathbf{F}}$ is not symmetric. An efficient method based on only six instead of these nine perturbations was proposed in [315, 316].

Another method for the computation of the macroscopic tangent operator is derived by means of the Lippmann-Schwinger equation and can be computed from a system of linear equations, as shown in [317]. To deduce the aforementioned system of linear equations, the linearized

stress increment (2.12) is transformed into

$$\Delta \bar{\sigma} = \frac{1}{\Omega} \left[\int_{\Omega} \mathbb{C} \, d\Omega + \int_{\Omega} \mathbb{C} : \frac{\partial \tilde{\epsilon}}{\partial \bar{\epsilon}} \, d\Omega \right] : \Delta \bar{\epsilon} \quad (2.15)$$

as shown in [173, 318]. This leads to the definition of the algorithmically consistent macroscopic tangent

$$\mathbb{C}^{\text{algo}} := \frac{1}{\Omega} \left[\int_{\Omega} \mathbb{C} \, d\Omega + \int_{\Omega} \mathbb{C} : \frac{\partial \tilde{\epsilon}}{\partial \bar{\epsilon}} \, d\Omega \right]. \quad (2.16)$$

Within this definition, the first part of the equation

$$\bar{\mathbb{C}}^V = \frac{1}{\Omega} \int_{\Omega} \mathbb{C} \, d\Omega \quad (2.17)$$

is the effective stiffness tensor as defined by Voigt [111]. In addition, the derivative of the fluctuation strain field $\tilde{\epsilon}$ with respect to the macroscopic strain field $\bar{\epsilon}$ can be determined by solving the following linear equation system:

$$\mathbb{I}^0 * [\mathbb{C} - \mathbb{C}^0] = \mathbb{I}^0 * \left[(\mathbb{C} - \mathbb{C}^0) : \frac{\partial \tilde{\epsilon}}{\partial \bar{\epsilon}} \right] - \frac{\partial \tilde{\epsilon}}{\partial \bar{\epsilon}}. \quad (2.18)$$

A straight forward extension of this definition of the algorithmically consistent macroscopic tangent operator to finite strains is given in [317] and leads to a speedup of 1.5 to 2 for different material behaviors compared to the aforementioned numerical tangent operator.

Since a two-scale full field simulation is computationally expensive, an efficient and accurate FE-FFT-based simulation procedure was proposed in [16, 110], while the FFT-based microstructure simulation is based on a Newton-Krylov solution scheme [195, 215, 216]. The efficient solution procedure is based on a pre-processing, a processing and a post-processing step. Within the pre-processing step different discretizations of a polycrystalline microstructure with different textures, number of grains and prescribed macroscopic strains are investigated. This leads to a minimal number of grid points, which is necessary to obtain an accurate macroscopic response. The resulting coarsely discretized microstructure is utilized within the actual two-scale simulation, while the history of the macroscopic strain of any point of particular interest is saved. Finally, in the post-processing step, this macroscopic strain and a finely discretized microstructure are used to generate highly resolved microstructural fields for these macroscopic points, see Figure 2.11. A generalization of this simulation procedure to finite strain kinematics is given in [319].

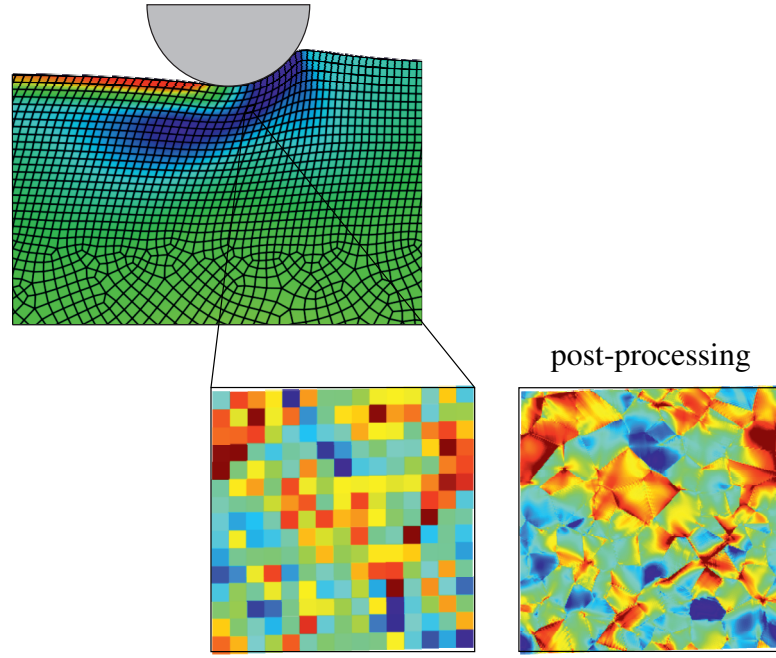


Figure 2.11: Efficient FE-FFT-based two-scale simulation with a coarse discretized microstructure, followed by a post-processing step to generate highly resolved microstructural data.

Another efficient simulation strategy is based on using highly resolved full field simulations only in macroscopic critical areas. In this context, an algorithm, which uses a database with certain tangent operators for the macroscopic simulation of fiberboards and switches to a full field FE-FFT-based two scale simulation if no appropriate tangent operator is available, was proposed in [246]. A similar approach is presented in [254, 320], in which a FFT-based simulation is used to train a database model in a pre-processing step. Within the actual two-scale FE-FFT-based simulation, this database model is used in general, except for macroscopic critical areas, in which a highly resolved full field simulation is performed to capture the viscoelastic and fatigue behavior of short fiber-reinforced polymers.

In contrast to the aforementioned fully coupled concurrent FE-FFT-based simulation approaches, a solution strategy based on an exclusively macroscopic FE simulation followed by an FFT-based simulation of distinct macroscopic integration points was applied in [129]. Doing that, a quantitative understanding of the load dependence of lattice strain evolution during monotonic loading was obtained. In addition, the intergranular strain evolution during biaxial loading [325] and the role of microstructural evolution, such as texture, anisotropy and dislocation density was investigated [326] in a similar manner. Finally, this two-scale simulation approach was used to predict and explain the lattice strain and intensity evolution of microstructures gained from in-situ diffraction experiments [327].

Table 2.3: FE-FFT-based algorithms and applications.

Algorithms and applications	Key references
Concurrent FE-FFT-based simulation	Spahn et al. [13], Sliseris et al. [246], Kochmann et al. [18], Kochmann et al. [16], Kochmann et al. [110], Kochmann et al. [316], Göküzüm and Keip [317], Rambašek et al. [321], Göküzüm et al. [293], Welschinger et al. [320], Fang et al. [322], Wang et al. [323], Han et al. [324], Köbler et al. [254], Gierden et al. [319]
Non-concurrent FE-FFT-based simulation	Upadhyay et al. [129], Upadhyay et al. [325], Upadhyay et al. [326], Upadhyay et al. [327], Liu et al. [328]
Macroscopic tangent operator - numerical tangent operator - algorithmically consistent tangent operator	Spahn et al. [13], Sliseris et al. [246], Kochmann et al. [18], Kochmann et al. [16], Kochmann et al. [110], Kochmann et al. [316], Fang et al. [322], Wang et al. [323], Gierden et al. [319] Göküzüm and Keip [317], Rambašek et al. [321], Göküzüm et al. [293]
Incorporating MOR techniques	Sliseris et al. [246], Kochmann et al. [16], Kochmann et al. [110], Welschinger et al. [320], Köbler et al. [254], Gierden et al. [319]
Simulation of composite microstructures	Spahn et al. [13], Göküzüm and Keip [317], Rambašek et al. [321], Göküzüm et al. [293], Welschinger et al. [320], Fang et al. [322], Wang et al. [323], Köbler et al. [254]
Simulation of polycrystalline microstructures	Kochmann et al. [18], Upadhyay et al. [325], Kochmann et al. [16], Kochmann et al. [110], Upadhyay et al. [326], Kochmann et al. [316], Upadhyay et al. [327], Liu et al. [328], Han et al. [324], Gierden et al. [319]

In the following, some more applications of the FE-FFT-based multiscale approach are listed. The utilization of the two-scale simulation approach to magneto-mechanically and electro-mechanically coupled materials at finite strains is given in [321] and [293], respectively. In addition, the FE-FFT-based method was used to investigate the process-structure-property relationship for additive manufacturing in a small strain regime in [328]. The application of the software DAMASK [259, 268] within a multiscale framework has recently been presented in [324]. Finally, investigating braided composite beams in terms of a FE-FFT-based two-scale simulation [322, 323], the FFT-based microstructure simulation based on variational methods [212, 214, 248] was used within the two-scale context, to overcome the poor convergence behavior of FFT-based solvers in terms of composites with high phase contrasts. An overview of the FE-FFT-based algorithms and their applications is also given in Table 2.3.

2.6 Conclusion

For periodic micro-heterogeneous materials, the FFT-based method represents a computational method which is a suitable alternative to classical FE-based methods. In the last two and a half decades this FFT-based method has proven to be a fast and accurate tool in regard of a computational microscale simulation. One major advantage of FFT-based simulations compared to FE-based simulations is the image processing-like character and, connected to that, the possibility to directly employ images of a real microstructure for the numerical simulation. This avoids the meshing of complex microstructures.

Possible problems of the FFT-based method concern the convergence behavior within simulations of microstructures incorporating infinite phase contrasts and artificial oscillations around discontinuities related to the Gibbs phenomenon. These problems were solved by developing accelerated solution methods (e.g. polarization based methods, methods based on augmented Lagrangians, gradient decent methods, or quasi-Newton methods) and using for example finite difference approximations of the Lippmann-Schwinger, composite voxels or a discrete Greens operator, respectively. This leads to a solution scheme, which is even more efficient than the classical FE-based microstructure simulation. Nevertheless, the FFT-based microstructure simulation is exclusively restricted to investigations on periodic microstructures, while there are no further restrictions for the FE-based microstructure simulation.

To generate an even more efficient simulation approach model order reduction techniques for FFT-based solvers were developed recently. These progresses and the intrinsic periodic character of the spectral solver including intrinsic periodic boundary conditions, lead to a well-suited scheme in terms of an efficient and accurate FE-FFT-based two-scale method.

3 | Article 2:

Efficient two-scale FE-FFT-based mechanical process simulation of elasto-viscoplastic polycrystals at finite strains

This article was published as:

Gierden, C., Kochmann, J., Waimann, J., Kinner-Becker, T., Sölter, J., Svendsen, B. and Reese, S. [2021], ‘Efficient two-scale FE-FFT-based mechanical process simulation of elasto-viscoplastic polycrystals at finite strains’, *Computer Methods in Applied Mechanics and Engineering* **374**, 113566.

Disclosure of the individual authors’ contributions to the article:

C. Gierden reviewed the relevant existing literature, implemented the framework of the FFT-based microstructure simulation of elasto-viscoplastic polycrystals at finite strains considered in this study into Abaqus / Standard (via the UMAT interface), performed all simulations, interpreted the results and wrote the article. J. Kochmann provided a Fortran stand-alone code for the FFT-based microstructure simulation of elasto-viscoplastic polycrystals at finite strains. T. Kinner-Becker and J. Sölter participated in the discussion regarding the setup of the deep rolling process. Everyone, including J. Waimann, B. Svendsen and S. Reese, gave conceptual advice, contributed to the discussion of the results, proofread the article and made valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

3.1 Abstract

The purpose of this work is the development of an efficient two-scale numerical scheme for the prediction of the local and overall mechanical behavior of polycrystalline materials with elasto-viscoplastic constitutive behavior at finite strains. Assuming scale separation, the microstructural deformations are prescribed by the kinematics of the macroscopic continuum body. The macroscopic constitutive behavior is in turn determined by the mean response of the point-wise linked microstructure which is represented by a periodic unit cell. The algorithmic formulation and numerical solution of the two locally coupled boundary value problems is based on the FE-FFT method. In particular, the presented work is concerned with the development of a CPU- and memory-efficient solution strategy for two-scale finite strain crystal plasticity simulations of polycrystalline aggregates which is based on a microstructural convergence analysis. This efficient solution strategy allows a two-scale simulation of complex macroscopic boundary value problems in a reasonable time period. In order to demonstrate the versatile use of the proposed method, three polycrystalline materials namely copper, aluminum and iron are studied with different textures for three distinct macroscopic loading conditions. On this basis, the micromechanical fields and the overall material response of an iron-based polycrystal are predicted for a deep rolling process, which serves as a testing example for a representative and application oriented simulation.

3.2 Introduction

The development of design optimization techniques for heterogeneous materials requires an appropriate description of statistical, topological and physical characteristics of the underlying microstructure and its overall constitutive response. To capture such microstructural details in a statistical fashion, an analytical homogenization like introduced by Voigt [111] or Reuss [112] may be used. Improved analytical homogenization approaches based on variational methods were first introduced by Hashin and Shtrikman [132]. Since we want to capture the microstructural details in a spatially resolved fashion, a two-scale full-field simulations are necessary. Most common in this context is the FE^2 method introduced by Smit et al. [113] and Feyel and Chaboche [123] which is based on representative volume elements [e.g., 154, 161, 163, 329] and computational homogenization [e.g., 124, 330]. Focussing on polycrystalline materials with elasto-viscoplastic constitutive behavior, various numerical results have been published by different authors assuming small [e.g., 123] and finite strain kinematics [e.g., 172, 174, 318]. However, technologically relevant two-scale simulations of complex microstructures with non-

linear constitutive behavior are still barely possible due to (i) the large amount of memory storage required for the high number of internal variables and (ii) the high computational effort for the solution of the local problem.

The large amount of memory storage (i) can significantly be reduced using statistically similar representative volume elements (RVEs) [e.g., 164, 331]. RVEs represent the morphology of the real microstructure by a lower complexity-based morphology which is generated based on statistical descriptors [e.g., 135, 136]. Additionally, it is well-known that even coarse discretizations of complex microstructures lead to quantitatively accurate predictions in terms of overall quantities [e.g., 16, 332].

The aforementioned computational effort (ii) - related to FE^2 simulations - can be significantly reduced using fast Fourier transform (FFT) methods for the numerical solution of the local problem. Comparisons between FE- and FFT-based crystal plasticity simulations of heterogeneous media have been documented by Prakash and Lebensohn [8], Liu et al. [9] and Eisenlohr et al. [194]. First, Moulinec and Suquet [11, 12] introduced such a FFT-based scheme for computing the effective response of linear and non-linear composites. Depending on the choice of an homogeneous reference material, this basic scheme which is based on fixed-point iterations leads only to a conditional convergence. Therefore, numerically more robust methods have been developed. Just to mention a few, such methods are based on augmented Lagrangians [e.g., 180, 196, 202], on Newton-Krylov solvers such as conjugate gradients [e.g., 195, 197, 215, 216] and as the general minimal residual method [e.g., 333], and polarization-based formulations [e.g., 20]. Resolution problems originally associated with Fourier spectral methods, such as spurious oscillations, have been solved using first- [30] and higher-order finite difference approximations [231] of the differential operators or composite-voxels [e.g., 32]. Fourier transforms are characterized by periodic global higher-order shape functions yielding a high-fidelity representation of micromechanical fields and periodic boundary conditions. Furthermore, such mesh-free or Voxel-based methods make the discretization of complex and fine-scale microstructures easily possible. Thus, Fourier spectral methods seem to be well-suitable for an efficient numerical solution of the local problem in the context of two-scale full-field simulations. Nevertheless the computational effort of solving the local boundary value problem is still high. Therefore, also model order reduction techniques like proposed in [17, 234, 235], or [236] could be used to solve the local boundary value problem.

However, only a few works have been published in the field of two-scale full-field FE-FFT-based simulations. First, Spahn et al. [13] proposed such an FE-FFT-based approach to model progressive damage in fiber-reinforced composite materials assuming linearized kinematics. Elastic phase-field [18] and elasto-viscoplastic constitutive modeling [16] of polycrystalline

aggregates has recently been addressed by the authors in previous works. Lately, Göküzüm and Keip [317] presented a finite strain extension focussing on composites with hyperelastic material behavior and the numerical treatment of the overall consistent algorithmic tangent moduli. More recently, Kochmann et al. [316] and Han et al. [334] proposed an algorithmic framework for two-scale FE-FFT-based modeling of elasto-viscoplastic polycrystals at finite strains.

This work deals with the development of a memory- and CPU-efficient solution strategy for two-scale full-field simulations of polycrystalline materials with elasto-viscoplastic constitutive behavior at finite strains. To this end, the solution scheme by Kochmann et al. [16] for linearized kinematics is extended to finite strains and validated for materials with different intrinsic anisotropy. In addition this solution scheme is applied to an application oriented simulation of a deep rolling process.

The paper is structured as follows: the two-scale boundary value problem (BVP) and scale transition are reviewed in Section 3.3. Section 3.4 deals with the kinematics of and the specific phenomenological constitutive model for finite strain elasto-viscoplasticity of single crystals. The algorithmic formulation and numerical solution of the macroscopic FE- and microscopic FFT-based BVP as well as the discretized set of local equilibrium equations are briefly explained in Section 3.5. In Section 3.6 the aforementioned solution strategy is explained and applied to a two-scale process simulation in Section 3.7. The paper ends with a conclusion and an outlook in Section 3.8.

Notation. A direct tensor notation is preferred throughout the text. Vectors and second-order tensors are represented by bold letters, e.g. $\mathbf{a}$ and $\mathbf{A}$, a tensor of fourth order by, e.g., $\mathbb{A}$. The linear mapping of a second-order tensor $\mathbf{B}$ by a fourth-order tensor $\mathbb{C}$ is denoted by $\mathbf{A} = \mathbb{C} : \mathbf{B}$. The scalar and dyadic product are denoted, e.g. by $\mathbf{a} \cdot \mathbf{b}$ as well as $\mathbf{A} : \mathbf{B}$, and $\mathbf{A} \otimes \mathbf{B}$, respectively. Furthermore, $\|\bullet\|$ represents the Frobenius norm. The Voigt representation of any second-order tensor $\mathbf{A}$ is denoted by $\mathbf{A}_v$ and a bar over any quantity $\bar{A}$ refers to the macroscopic BVP, whereas the absence of a bar is related to quantities on the microstructural level. Additional notation will be introduced when needed.

3.3 Two-scale boundary value problem (BVP)

Considering a two-scale boundary value problem the BVP is split into a microscopic BVP concerning the description of the material behavior and a macroscopic BVP related to the structural behavior.

3.3.1 Macroscopic continuum relations

Let us consider the macroscopic continuum $\bar{\mathcal{B}}_t$ at time $t \in T$, where $T \subset \mathbb{R}$ denotes the time interval of interest $T = [t_0, t_{\text{end}}]$. The reference configuration $\bar{\mathcal{B}}_0 \subset \mathbb{R}^3$ at $t = 0$ is identified by the position vector $\bar{\mathbf{X}} \in \bar{\mathcal{B}}_0$. The macroscopic structure is subjected to displacement and/or traction boundary conditions, i.e.,

$$\bar{\mathbf{u}} = \check{\bar{\mathbf{u}}} \text{ on } \partial_{\bar{\mathbf{u}}} \bar{\mathcal{B}}_0, \quad \bar{\mathbf{t}} = \check{\bar{\mathbf{t}}} \text{ on } \partial_{\bar{\mathbf{t}}} \bar{\mathcal{B}}_0 \quad (3.1)$$

such that $\partial \bar{\mathcal{B}}_0 = \partial_{\bar{\mathbf{u}}} \bar{\mathcal{B}}_0 \cup \partial_{\bar{\mathbf{t}}} \bar{\mathcal{B}}_0$ and $\partial_{\bar{\mathbf{u}}} \bar{\mathcal{B}}_0 \cap \partial_{\bar{\mathbf{t}}} \bar{\mathcal{B}}_0 = \emptyset$. The macroscopic non-linear mapping $\bar{\varphi}_t(\bar{\mathbf{X}}, t)$ maps points $\bar{\mathbf{X}}$ of the reference configuration $\bar{\mathcal{B}}_0$ onto points $\bar{\mathbf{x}}$ in the current configuration $\bar{\mathcal{B}}_t$, see Figure 3.1.

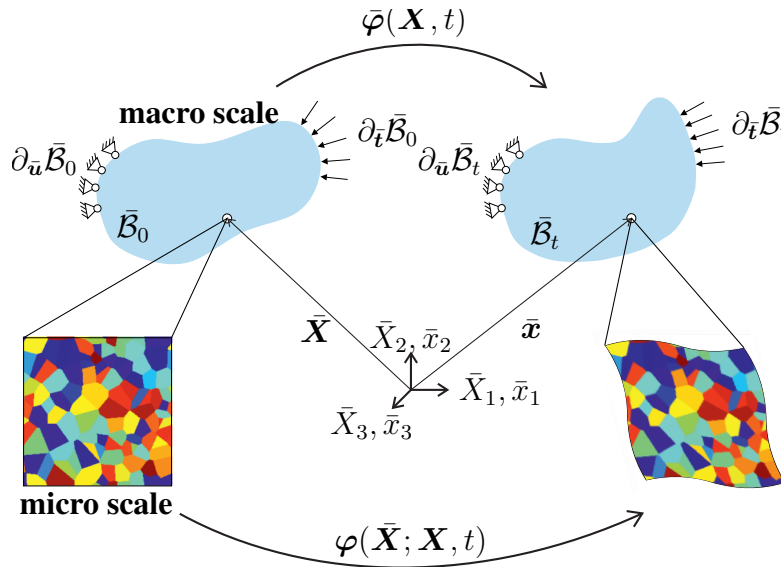


Figure 3.1: Relations between current and reference configurations of the micro and macroscale.

The macroscopic deformation gradient $\bar{\mathbf{F}}(\bar{\mathbf{X}}, t) = \text{Grad}_{\bar{\mathbf{X}}} \bar{\varphi}_t(\bar{\mathbf{X}}, t)$ and the first Piola-Kirchhoff stress tensor $\bar{\mathbf{P}}(\bar{\mathbf{X}}, t) = \bar{\mathbf{P}}(\bar{\mathbf{X}}, \bar{\mathbf{F}})$ are introduced to define the macroscopic quasi-static balance of linear momentum, which is given in the absence of body forces by

$$\text{Div}_{\bar{\mathbf{X}}} \bar{\mathbf{P}}(\bar{\mathbf{X}}, t) = \mathbf{0} \quad \text{in } \bar{\mathcal{B}}_0 \quad (3.2)$$

where $\text{Div}_{\bar{\mathbf{X}}}$ and $\text{Grad}_{\bar{\mathbf{X}}}$ denote the divergence and gradient operator with respect to the reference configuration.

3.3.2 Microscopic field relations

The reference configuration of the microstructural domain $\mathcal{B}_0 \subset \mathbb{R}^3$ is parameterized in $\mathbf{X}$ and the current configuration $\mathcal{B}_t$ in $\mathbf{x}$ at the time t . The microscopic mapping $\varphi_t(\bar{\mathbf{X}}, \mathbf{X}, t) = \bar{\mathbf{F}}(\bar{\mathbf{X}}, t)\mathbf{X} + \tilde{\mathbf{u}}(\mathbf{X}, t)$ is defined using two contributions: the first one is the deformation gradient $\bar{\mathbf{F}}(\bar{\mathbf{X}}, t)$ which is spatially homogeneous at a macroscopic point given by $\bar{\mathbf{X}}$; the second contribution is the locally fluctuating displacement field $\tilde{\mathbf{u}}(\mathbf{X}, t)$ which is depending on the position $\mathbf{X}$ on the micro scale. Consequently, the microscopic deformation gradient reads

$$\mathbf{F}(\bar{\mathbf{X}}, \mathbf{X}, t) = \text{Grad}_{\mathbf{X}} \varphi_t(\bar{\mathbf{X}}, \mathbf{X}, t) = \bar{\mathbf{F}}(\bar{\mathbf{X}}, t) + \tilde{\mathbf{H}}(\mathbf{X}, t) \quad (3.3)$$

where $\tilde{\mathbf{H}}(\mathbf{X}, t) = \text{Grad}_{\mathbf{X}} \tilde{\mathbf{u}}(\mathbf{X}, t)$ denotes the spatially heterogeneous displacement field gradient. Having introduced the kinematic relations, the material response at each $\mathbf{X} \in \mathcal{B}_0$ is assumed to be governed by an arbitrary rate-dependent constitutive law $\mathbf{P}(\bar{\mathbf{X}}, \mathbf{X}, t) = \mathbf{P}(\mathbf{F}(\bar{\mathbf{X}}, \mathbf{X}, t), \chi)$. Internally evolving state variables are denoted by χ . They are specified in Section 3.4.2 in the context of constitutive modeling. In analogy to (3.2), the quasi-static microscopic balance of linear momentum in absence of body forces is defined as

$$\text{Div}_{\mathbf{X}} \mathbf{P}(\bar{\mathbf{X}}, \mathbf{X}, t) = \mathbf{0} \quad \text{in } \mathcal{B}_0. \quad (3.4)$$

Assuming periodic micromechanical fields, periodic deformations $\mathbf{x}^+ - \mathbf{x}^- = \bar{\mathbf{F}}(\mathbf{X}^+ - \mathbf{X}^-)$ and antiperiodic tractions $\mathbf{t}^+ = -\mathbf{t}^-$ are prescribed on opposite faces of the boundary $\partial\mathcal{B}_0^+$ and $\partial\mathcal{B}_0^-$.

3.3.3 Scale bridging

Figure 3.2 schematically shows the connection between the micro and the macro scale: The microscopic $\mathbf{F}(\bar{\mathbf{X}}, \mathbf{X}, t)$ and $\mathbf{P}(\bar{\mathbf{X}}, \mathbf{X}, t)$ are computed in dependence of the macroscopic $\bar{\mathbf{F}}(\bar{\mathbf{X}}, t)$. In the following, by calculating the resulting macroscopic $\bar{\mathbf{P}}(\bar{\mathbf{X}}, t)$ depending on $\mathbf{F}(\bar{\mathbf{X}}, \mathbf{X}, t)$ and $\mathbf{P}(\bar{\mathbf{X}}, \mathbf{X}, t)$, the microstructural information is transferred back to the macrostructure.

The macroscopic deformation gradient $\bar{\mathbf{F}}(\bar{\mathbf{X}}, t)$ and stress tensor $\bar{\mathbf{P}}(\bar{\mathbf{X}}, t)$ are defined via the volume averages [e.g., 137, 335] of their microscopic counterparts:

$$\bar{\mathbf{F}}(\bar{\mathbf{X}}, t) = \frac{1}{V} \int_{\mathcal{B}_0} \mathbf{F}(\bar{\mathbf{X}}, \mathbf{X}, t) dV \quad \text{and} \quad \bar{\mathbf{P}}(\bar{\mathbf{X}}, t) = \frac{1}{V} \int_{\mathcal{B}_0} \mathbf{P}(\bar{\mathbf{X}}, \mathbf{X}, t) dV \quad (3.5)$$

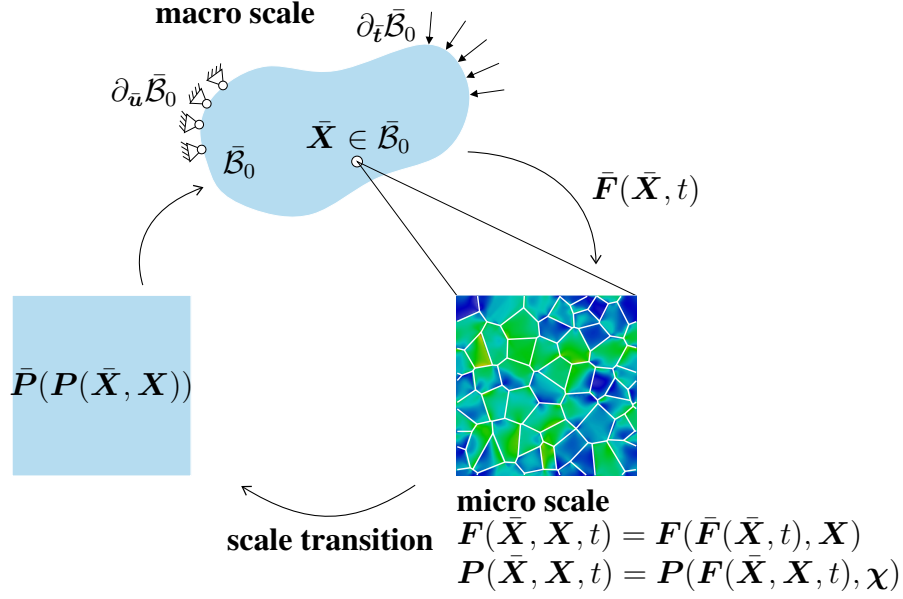


Figure 3.2: Coupling between micro and macro scale.

3.4 Constitutive model

The kinematics of and the specific phenomenological constitutive model for elasto-viscoplastic single crystals are reviewed in Section 3.4.1 and 3.4.2. All quantities are referred to the microscopic BVP and for a better readability the dependencies of $\bar{X}$, X , χ and t are neglected in what follows.

3.4.1 Finite strain kinematics

Following Asaro [336], Kröner [337], Lee [338], Rice [339], Asaro and Rice [340] and others, we assume the deformation gradient $F = F_e F_p$ to be multiplicatively decomposed into an elastic part F_e and a plastic part F_p . Therein, F_e is used to consider small elastic stretches as well as rigid body rotations and F_p accounts for plastic deformations. Following Peirce et al. [341] and Rice [339] and considering dislocation slip as the only deformation process, the plastic velocity gradient L_p is assumed to be defined by the superposition of the contribution of crystallographic slip systems $\alpha = 1, \dots, n_{\text{slip}}$ such that

$$L_p := \sum_{\alpha=1}^{n_{\text{slip}}} \dot{\gamma}_{\alpha} d_{\alpha} \otimes n_{\alpha} = \dot{F}_p F_p^{-1} \quad (3.6)$$

holds, where $\dot{\gamma}_{\alpha}$ denotes the plastic slip rates. The individual slip systems are defined by the slip direction d_{α} and for the slip plane normal n_{α} , respectively.

3.4.2 Single crystal plasticity constitutive model

The elastic deformation gradient $\mathbf{F}_e = \mathbf{F} \mathbf{F}_p^{-1}$ is related to the second Piola-Kirchhoff stress tensor $\mathbf{S}_e = \mathbb{C} : \mathbf{E}_e$ in the intermediate configuration, where $\mathbf{E}_e = \frac{1}{2}(\mathbf{C}_e - \mathbf{I})$ denotes the elastic Green-Lagrange strain tensor, $\mathbb{C}$ the elastic stiffness tensor and $\mathbf{C}_e = \mathbf{F}_e^T \mathbf{F}_e$ the elastic right Cauchy-Green tensor. If the resolved shear stress of any slip system α

$$\tau_\alpha(\mathbf{M}_e) := \mathbf{M}_e \cdot (\mathbf{d}_\alpha \otimes \mathbf{n}_\alpha) \quad (3.7)$$

exceeds the critical resolved shear stress τ^c , the material is considered to flow which yields to irreversible deformations. Here, $\mathbf{M}_e := \mathbf{C}_e \mathbf{S}_e$ denotes the Mandel stress tensor. The critical resolved shear stress is related to the accumulated plastic slip $\gamma_{\text{acc}} = \sum_\alpha \int |\dot{\gamma}_\alpha| dt$ through

$$\tau^c(\gamma_{\text{acc}}) = \tau_0^c + q_h(\gamma_{\text{acc}}), \quad (3.8)$$

where τ_0^c denotes the initial critical resolved shear stress and $q_h(\gamma_{\text{acc}})$ an isotropic hardening function. The rate sensitivity parameter p , drag stress τ^D and reference shear rate $\dot{\gamma}_0$ are introduced to define the Perzyna-type [342] flow rule

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \left\langle \frac{|\tau_\alpha| - \tau^c}{\tau^D} \right\rangle^p \text{sgn}(\tau_\alpha). \quad (3.9)$$

Assuming a Voce-type hardening behavior, the hardening function

$$q_h(\gamma_{\text{acc}}) = \tau_0^c + (\tau_\infty - \tau_0) \tanh\left[\frac{(h_0 - h_\infty) \gamma_{\text{acc}}}{(\tau_\infty - \tau_0^c)}\right] + h_\infty \gamma_{\text{acc}} \quad (3.10)$$

is defined in terms of the initial and saturation hardening parameters h_0 and h_∞ . The flow stress saturation is described by τ_∞ . The internal variables which are already introduced in Section 3.3 are now specified as $\chi = [\mathbf{F}_p^{-1}, \gamma_{\text{acc}}]^T$.

3.4.3 Discretized set of local equilibrium equations

The flow rule (3.9) is assumed to be discretized using an implicit time integration scheme (e.g. backward Euler). The robustness of the numerical solution of this equation is strongly depending on the rate sensitivity parameter p . For moderate and high rate-sensitivity parameters p , small time increments Δt are required to ensure convergence of the local return mapping algorithm, in general. Following Wulfinghoff and Böhlke [343], we assume a continuously differentiable transition between the powerlaw and a linear approximation with slope m which

leads to the modified flow rule

$$\Delta\gamma_\alpha = \begin{cases} 0 & |\tau_\alpha| \leq \tau^c \\ \Delta\gamma_0 \left(\frac{|\tau_\alpha| - \tau^c}{\tau^D} \right)^p \text{sgn}(\tau_\alpha) & \tau^c < |\tau_\alpha| \leq \tau^R \\ \left[m(|\tau_\alpha| - \tau^R) + \Delta\gamma_0 \left(\frac{\Delta\tau^R}{\tau^D} \right)^p \right] \text{sgn}(\tau_\alpha) & |\tau_\alpha| > \tau^R \end{cases} \quad (3.11)$$

with $\Delta\gamma_0 = \Delta t \dot{\gamma}_0$. The point where the original power law is replaced by the linear approximation is denoted by τ^R . The regularized powerlaw gives an improved initial guess for the non-regularized solution. If the solution algorithm is not converging, the slope $m^{(i)}$ is decreased. If the regularized solution does not coincide with the original powerlaw solution at convergence, the slope of the linear approximation $m^{(i)}$ is increased and a new local iteration step $i + 1$ is performed with slope $m^{(i+1)}$ (see Figure 3.3).

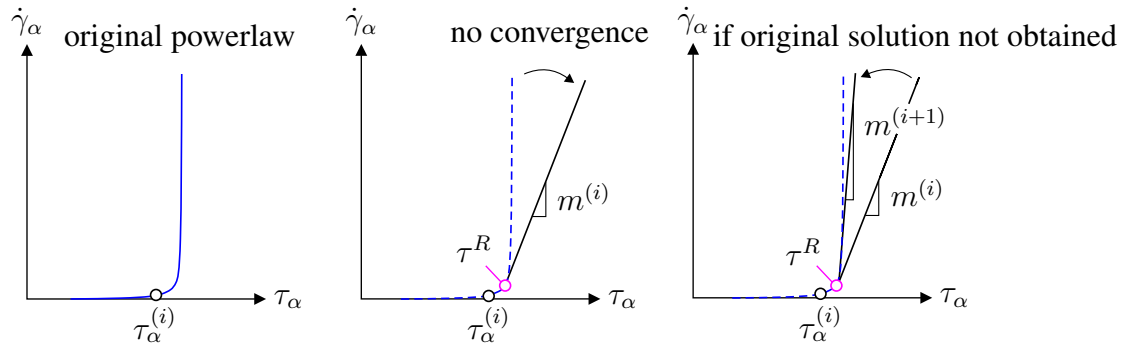


Figure 3.3: *Left*: original powerlaw, *center*: no convergence $\rightarrow m^{(i)}$ is reduced to get a regularized powerlaw (*black*), *right*: regularized powerlaw (*black*) does not coincide with original powerlaw (*dashed blue*) $m^{(i)}$ is increased to $m^{(i+1)}$. See text for details.

This procedure is repeated until the regularized solution coincides with the original solution and local convergence is achieved¹. The local set of equilibrium equations

$$\mathbf{r}(\mathbf{S}_e, \tau^c) = \begin{pmatrix} \mathbf{r}^{\mathbf{S}_e} \\ r^{\tau^c} \end{pmatrix} = \begin{pmatrix} \mathbf{E}_e - \mathbb{C}^{-1} : \mathbf{S}_e \\ \tau_f^c - \tau^c \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix} \quad (3.12)$$

is solved for the primary unknowns $\mathbf{S}_e$ and τ^c using Newton's method with accuracy tol_χ , see

¹If still no convergence is obtained within an admissible number of iterations, Δt is decreased at the FE level and the same loadstep is computed again.

Algorithm 1.

```

Set:  $iter = 0$ 
do
  Set:  $iter = iter + 1$ 
  Calc:  $\tau^C, \Delta\tau^R$ 
  Calc: Point of linear approximation:  $\tau^R = \tau^C + \Delta\tau^R$ 
  Calc: Residuuum:  $r$ 
  if  $\|r\| > tol_x$  then
    Calc:  $S_e, \tau^C$ 
    if  $iter > iter_{max}$  then
      Set:  $m = m/m_{dec}$ 
      Set:  $iter = 0$ 
      Reset:  $S_e, \tau^C$ 
      Update:  $\Delta\tau^R$ 
    end
  else if  $\|\tau\| > \tau^R$  then
    Set:  $m = m \cdot m_{inc}$ 
    Set:  $iter = 0$ 
    Update:  $\Delta\tau^R$ 
  else
    | End of Newton iteration
  end
end

```

Algorithm 1: Newton iteration to solve the local set of equilibrium equations with the modified flow rule, while the maximum number of iterations before the modified flow rule is used is set to $iter_{max} = 10$ and the factor to decrease or increase the slope m is set to $m_{dec} = 3$ and $m_{inc} = 1.3$, respectively.

On this basis, other stress measures such as the Kirchhoff $\tau = F_e S_e F_e^T$ or first Piola Kirchhoff stress tensor $P = \tau F^{-T}$ can be computed.

3.5 Numerical Methods

As mentioned above, the numerical treatment of the present two-scale problem is based on the FE-FFT method [13, 16, 18]. The algorithmic formulation and numerical solution of the FE-based macroscopic and FFT-based microscopic boundary value problem are presented in Sections 3.5.1 and 3.5.2.

3.5.1 Finite element discretization of macroscopic equations

The basis of the finite element formulation of the macroscopic boundary value problem is the weak form of the balance of linear momentum in (3.2)

$$\bar{g}(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}) = \int_{\bar{\mathcal{B}}_0} \bar{\mathbf{S}} \cdot \delta\bar{\mathbf{E}} dV - \int_{\partial_{\bar{\mathbf{t}}}\bar{\mathcal{B}}_0} \bar{\mathbf{t}} \cdot \delta\bar{\mathbf{u}} dA = 0 \quad \forall \delta\bar{\mathbf{u}}, \quad (3.13)$$

which is constructed using the virtual Green-Lagrange strain tensor $\delta\bar{\mathbf{E}} = (\bar{\mathbf{F}}^T \text{Grad}_{\bar{\mathbf{X}}} \delta\bar{\mathbf{u}} + \text{Grad}_{\bar{\mathbf{X}}} \delta\bar{\mathbf{u}}^T \bar{\mathbf{F}})/2$ and with use of an arbitrary test function $\delta\bar{\mathbf{u}}$ which fulfills the constraint $\delta\bar{\mathbf{u}} = 0$ on $\partial_{\bar{\mathbf{u}}}\bar{\mathcal{B}}_0$. The displacement and traction boundary conditions are given by $\bar{\mathbf{u}} = \bar{\mathbf{u}}$ on $\partial_{\bar{\mathbf{u}}}\bar{\mathcal{B}}_0$ and $\bar{\mathbf{t}} = \bar{\mathbf{P}}\bar{\mathbf{n}}$ on $\partial_{\bar{\mathbf{t}}}\bar{\mathcal{B}}_0$. Linearization of (3.13) with respect to $\bar{\mathbf{u}}$ induces the approximation

$$\begin{aligned} \int_{\bar{\Omega}} \text{Grad} \delta\bar{\mathbf{u}} \cdot (\text{Grad} \Delta\bar{\mathbf{u}} \bar{\mathbf{S}}) dV + \int_{\bar{\Omega}} \delta\bar{\mathbf{E}} \cdot \partial_{\bar{\mathbf{E}}} \bar{\mathbf{S}}[\Delta\bar{\mathbf{E}}] dV = \\ - \int_{\bar{\Omega}} \delta\bar{\mathbf{E}} \cdot \bar{\mathbf{S}} dV + \int_{\partial_{\bar{\mathbf{t}}}\bar{\Omega}} \bar{\mathbf{t}} \cdot \delta\bar{\mathbf{u}} dA \quad \forall \delta\bar{\mathbf{u}}, \end{aligned} \quad (3.14)$$

which is non-linear in the sought quantity $\Delta\bar{\mathbf{u}}$. In the following the well-known finite element discretization and thus a subdivision of the body $\bar{\Omega}$ into n_{elem} elements with volume $\bar{\Omega}^e$ is performed. Additionally, the approximation of the displacement and virtual displacement field of any element e using the shape functions $N_{\bar{\mathbf{u}}}^e$ is introduced: $\bar{\mathbf{u}} \approx N_{\bar{\mathbf{u}}}^e \bar{\mathbf{u}}^e$, $\delta\bar{\mathbf{u}} \approx N_{\bar{\mathbf{u}}}^e \delta\bar{\mathbf{u}}^e$. This results in the following expression:

$$\begin{aligned} \sum_{e=1}^{n_{\text{elem}}} \delta\bar{\mathbf{u}}^{eT} \left\{ \underbrace{\int_{\bar{\Omega}^e} \mathbf{B}_{\bar{\mathbf{u}}}^{eT} \mathbb{D}^e \mathbf{B}_{\bar{\mathbf{u}}}^e dV + \int_{\bar{\Omega}^e} \mathbf{G}_{\bar{\mathbf{u}}}^{eT} (\partial_{\bar{\mathbf{E}}_v} \bar{\mathbf{S}}_v)^e \mathbf{G}_{\bar{\mathbf{u}}}^e dV}_{\mathbf{k}_{\bar{\mathbf{u}}}^e} \right\} = \\ - \sum_{e=1}^{n_{\text{elem}}} \delta\bar{\mathbf{u}}^{eT} \left\{ \underbrace{\int_{\bar{\mathcal{B}}^e} \mathbf{G}_{\bar{\mathbf{u}}}^{eT} \bar{\mathbf{S}}_v^e dV - \int_{\partial_{\bar{\mathbf{t}}}\bar{\Omega}^e} \mathbf{N}_{\bar{\mathbf{u}}}^{eT} \bar{\mathbf{t}}_0 dA}_{\mathbf{r}_{\bar{\mathbf{u}}}^e} \right\}, \end{aligned} \quad (3.15)$$

where $D_{ijkl}^e = S_{jl}^e \delta_{ik}$ holds. In (3.15), $\mathbf{B}_{\bar{\mathbf{u}}}^e := \text{Grad}_{\bar{\mathbf{X}}} (N_{\bar{\mathbf{u}}}^e)$ denotes the B-operator and the matrix $\mathbf{G}_{\bar{\mathbf{u}}}^e$ is introduced such that $\Delta\bar{\mathbf{E}} \approx \mathbf{G}_{\bar{\mathbf{u}}}^e \bar{\mathbf{u}}^e$ and $\delta\bar{\mathbf{E}} \approx \mathbf{G}_{\bar{\mathbf{u}}}^e \delta\bar{\mathbf{u}}^e$.

The assembly of Equation (3.15) leads to a linear system of equations, which is solved in terms of the global nodal displacement increments. To obtain quadratic convergence within the Newton-Raphson scheme to solve this equation, a consistent linearization of Equation (3.13) is necessary. The resulting consistent algorithmic tangent operator $\bar{\mathbf{A}}^e = (\partial_{\bar{\mathbf{E}}} \bar{\mathbf{S}})^e$ is expressed in terms of the macroscopic second Piola-Kirchhoff stress tensor $\bar{\mathbf{S}}^e$ and the

Green-Lagrange strain tensor $\bar{\mathbf{E}}^e$. This tangent operator is computed by means of numerical derivatives constructed from forward finite differences based on the algorithmic formulation proposed by Miehe [315]. Since the local fields $\mathbf{F}^{(e,i)}$, $\mathbf{P}^{(e,i)}$ and $\mathbb{A}^{(e,i)}$ are known from the evaluation of the constitutive response at each $\mathbf{X} \in \mathcal{B}_0$, the constitutive relation is replaced by its linearized version

$$\mathbf{P}^{(e,i+1)} = \mathbf{P}^{(e,i)} + \mathbb{A}^{(e,i)} : (\mathbf{F}^{(e,i+1)} - \mathbf{F}^{(e,i)}) \quad (3.16)$$

for the numerical tangent computation yielding a linear system of equations to be solved for each macroscopic perturbation in $\bar{\mathbf{F}}$. Following Miehe [315] or Kochmann et al. [316], three (2D) or six (3D) stress computations are required for the numerical construction of $\bar{\mathbb{A}}^e$ for the geometrically non-linear theory.

3.5.2 Fourier-based discretization of microscopic field equations

Small strains. In the theory of linear composites the micromechanical fields are assumed to satisfy an integral equation [118, 119] which is known as the Lippmann-Schwinger equation:

$$\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \mathbb{T}^{(0)} * \boldsymbol{\tau} \quad \text{in } \mathcal{B}_0, \quad (3.17)$$

where $\boldsymbol{\varepsilon}$ is the microscopic and $\bar{\boldsymbol{\varepsilon}}$ the macroscopic strain and

$$(\mathbb{T}^{(0)} * \boldsymbol{\tau})(\mathbf{X}) = \int_{\Omega} \mathbb{T}^{(0)}(\mathbf{X}, \mathbf{X}') : \boldsymbol{\tau}(\mathbf{X}') \, d\mathbf{X}' \quad (3.18)$$

denotes the convolution integral between the Green's operator $\mathbb{T}^{(0)}$ and $\boldsymbol{\tau}$. Assuming an isotropic reference medium with elastic constants $\mu^{(0)}$ and $\lambda^{(0)}$, closed-form expressions for the Green's function tensor $\mathbf{G}^{(0)}$ and Green's operator $\mathbb{T}^{(0)}$ are available in Fourier space which is parameterized by the wave vector $\boldsymbol{\xi}$:

$$\left(\hat{G}_{ik}^{(0)}(\boldsymbol{\xi}) \right)^{-1} = C_{ijkl}^{(0)} \xi_j \xi_l, \quad \hat{\Gamma}_{ijkl}^{(0)}(\boldsymbol{\xi}) = \hat{G}_{ik}^{(0)}(\boldsymbol{\xi}) \xi_j \xi_l \quad \text{for } \boldsymbol{\xi} \neq \mathbf{0}. \quad (3.19)$$

By introducing an homogeneous reference material with elastic stiffness $\mathbb{C}^{(0)}$ the constitutive relation $\boldsymbol{\sigma}(\boldsymbol{\varepsilon}) = \mathbb{C} : \boldsymbol{\varepsilon}$ is reformulated in terms of a polarization field $\boldsymbol{\tau} = \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) - \mathbb{C}^{(0)} : \boldsymbol{\varepsilon}$ which defines the difference between the material properties of the composite and the homogeneous reference material. Making use of Green's operator $\mathbb{T}^{(0)}$ associated with $\mathbb{C}^{(0)}$ solves the reformulated local problem and thus, results in the fundamental solutions for $\mathbf{u}$ and

$\varepsilon = \text{sym}(\nabla \mathbf{u})$. First, Moulinec and Suquet [11] proposed an efficient computational approach to solve the Lippmann-Schwinger equation in an iterative fashion using fast Fourier transforms and fixed-point methods [e.g., 152, 190, 344].

Finite strains. Lahellec et al. [192] proposed an extension to hyperelastic material behavior and [194, 333] to finite strain crystal plasticity. In this case the polarization stress

$$\boldsymbol{\tau} = \mathbf{P} - \mathbb{C}^{(0)} : \mathbf{F} \quad (3.20)$$

is formulated in terms of the deformation gradient $\mathbf{F}$ and its work conjugate stress measure $\mathbf{P}$ which leads to the reformulated local problem

$$\text{div}(\mathbb{C}^{(0)} : \mathbf{F}) = -\text{div}(\boldsymbol{\tau}) \quad \text{in } \mathcal{B}_0. \quad (3.21)$$

Recalling (3.3) and making use of Green's function $\mathbf{G}^{(0)}$, the Lippmann-Schwinger equation is assumed to take the following form

$$\mathbf{F} = \bar{\mathbf{F}} - \mathbb{I}^{(0)} * \boldsymbol{\tau} \quad \text{in } \mathcal{B}_0 \quad (3.22)$$

The Fourier transformation of (3.22) yields

$$\hat{\mathbf{F}}(\boldsymbol{\xi}) = \begin{cases} -\hat{\mathbb{I}}^{(0)}(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) & \text{for } \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\mathbf{F}} & \text{for } \boldsymbol{\xi} = \mathbf{0} \end{cases}. \quad (3.23)$$

In order to ensure numerically robust computations an FFT- and conjugate gradient-based iterative solver [e.g., 195, 197, 215] is implemented and used in this work. To this end, the linearized version of (3.23)

$$\Delta \mathbf{F}^{(i+1)} + \mathbb{I}^{(0)} * (\mathbb{C}^{*(i)} - \mathbb{C}^{(0)}) : \Delta \mathbf{F}^{(i+1)} = \bar{\mathbf{F}} - \mathbb{I}^{(0)} * \mathbf{P}^{(i)}(\mathbf{F}^{(i)}, \boldsymbol{\chi}) \quad (3.24)$$

is solved numerically for $\Delta \mathbf{F}^{(i+1)}$ with an accuracy tol_{CG} of the conjugate gradient solver, where $\mathbb{C}^{*(i)} = \partial_{\mathbf{F}} \mathbf{P}|_{\mathbf{F}^{(i)}}$ denotes the local algorithmic tangent operator. In order to improve the numerical robustness of the local solver, a finite number of fixed-point iterations is performed before each Newton step. Once $\|\Delta \mathbf{F}^{(i+1)}\| / \|\bar{\mathbf{F}}\| < \text{tol}_{\Delta \mathbf{F}}$ is fulfilled, the microscopic boundary value problem is considered to be converged, while $\text{tol}_{\Delta \mathbf{F}}$ is the tolerance of the Newton solver. Details on the algorithmic formulation and implementation can be found in [16].

3.6 Solution strategy

Recently, Kochmann et al. [16] showed among others that even coarse discretizations of polycrystalline microstructures lead to quantitatively accurate predictions in terms of overall quantities (e.g. first and second moments of stress). This observation was confirmed for different microstructure realizations (e.g. different grain orientation distributions and number of grains). On this basis, the authors developed a CPU-efficient solution strategy for two-scale full-field simulations of polycrystalline materials with elasto-viscoplastic constitutive behavior at small strains. This solution strategy contains the following three computational stages:

1. *Pre-processing*: Identification of the minimal number of microscopic grid points $N_{\min}$ (for different loading cases) which are required to get an error in the effective quantities (e.g. $\|\bar{\sigma}\|$) smaller than a prescribed tolerance (e.g. 2 %).
2. *Processing*: Two-scale simulation with coarse mesh ($N = N_{\min}$) and storage of macroscopic deformation gradient $\bar{\mathbf{F}}$ for each converged macroscopic load step $k = 1, \dots, n_{\text{load}}$ in each integration point of particular interest of the macroscopic structure $\bar{\mathbf{x}} \in \bar{\mathcal{B}}_0$.
3. *Post-processing*: Reconstruction of highly resolved micromechanical fields of the investigated integration points $\bar{\mathbf{x}}^* \subset \bar{\mathbf{x}} \in \bar{\mathcal{B}}_0$ in stand-alone computations with $N \gg N_{\min}$ based on the deformation gradient history data $\bar{\mathbf{F}}(k)$ obtained from the *processing* stage.

This simple solution scheme ensures both, a high fidelity representation of local fields as well as moderate overall computation times. The pre-processing step may also be based on an analytical homogenization procedure to achieved even better computing times; see e.g., the works of Castaneda and Suquet [156], Lebensohn et al. [180] and Song and Castaneda[160]. However, to generate an easy and convenient solution strategy the same two-scale simulation is used in all three stages of the solution strategy. However, our group's previous work is only related to small strains. In the following Section 3.7, we show the approach's applicability for finite strain crystal plasticity simulations and examine different metals with different crystal structures and intrinsic anisotropy.

3.7 Algorithmic treatment and numerical examples

3.7.1 Algorithmic setting

In order to increase the efficiency of the proposed two-scale model, a reduced FE formulation with hourglass stabilization [e.g., 345, 346] is used as an element routine in the finite element analysis program Abaqus 2017². The macroscopic BVP (3.2) is solved implicitly using the Newton-Raphson method. The numerical computation of the overall consistent tangent moduli is based on a perturbation value of $\zeta = 10^{-8}$. The tolerance for the residual force-based convergence at the FE level is chosen as $\text{tol}_{f_M} = 5 \cdot 10^{-3} \text{ N}$ (see [18] for details). At the FFT-level, three fixed-point-based precomputations are performed, first. The tolerances for the conjugate gradient solver [347] and for the mechanical equilibrium on the macro scale are set to $\text{tol}_{CG} = 10^{-18}$ and $\text{tol}_{\Delta F} = 10^{-10}$, respectively. The local set of equilibrium equations (3.12) is considered to be converged if the tolerance of $\text{tol}_\chi = 10^{-13}$ is satisfied.

In the following, two-dimensional plane-strain problem settings are investigated. The squared microstructural unit cell of side length L is discretized using N grid points in each spatial direction. This yields an equidistant grid spacing $\Delta x = L/N$. In order to reduce the influence of spurious oscillations, an averaged forward-backward finite difference approximation for the differential operators is employed [cf. 30]. Optimal spatial resolution and convergence is obtained for this approach using odd N , which is used for all computational examples. The (inverse) Fourier transform of any local field is performed using the FFTW-library³.

3.7.2 Material data

The material parameters for the stiffness and related to the slip systems are taken from [202, 348, 349] and [16]. For fcc metals the $\mathbf{d}_\alpha = \{111\}$ and $\mathbf{n}_\alpha = [110]$ slip systems are considered. Two families of slip systems which are characterized by nearly identical activation energies, are taken into account for bcc metals: the $\mathbf{d}_\alpha = \{110\}$, $\mathbf{n}_\alpha = [111]$ and $\mathbf{d}_\alpha = \{211\}$, $\mathbf{n}_\alpha = [111]$ systems. Pure Copper (Cu), Aluminum (Al) and Iron (Fe) are investigated which are characterized by a different intrinsic anisotropy. The latter can be expressed by the factor $A = 2 C_{44}/(C_{11} - C_{12})$ which leads to $A_{Cu} = 2.21$, $A_{Al} = 1.21$ and $A_{Fe} = 2.33$ based on the used material parameters listed in Table 3.1.

²www.3ds.com/products-services/simulia/products/abaqus/

³www.fftw.org

	C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]	τ_0^c [MPa]	τ^D [MPa]	τ_∞ [MPa]	h_0 [MPa]	p [-]
Cu	170.2	114.9	61.0	0.1	10	31.0	50.0	20
Al	112.0	66.0	28.0	0.3	6.0	138.8	100.0	50
Fe	236.0	134.0	119.0	1.0	149.0	400.0	500.0	20

Table 3.1: Used material parameters for Copper [202], Aluminum [348] and Iron [16, 349] with $\dot{\gamma}_0 = 10^{-3}$ 1/s.

3.7.3 Microstructural convergence analysis of the overall quantities

Let us consider a periodic polygrain microstructure consisting of 100 grains which are characterized by the three Eulerian angles $\{\phi_1, \phi_2, \phi_3\}$ based on which the rotation matrix (Bunge notation) is computed for each single grain. The polycrystal is assumed to exhibit three different random textures which are visualized in Figure 3.4.

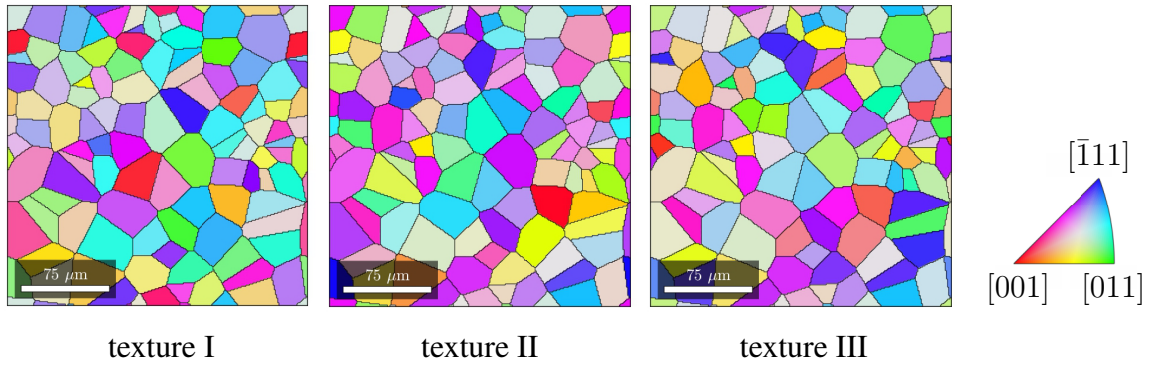


Figure 3.4: Polygrain microstructure consisting of 100 grains with different textures.

The influence of these three different textures is given in Figure 3.5 for a copper unit cell undergoing a simple shear load case. These results indicate that the different orientations of the grains do have a certain influence on the microscopic and therefore also in the resulting macroscopic response of the material behavior. Due to that and since we want to consider these different textures and also different phases and grain evolutions in future works, a two-scale simulation is necessary to capture the detailed microscopic and resulting macroscopic material behavior.

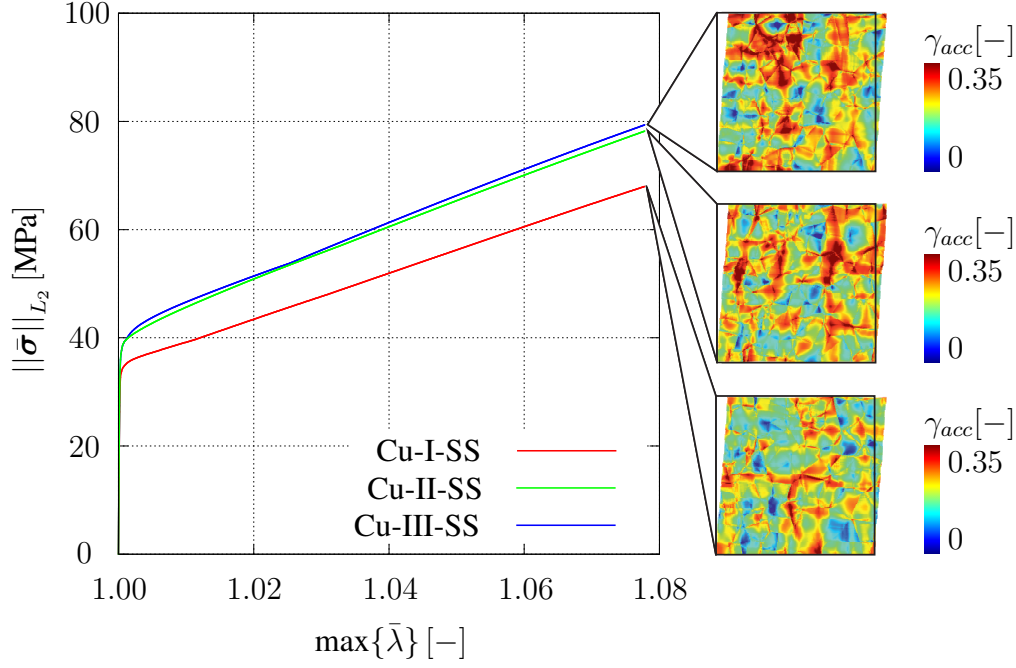


Figure 3.5: Effective response in terms of the L_2 -norm of the Cauchy stress $\|\boldsymbol{\sigma}\|_{L_2}$ over the maximum stretch $\max\{\bar{\lambda}\}$ for a pure copper unit cell discretized by 255×255 grid points with the three different textures subjected to a simple shear load case and the corresponding microscopic accumulated plastic slip in the deformed configuration.

The aforementioned polycrystal with textures I-III is subjected to the following three deformation gradients which correspond to uniaxial tension (UT), simple shear (SS) and a mixed loading (ML) with $F_{\max} = 0.15$, $\dot{F} = 1/\text{s}$ and $\Delta t = 5 \cdot 10^{-8}$. Since the material behavior is plastically incompressible only volume preserving deformation gradients ($\det \mathbf{F} = 1$) are investigated.

In order to test the plausibility of our model, we compared the the macroscopic material response of the presented finite strain model with the small strain model presented in [316]. In Figure 3.6, the stress-strain behavior $\bar{\sigma}_{12} - \bar{\varepsilon}_{12}$ considering small strain kinematics and the stress-strain behavior $\bar{\sigma}_{12} - \bar{E}_{12}$ considering finite strain kinematics are shown. As expected, these solutions coincide in the beginning, while a difference rises with rising strain.

For the unit cell, seven different discretizations are considered which are defined by $N \in \{7, 15, 31, 63, 127, 255\}$ grid points in each spatial direction, respectively. Since the focus here is on the convergence analysis of the overall quantities based on the microstructural discretization level $N = 255$ grid points are related to a converged overall constitutive response.

In Figure 3.7 the effective response in terms of the L_2 -norm of the Cauchy stress $\|\boldsymbol{\sigma}\|_{L_2}$ over the maximum stretch $\max\{\bar{\lambda}\}$ of two exemplary microstructures is shown. Illustrated is

$$\mathbf{F}^{(SS)} = \begin{pmatrix} 1 & F_{\max} \\ 0 & 1 \end{pmatrix}$$

$$\mathbf{F}^{(UT)} = \begin{pmatrix} 1 + F_{\max} & 0 \\ 0 & 1/F_{11}^{(UT)} \end{pmatrix}$$

$$\mathbf{F}^{(ML)} = \begin{pmatrix} 1 + F_{\max} & F_{\max} \\ 0 & 1/F_{11}^{(ML)} \end{pmatrix}$$

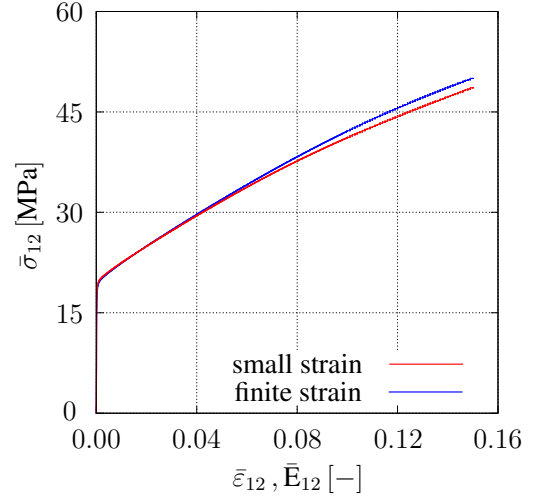


Figure 3.6: Considered deformation gradients corresponding to uniaxial tension (UT), simple shear (SS) and a mixed loading (ML) (left) and comparison of small and finite strain kinematics for a Copper unit cell with texture III submitted to the simple shear loading (right).

the effective response of an iron-based microstructure with texture II submitted to the simple shear load case as well as another iron-based microstructure with texture III submitted to the uniaxial tension load case. The results of the two different problems show that already coarse discretizations (e.g. with $N = 15$ grid points) lead to an accurate effective response of the considered microstructure.

In addition Table 3.2 shows the computing times of the six different considered discretizations of the iron-based microstructure with texture II submitted to the simple shear load case. These computing times are exponentially increasing, related to the exponential increase in the number of considered grid points. Due to that a coarse discretized microstructure is necessary to get reasonable computing times in terms of a complex two-scale simulation.

	N = 7	N = 15	N = 31	N = 63	N = 127	N = 255
time [h]	0.04	0.15	0.70	3.14	12.45	51.20

Table 3.2: Computing time of the iron-based microstructure with texture II submitted to the simple shear load case.

To determine which minimal number of grid points is necessary to get an accurate macroscopic response, a convergence analysis in terms of the macroscopic stress is performed.

In the following, the error of the macroscopic stress is analyzed for different number of grid points N . Since we consider finite strains we use the relative error in the macroscopic first Piola-Kirchhoff stress $\bar{\mathcal{E}} = \|\bar{\mathbf{P}}\|_{L_2} / \|\bar{\mathbf{P}}_{255}\|_{L_2}$, where $\bar{\mathbf{P}}_{255}$ represents the macroscopic

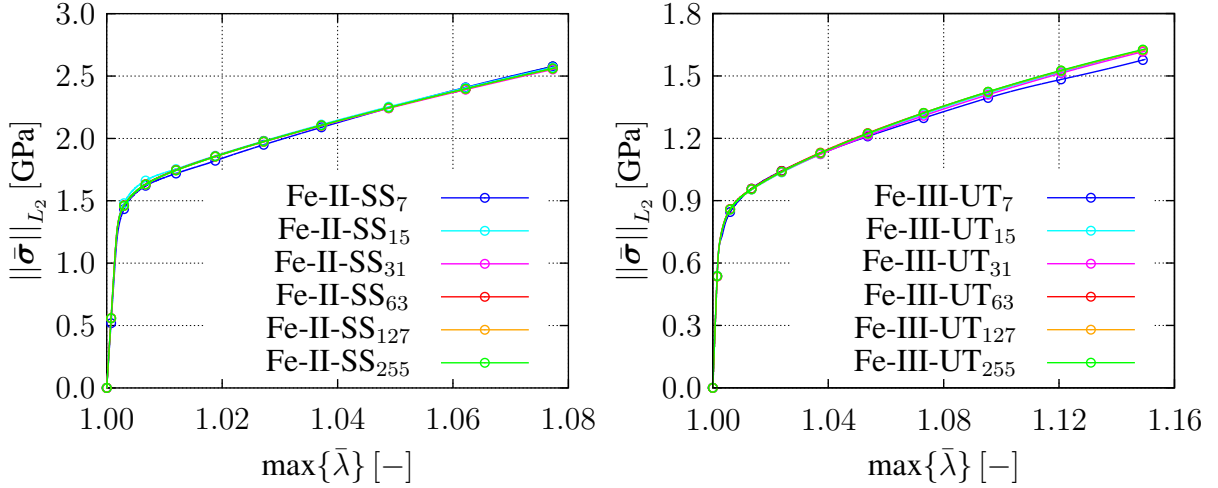


Figure 3.7: Effective response in terms of the L_2 -norm of the Cauchy stress $\|\bar{\sigma}\|_{L_2}$ over the maximum stretch $\max\{\bar{\lambda}\}$ for an pure iron unit cell with texture II subjected to the simple shear load case (*left*) and with texture III subjected to the uniaxial tension load case (*right*).

first Piola-Kirchhoff stress corresponding to $N = 255$ grid points, for the different materials, textures and load cases, respectively.

The error in the overall constitutive response of an Fe-, an Al- and a Cu-based polycrystal is plotted in Figure 3.8. As seen before, coarse discretizations ($N < 15$) lead to large errors in the norm of the macroscopic stress, which may for example be related to hitting a particular material behavior under the grid point while discretizing the unit cell which may not be representative in this area. Nevertheless, the error in the macroscopic stresses for all investigated loading cases (UT, SS, ML), textures (texture I-III) and materials (Cu, Al, Fe) is always smaller than 2% even if only $N=15$ grid points in each spatial direction are used for the discretization. Due to that a discretization with $N = N_{\min} = 15$ grid points in x_1 - and x_2 -direction is fine enough to get an accurate global response of the material behavior in the processing step.

These basic results show that coarse discretizations are capable of predicting a sufficiently accurate overall constitutive response which is barely affected by the underlying texture, material and loading case. This observation is in agreement with small strain crystal plasticity results published by Kochmann et al. [16]. Up to this point, all simulation examples were restricted to integration point studies only. Next, a macroscopic FE-structure is investigated to demonstrate that the proposed solution strategy, which was introduced in Section 3.6, is capable of giving accurate predictions in terms of micromechanical fields and overall quantities for more complex macroscopic BVPs and finite strain elasto-viscoplasticity.

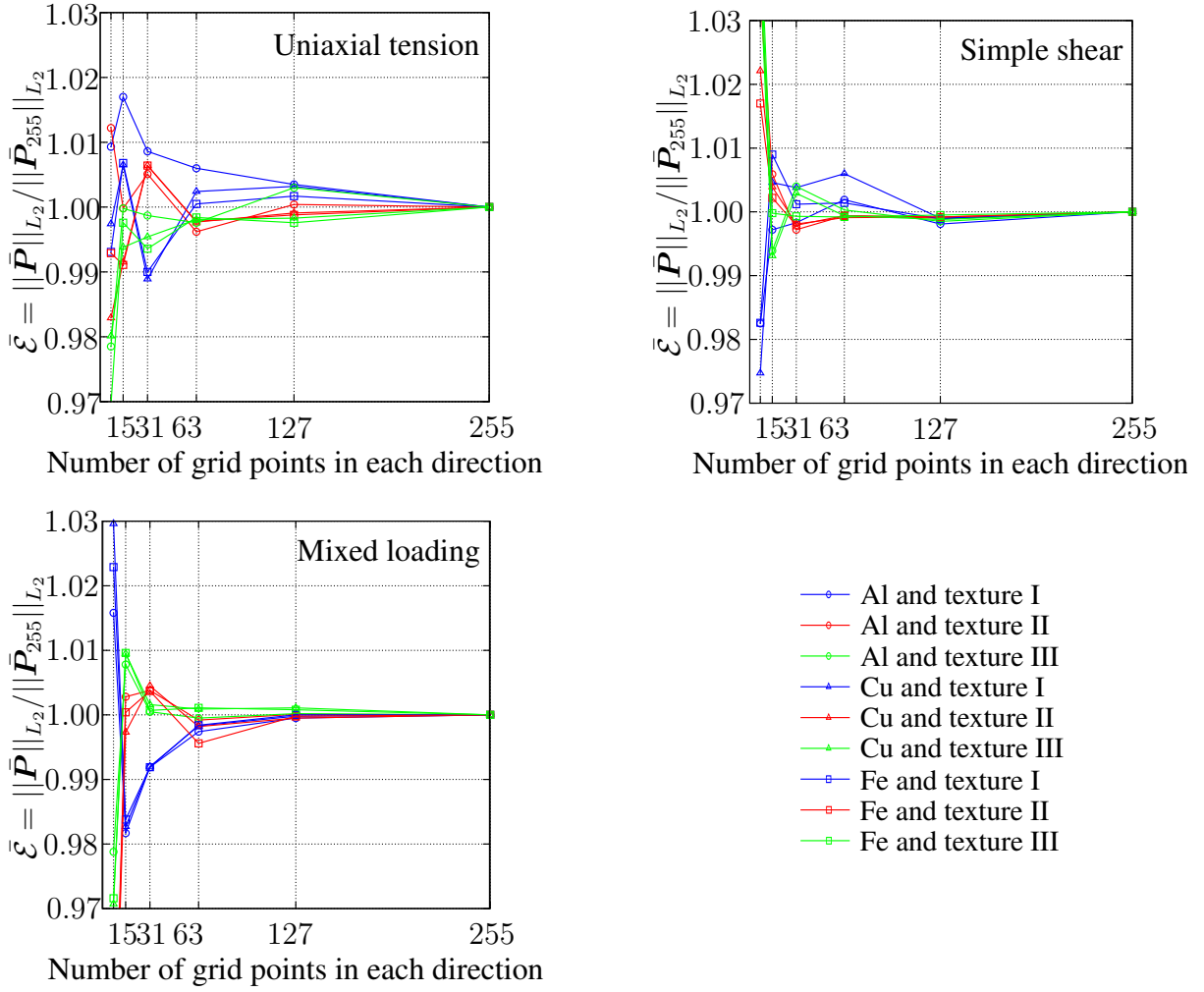


Figure 3.8: Convergence of $\bar{\mathbf{P}}$ depending on microstructural discretization for different polycrystals with different textures undergoing different deformations ($F^{(UT)}$, $F^{(SS)}$ and $F^{(ML)}$).

3.7.4 Two-scale modeling of the deep rolling process

As mentioned before, the finite element analysis program Abaqus is used to solve the macroscopic BVP. Therefore, a user material is defined to solve the microscopic BVP by using an FFT-based solver.

We consider a deep rolling process within a plane strain setting as a numerical two-scale example. The investigated specimen has a dimension of $12 \times 6 \text{ mm}^2$ and is discretized by 6125 bi-linear plane strain CPE4R elements with reduced integration and hourglass stabilization [e.g., 345, 346]. The nodes at the bottom of the workpiece are fixed in all degrees of freedom, while the nodes at the side are restricted to symmetry boundary conditions to account for the surrounding material. Friction during hydrostatic deep rolling is negligibly small. Therefore,

the contact interaction between the deep rolling tool, which is modeled as an analytical rigid body, and the workpiece is assumed to be frictionless.

The displacement controlled deep rolling sequence is defined as follows: in the first step, the deep rolling tool is pushed down $16\ \mu\text{m}$ into the bulk material. Thereafter, in the second step, the deep rolling tool is moved $8\ \text{mm}$ along the specimen at a feed rate of $8\ \text{mm/s}$ before it is finally released. A fully automatic time incrementation is used for the simulation in Abaqus.

At each macroscopic integration point a polycrystalline microstructure ($250 \times 250\ \mu\text{m}^2$) is attached. For simplicity, it is the same microstructure at each integration point. It consists of 100 grains with texture II and the material properties of iron (see Section 3.7.3). In Figure 3.9, the orientation of the first Eulerian angle ϕ_1 is shown. The results of the pre-processing step considering this microstructure are already presented in Figure 3.8. Following these results, a microstructure with only 15 grid points in each direction is attached to each macroscopic integration point.

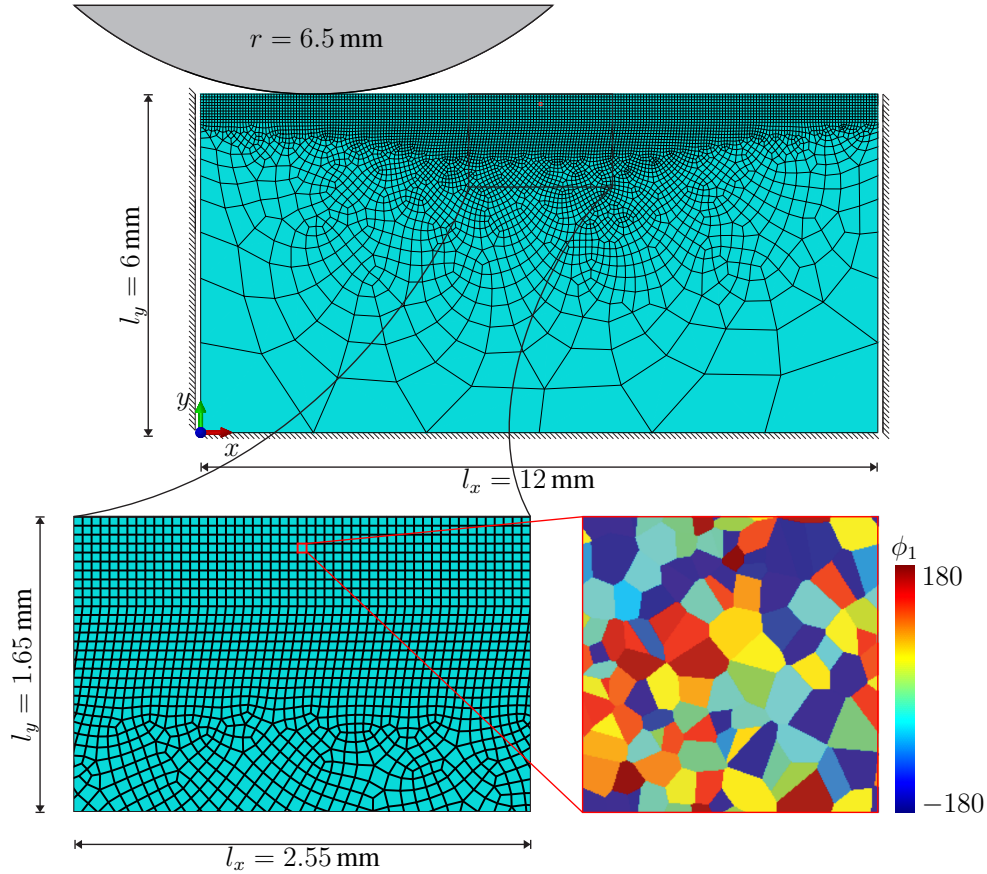


Figure 3.9: Mesh, dimensions and boundary conditions of the deep rolling process and orientation of the first Eulerian angle ϕ_1 of the microstructure which is discretized with 255 grid points in each direction.

Considering the coarsely discretized microstructure and a macroscopic parallel processing with 16 CPUs it is possible to solve this complex macroscopic boundary value problem within a reasonable time period, while the computing time of the same example but with a fine discretized microstructure would be way too long. The results of the processing step and hence the deep rolling process simulation itself, are given in Figure 3.10 and Figure 3.11. For the processing industry, the most interesting result of a deep rolling process is the evolution of the residual stress component $\bar{\sigma}_{xx}$, since the residual stress of the other stress components ($\bar{\sigma}_{yy}$ and $\bar{\sigma}_{xy}$) is negligibly small. In Figure 3.10, the macroscopic residual stress component $\bar{\sigma}_{xx}$ at the end of the simulation, when the deep rolling tool is released, is shown. As expected, the maximum residual stress occurs near the surface (0 – 1 mm), while the effect of the deep rolling process in regions of 2 – 3 mm below the surface is negligibly small.

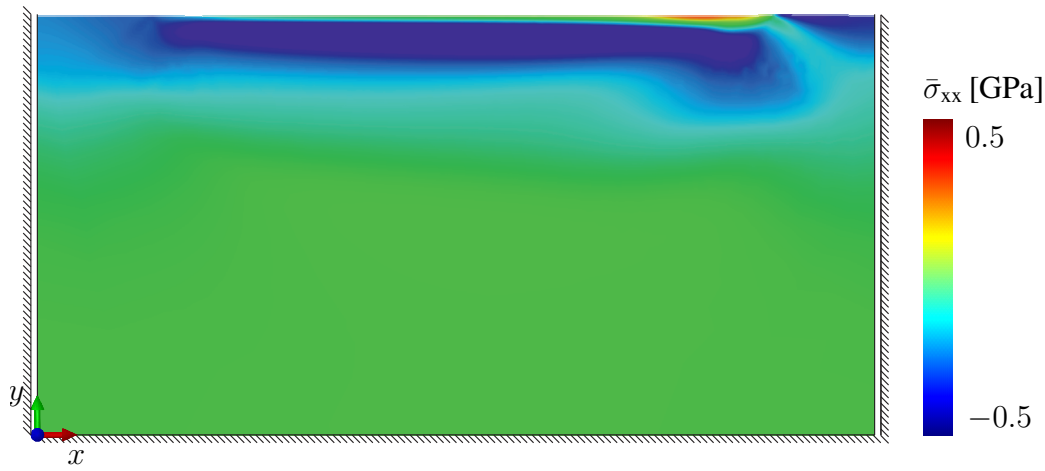


Figure 3.10: Macroscopic residual stress of the σ_{xx} component due to the deep rolling process at the end of the simulation when the deep rolling tool is released.

In order to be able to recognize the details during the simulation, the enlarged section of the specimen (see Figure 3.9) for four different process time steps is shown in Figure 3.11 in the left column. Here, the macroscopic stress component $\bar{\sigma}_{xx}$ and the macroscopic deformations (10-times scaled) are presented. The macroscopic residual stress results from the plastic slip on the micro scale. Therefore, the evolution of the accumulated plastic slip of the considered microstructure for the processing step with 15 grid points in each direction (*centered column*) as well as for the post-processing step with 255 grid points in each direction (*right column*) is shown for the same process time steps and for one macroscopic element with reduced integration (highlighted by a red frame).

At a process time of $t = 1.308$ s, the lower tip of the deep rolling tool reaches the plotted section of interest. Since the integration point for which the microstructure is shown in

Figure 3.11 is too far away from the processing zone at this point, no plastic slip will occur here. Moving the deep rolling tool further in x -direction, it reaches the highlighted element. At $t = 1.442$ s plastic slip is evolving in the investigated microstructure [see Figure 3.11, *centered column, second row*]. Since the coarse discretized microstructure consequently leads to coarse microstructural data, the post-processing step is necessary to obtain highly resolved microstructural data of the investigated microstructure. Therefore, the history of the macroscopic deformation gradient $\bar{\mathbf{F}}$ and a fine discretized microstructure with $N = 255$ grid point in each direction is used in a stand-alone code, which leads to the desired highly resolved microstructural data of the plastic slip, see right column in Figure 3.11. This plastic slip of the investigated macroscopic integration point will rise until the lower tip of the deep rolling tool reaches roughly the investigated elements x -position ($t = 1.480$ s). A further movement of the deep rolling tool in x -direction has no longer much influence on the evolution of the plastic slip of the investigated microstructure, see e.g. process time step $t = 1.535$ s.

The described solution strategy may be used for any macroscopic integration point of special interest, so that the two-scale simulation itself may be performed in a reasonable time period with the coarse discretized microstructure followed by the post-processing step which leads to highly resolved microstructural data of any macroscopic integration point.

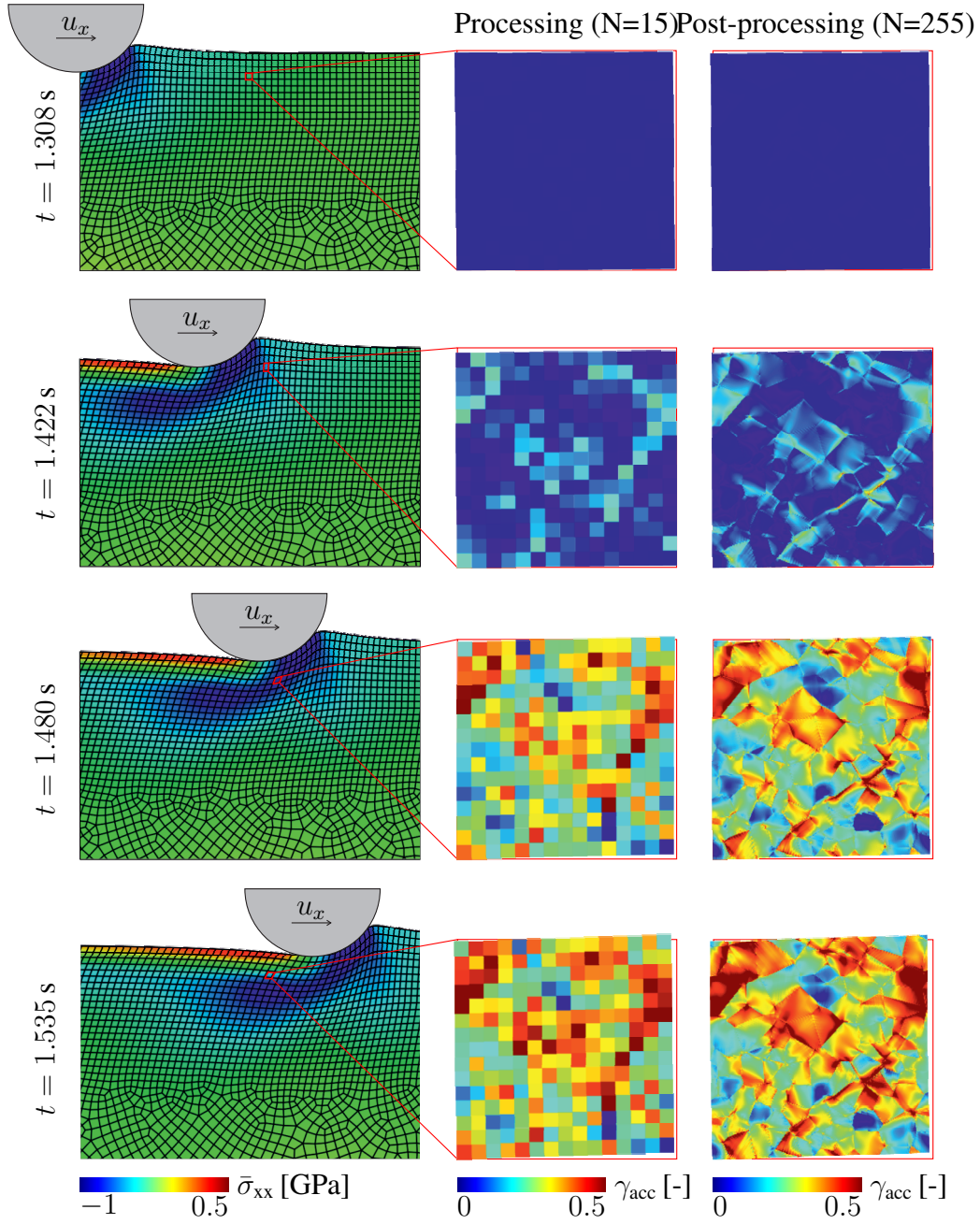


Figure 3.11: Macroscopic stress component $\bar{\sigma}_{xx}$ and 10-times scaled deformations on the macro scale and accumulated plastic slip γ_{acc} in the deformed configuration on the micro scale for four different process time steps. Therein, the coarse discretization refers to the processing step and the fine discretization refers to the post-processing step.

3.8 Conclusion and outlook

We presented an efficient two-scale FE-FFT-based framework for elasto-viscoplastic polycrystalline material behavior at finite strains for the simulation of complex macroscopic boundary value problems in reasonable time periods. A two-scale simulation of a complex macroscopic BVP with a fine discretized microstructure at every integration point will lead to far too high computing times. To overcome this problem, we introduced a solution strategy based on a microstructural convergence analysis. This leads to a minimal number of grid points, which needs to be considered to get sufficient accurate macroscopic results. Since this coarse microstructural discretization consequently leads to poor microstructural results, a post-processing step is used to reconstruct highly resolved microstructural data. Therefore, the history of the macroscopic deformation gradient $\bar{\mathbf{F}}$ of any integration point of special interest and a finely discretized microstructure is used. In further works this solution strategy will be used for the simulation of different mechanical and thermo-mechanical processes to generate a better understanding of the polycrystalline material behavior undergoing processes like deep rolling, induction hardening or precision machining. This should result in the characterization of new process signatures, which is the relation between material loads and material modifications, like (residual) micro-stresses of the II. and III. type, statistics about grain size and shape, misorientation and dislocation density. The inclusion of their computation is planned in future works and will facilitate the assessment of the influence of different manufacturing processes on the mentioned properties. In this context, the derivation of process signatures for microstructural modifications will become possible. In addition to that the numerical results of these process simulations will be compared to experimental results in future works.

4 | Article 3:

Efficient thermomechanically coupled FE-FFT-based multiscale simulation of polycrystals

This article was published as:

Gierden, C., Schmidt, A., Waimann, J., Svendsen, B. and Reese, S. [2023], ‘Efficient thermomechanically coupled FE-FFT-based multiscale simulation of polycrystals’, *Proceedings in Applied Mathematics and Mechanics (PAMM)*, **23** (2), e202300058.

Disclosure of the individual authors’ contributions to the article:

C. Gierden reviewed the relevant existing literature, implemented the framework of the FFT-based microstructure simulation of elasto-viscoplastic polycrystals at finite strains for the pure mechanical case into Abaqus / Standard (via the UMAT interface), performed the simulations, interpreted the results and wrote the article. A. Schmidt implemented the thermomechanical coupling. Furthermore, she, J. Waimann, B. Svendsen and S. Reese gave conceptual advice, contributed to the discussion of the results, proofread the article and made valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

4.1 Abstract

In general, the overall macroscopic material behavior of any structural component is directly dependent on its underlying microstructure. For metal components, the associated microstructure is given in terms of a polycrystal. To enable the simulation of the related microstructural and overall elasto-viscoplastic material behavior, a two-scale simulation approach can be used. In this context, we use a FE-FFT-based two-scale method, which is an efficient alternative to the classical FE^2 method for the simulation of periodic microstructures. In addition, we consider a thermomechanically coupled framework to account for both thermal and mechanical loads. Finally, we incorporate a model order reduction technique based on a coarsely discretized microstructure to develop an efficient two-scale simulation technique. As a demonstration of the feasibility of the proposed simulation framework, a numerical example will be investigated.

4.2 Introduction

When studying the overall material behavior of a structural component, this behavior is directly determined by the underlying microstructure and its properties. For example, when analyzing metals, the microscale is represented by a polycrystal and its characteristics. In order to investigate both the macroscopic as well as the microscopic material behavior in a high resolution manner, several multiscale approaches have been developed [124]. The most common in this context is the application of the FE^2 method, which refers to the use of the finite element method on both scales [113, 123]. An alternative to this two-scale method is the FE-FFT-based method introduced in [13]. In this approach, the finite element simulation on the microscale is replaced by a Fast Fourier Transform (FFT)-based approach [11, 12]. This two-scale simulation method has been applied to the multiscale simulation of polycrystalline microstructures at small strains in [18] and generalized to finite strains in [16, 324]. Furthermore, an extension considering additionally a thermomechanical coupling with a constant temperature field on the microscale at finite strains was introduced in [68]. A general review on FE-FFT-based two-scale methods is given in [15].

Considering only the microscale simulation, the FFT-based method was first applied to the simulation of polycrystalline microstructures considering rigid-viscoplastic material behavior at small strains in [350] and was found to be an efficient solution method for the simulation of periodic microstructures compared to the finite element method [8, 9]. A generalization of this approach to elasto-viscoplastic material behavior at small strains and further to finite strains can be found in [202] and [194], respectively. To increase the accuracy and efficiency of an

FFT-based microscale simulation, several methods have been introduced. To mention some of them, finite difference approximations can be used to reduce the effect of Gibbs oscillations [29, 30] or efficient solvers such as conjugate gradient based solvers are applied to reduce the computational effort either in a small strain setting [215, 216] or in a finite strain setting [195]. A comprehensive review of the FFT-based microscale simulation technique can be found in [10, 14].

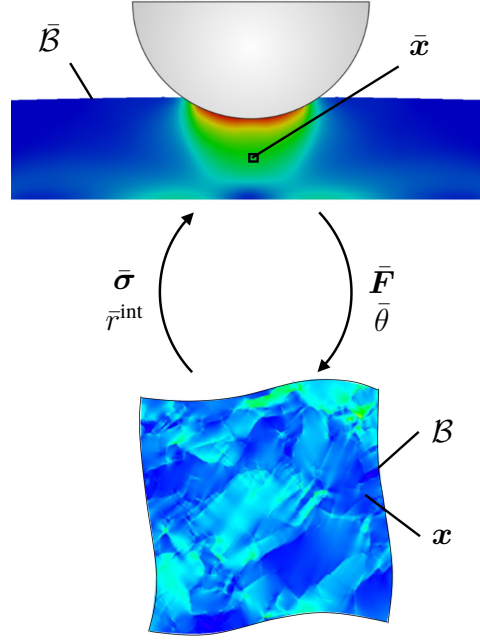
Since two-scale simulation methods are generally computationally demanding, several efficient solution strategies and model order reduction techniques have been developed to reduce this computational burden. Efficient solution strategies include methods based on a coarsely discretized microstructure for the two-scale simulation, while high-resolution results can be generated in a post-processing step [16, 319], or methods using a pre-calculated database in general, while the high-resolution two-scale simulation is performed only in macroscopic critical areas [254]. Other model order reduction techniques reduce the computational effort at either the macro- or microscale. Since model order reduction techniques are widely used for macroscale simulations, only specific model order reduction techniques applied to FFT-based microscale simulations are addressed here. In this context, the computational costs of FFT-based microscale simulations have been reduced using proper orthogonal decomposition [234], low-rank tensor approximations [282], or a reduced set of Fourier modes [17] with a fixed [17], geometrically adapted [237], or strain-based [38] sampling pattern, or additionally combined with a clustered microstructure [351].

In this work, we use the thermomechanically coupled FE-FFT-based two-scale method incorporating finite strains introduced in [68] to compute fluctuating temperature fields at the microscale, similar to what was done in [352, 353], using a FE-based microstructure simulation. Here, the FFT-based microscale simulation is utilized and optimized using the finite difference approximation presented in [30] and a Newton-Krylov solver as introduced in [195]. In addition, the efficient solution strategy based on a coarsely discretized microstructure for the two-scale simulation [16, 319] is applied.

The paper is organized as follows: In Section 4.3 the thermomechanically coupled two-scale boundary value problem is briefly discussed. This is followed by the introduction of the microstructural constitutive relations in Section 4.4. After discussing the microscale simulation using spectral solvers in Section 4.5 and the numerical results in Section 4.6, the paper ends with a conclusion and an outlook in Section 4.7.

4.3 Two-scale boundary value problem

To perform a thermomechanically coupled two-scale simulation, the balance of linear momentum and the balance of internal energy must be solved at the macro- as well as the microscale. Considering finite strains, these balance equations with respect to the reference configuration are given below, while a sketch of the two-scale boundary value problem considering deformed bodies is given on the left:



Balance of linear momentum

Macroscale

$$\begin{aligned} \text{Div}(\bar{\mathbf{F}}\bar{\mathbf{S}}) + \bar{\mathbf{f}}_0 &= \mathbf{0} & \text{in } \bar{\mathcal{B}}_0 \\ \bar{\mathbf{F}}\bar{\mathbf{S}} \cdot \bar{\mathbf{N}} &= \bar{\mathbf{t}}_0 & \text{on } \partial_t \bar{\mathcal{B}}_0 \\ \bar{\mathbf{u}} &= \bar{\mathbf{u}}_0 & \text{on } \partial_u \bar{\mathcal{B}}_0 \end{aligned}$$

Microscale

$$\begin{aligned} \text{Div}(\mathbf{F}\mathbf{S}) &= \mathbf{0} & \text{in } \mathcal{B}_0 \\ \mathbf{S} &= \mathbf{S}(\bar{\mathbf{X}}, \mathbf{X}, \mathbf{F}(\bar{\mathbf{X}}, \mathbf{X}), \theta(\bar{\mathbf{X}}), \zeta_k(\bar{\mathbf{X}}, \mathbf{X})) & r_0^{\text{int}} = r_0^{\text{int}}(\bar{\mathbf{X}}, \mathbf{X}, \mathbf{F}(\bar{\mathbf{X}}, \mathbf{X}), \theta(\bar{\mathbf{X}}), \zeta_k(\bar{\mathbf{X}}, \mathbf{X})) \\ \mathbf{F} &= \bar{\mathbf{F}}(\bar{\mathbf{X}}) + \tilde{\mathbf{H}}(\bar{\mathbf{X}}, \mathbf{X}) & \theta = \bar{\theta}(\bar{\mathbf{X}}) + \tilde{\theta}(\bar{\mathbf{X}}, \mathbf{X}) \end{aligned}$$

Balance of internal energy

Macroscale

$$\begin{aligned} -\dot{\bar{e}} + \bar{\mathbf{S}} : \dot{\bar{\mathbf{E}}} - \text{Div}(\bar{\mathbf{q}}_0) + \bar{r}_0^{\text{ext}} &= 0 & \text{in } \bar{\mathcal{B}}_0 \\ \bar{\mathbf{q}}_0 \cdot \bar{\mathbf{N}} &= -\bar{q}_0 & \text{on } \partial_q \bar{\mathcal{B}}_0 \\ \bar{\theta} &= \bar{\theta}_0 & \text{on } \partial_\theta \bar{\mathcal{B}}_0 \end{aligned}$$

Microscale

$$\begin{aligned} -\dot{e} + \mathbf{S} : \dot{\mathbf{E}} - \text{Div}(\mathbf{q}_0) &= 0 & \text{in } \mathcal{B}_0 \end{aligned}$$

Here $\mathbf{X}$ represents the position vector, $\mathbf{F}$ is the deformation gradient, $\mathbf{E}$ is the Green-Lagrange strain, $\mathbf{S}$ is the second Piola-Kirchhoff stress, $\mathbf{f}_0$ is an external body force, $\mathbf{t}_0$ is a surface traction, e is the total energy, $\mathbf{q}_0$ is the heat flux, r_0^{ext} and r_0^{int} define the external and internal heat

sources, and ζ_k represents a set of internal variables. The bar above any quantity refers to the macroscale, and the absence of the bar therefore refers to the microscale. Furthermore the macroscopic balance equations must be fulfilled within the body $\bar{\mathcal{B}}_0$ and satisfy the macroscopic boundary conditions as given on $\partial\bar{\mathcal{B}}_0$, while the microscopic balance equations must be fulfilled within the unit cell $\mathcal{B}_0$ assuming periodic boundary conditions. Finally, $\tilde{\mathbf{H}}$ and $\tilde{\theta}$ are the microscopic fluctuating displacement gradient and temperature, which denote the primary unknowns.

As introduced in [352], the microscopic boundary value problem is solved in a staggered manner. First, the balance of linear momentum is solved by applying $\bar{\mathbf{F}}$ and considering the temperature field $\theta = \bar{\theta}$ to be constant, to compute the averaged stress $\bar{\mathbf{S}}$ and internal heat sources $\bar{r}_0^{\text{int}}$ (which are involved in the macroscopic balance of internal energy, cf. Equation (4.6)). Then, the balance of internal energy is solved by employing the macroscopic temperature gradient $\text{Grad}(\bar{\theta})$ to compute the averaged heat flux $\bar{\mathbf{q}}_0$. However, since we only consider an isotropic and homogeneous conductivity K_θ within the microstructure, the microstructural fluctuations can be neglected. Thus, in contrast to [352], the macroscopic heat flux $\bar{\mathbf{q}}_0$ can be computed directly from the macroscopic quantities without solving the microscopic balance of internal energy. Therefore, the scale transition back to the macroscale is performed by calculating only the macroscopic second Piola-Kirchhoff stress $\bar{\mathbf{S}}$ and the macroscopic heat sources $\bar{r}_0^{\text{int}}$ as volume averages of their microscopic counterparts, where $\mathcal{V}_0$ is the volume of the microstructure:

$$\bar{\mathbf{S}}(\bar{\mathbf{X}}) = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} \mathbf{S}(\bar{\mathbf{X}}, \mathbf{X}) \, d\mathcal{V} \quad \text{and} \quad \bar{r}_0^{\text{int}}(\bar{\mathbf{X}}) = \frac{1}{\mathcal{V}_0} \int_{\mathcal{B}_0} r_0^{\text{int}}(\bar{\mathbf{X}}, \mathbf{X}) \, d\mathcal{V}.$$

4.4 Microstructural constitutive model

Considering a two-scale simulation of metals, the associated microstructure is defined as a polycrystal. Taking into account finite deformations, the deformation gradient $\mathbf{F} = \mathbf{F}_e \mathbf{F}_p$ is multiplicatively split into an elastic part $\mathbf{F}_e$ and a plastic part $\mathbf{F}_p$. Furthermore, in the context of crystal plasticity, where dislocation slip is assumed to be the only plastic deformation process, the plastic velocity gradient $\mathbf{L}_p = \dot{\mathbf{F}}_p \mathbf{F}_p^{-1}$ is given as the sum of each shear rate $\dot{\gamma}_\alpha$ over all slip systems n_α defined by the slip plane normal $\mathbf{n}_\alpha$ and the slip plane direction $\mathbf{d}_\alpha$ [339, 340]:

$$\mathbf{L}_p = \sum_{\alpha}^{n_\alpha} \dot{\gamma}_\alpha \mathbf{d}_\alpha \otimes \mathbf{n}_\alpha. \quad (4.1)$$

Since elastic deformations in metals are generally small, we applied a St. Venant-Kirchhoff law, taking into account the effect of temperature changes, which defines the elastic second Piola-Kirchhoff stress in the intermediate configuration as

$$\mathbf{S}_e = \mathbb{C}^{\text{gra}} : \mathbf{E}_e - \mathbb{C}^{\text{gra}} : \mathbf{A}_t (\theta - \theta^{\text{ref}}). \quad (4.2)$$

In the previous equation, the rotated cubic anisotropic elasticity tensor $\mathbb{C}^{\text{gra}}$ depending on the grain orientation, the elastic Green-Lagrange strain $\mathbf{E}_e$, the reference temperature θ^{ref} and the thermal expansion tensor $\mathbf{A}_t = \alpha_t \mathbf{I}$ were introduced with α_t denoting the thermal expansion coefficient and $\mathbf{I}$ referring to the second order identity tensor. Furthermore, we considered an isotropic hardening $q_p(\gamma_{\text{acc}})$ of Voce-type plus an additional linear term depending on the accumulated plastic slip γ_{acc} , which is defined as the time integral over the sum of all shear rates. Finally, the evolution equation for the shear rate in each slip system is assumed to be of Perzyna-type yielding

$$\dot{\gamma}_\alpha = \begin{cases} 0 & \text{if } \tau_\alpha \leq \tau^c \\ \text{sgn}(\tau_\alpha) \dot{\gamma}_0 \left(\frac{|\tau_\alpha| - \tau^c}{\tau^D} \right)^p & \text{if } \tau_\alpha > \tau^c \end{cases}, \quad (4.3)$$

with the resolved shear stress $\tau_\alpha = \mathbf{M}_e : (\mathbf{d}_\alpha \otimes \mathbf{n}_\alpha)$ in slip system α , the critical shear stress τ^c , the drag stress τ^D , the rate sensitivity parameter p and the reference shear rate $\dot{\gamma}_0$.

4.5 Microscale simulation using a spectral solver

Since solving the macroscopic boundary value problem by means of the finite element method is a very common procedure, in the following we will focus only on solving the microscopic boundary value problem by means of a spectral solver. As mentioned before, the solutions of the mechanical and thermal boundary value problems are computed in a staggered manner. Starting from the mechanical boundary value problem and using the FFT-based simulation approach [11, 12], the microscopic balance equation has to be reformulated by introducing the polarization stress $\boldsymbol{\tau}$ [131], which defines the difference between the stress in the real microstructure and the stress in an isotropic homogeneous reference material defined by the

stiffness tensor $\mathbb{C}^0$:

$$\begin{aligned}\text{Div}(\boldsymbol{\tau} + \mathbb{C}^0 : \mathbf{F}) &= \mathbf{0} \quad \text{in } \mathcal{B}_0 \\ \boldsymbol{\tau} &= \mathbf{F} \mathbf{S} - \mathbb{C}^0 : \mathbf{F} \\ \mathbf{F} &= \bar{\mathbf{F}} + \tilde{\mathbf{H}}\end{aligned}$$

This reformulated boundary value can be solved using the Lippmann-Schwinger equation [337] yielding

$$\mathbf{F} = \bar{\mathbf{F}} - \Gamma^0 * \boldsymbol{\tau}, \quad (4.4)$$

where Γ^0 is the Green's operator and $*$ represents the convolution of the Green's operator and the polarization stress, which considers the influence of $\boldsymbol{\tau}$ on $\mathbf{F}$ at each position. Transferring this equation in Fourier space results in

$$\hat{\mathbf{F}}(\boldsymbol{\xi}) = \begin{cases} -\hat{\Gamma}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) & \text{for } \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\mathbf{F}} & \text{for } \boldsymbol{\xi} = \mathbf{0} \end{cases}. \quad (4.5)$$

Here, the hat over any quantity refers to its Fourier transform depending on the Fourier modes $\boldsymbol{\xi}$. In Fourier space, the convolution results in a simple multiplication and the Green's operator is explicitly known in Fourier space, depending only on the reference material behavior and the Fourier modes. In order to solve this equation, we use a Newton-Krylov solver as introduced in [195].

To compute microstructural fluctuations in the temperature field, the thermal boundary value problem is also solved in Fourier space. Therefore the balance of internal energy with respect to the reference configuration is reformulated as

$$-\theta \frac{\partial^2 \check{\psi}}{\partial \theta^2} \dot{\theta} = \underbrace{\theta \frac{\partial \mathbf{S}}{\partial \theta} : \dot{\mathbf{E}}}_{r_0^e} + \underbrace{\left[\sum_{\alpha=1}^n \dot{\gamma}_\alpha \left(\tau_\alpha - \theta \frac{\partial \tau_\alpha}{\partial \theta} \right) \right]}_{r_0^p} - \left(q_p - \theta \frac{\partial q_p}{\partial \theta} \right) \dot{\gamma}_{\text{acc}} - \text{Div}(\mathbf{q}_0). \quad (4.6)$$

with the total energy $\check{\psi}$. By considering a constant temperature field in time during the microscale simulation and by neglecting the elastic heat sources r_0^e , while simplifying the

plastic heat sources r_0^p to

$$r_0^p \approx \beta \left(\sum_{\alpha=1}^n \dot{\gamma}_\alpha \tau_\alpha - q_p \dot{\gamma}_{\text{acc}} \right) \quad (4.7)$$

using the Taylor-Quinney coefficient β [354], the balance of internal energy in the current configuration reduces to

$$\text{div}(\mathbf{q}) - r^p = 0 \quad (4.8)$$

with $r^p = 1/\det(\mathbf{F}) r_0^p$. Considering $\mathbf{q} = -K_\theta \text{grad}(\theta)$ and an isotropic and homogeneous conductivity K_θ for each crystal, this equation can directly be solved in Fourier space:

$$\hat{\theta}(\boldsymbol{\xi}) = \begin{cases} -\frac{\hat{r}^p(\boldsymbol{\xi})}{K_\theta \boldsymbol{\xi} \cdot \boldsymbol{\xi}} & \text{for } \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\theta} & \text{for } \boldsymbol{\xi} = \mathbf{0} \end{cases} \quad (4.9)$$

and later transferred back to real space.

4.6 Numerical results

To demonstrate the applicability of the thermomechanically coupled FE-FFT-based two-scale method, we investigate the multiscale simulation of a four-point bending test considering a polycrystalline microstructure and the material parameters of copper, chosen in line with the literature. The dimensions, boundary conditions and discretization of the macroscopic boundary value problem are depicted in Figure 4.1. The polycrystalline microstructure with the orientation of the first Euler angle is shown on the right. A displacement of $u_2 = 0.5$ mm is applied within one second, and the simulation is performed at room temperature $\theta^{\text{ref}} = 293.15$ K. The two-scale simulation is performed using Abaqus, with the FFT-based microstructure simulation implemented as a user material. On the macroscale, a fully coupled thermomechanical finite element analysis is performed. In this context, a plane strain setting and reduced integration with hourglass stabilization are considered.

Regarding the microscale simulation, we use an efficient solution strategy [16, 319] based on using only a coarsely discretized microstructure during the two-scale simulation, which is attached to each macroscopic integration point. Since this only provides accurate macroscopic results, highly resolved microstructural results are generated in a post-processing step by applying the macroscopic deformation gradient of any integration point of particular interest to

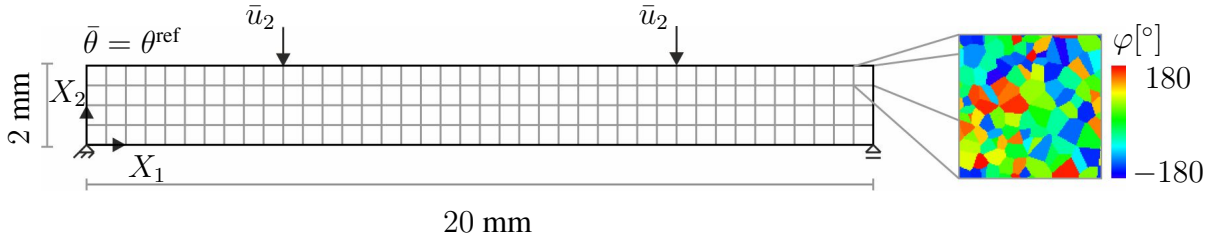


Figure 4.1: Macroscopic boundary value problem with dimensions, boundary conditions and discretization of the four-point bending test and orientation of the first Euler angle of the polycrystalline microstructure.

a finely discretized microstructure.

The results of the two-scale simulation are given in Figure 4.2. At the macroscale, the logarithmic strain $\overline{LE}_{11}$, the Cauchy stress $\bar{\sigma}_{11}$, the accumulated plastic slip $\bar{\gamma}_{\text{acc}}$, and the change in the temperature $\Delta\bar{\theta} = \bar{\theta} - \theta^{\text{ref}}$ are shown, whereas at the microscale, the Green-Lagrange strain E_{11} , the Cauchy stress σ_{11} , the accumulated plastic slip γ_{acc} , and the fluctuating temperature field $\tilde{\theta}$ are plotted. The microscopic results are generated for the highlighted element at the macroscale.

As expected, the maximum values within the macroscopic fields are located between the two loads and are more or less constant in the four-point bending test. Looking at the strain in horizontal direction, the compressive strains are located at the top of the specimen, while the tensile strains occur at the bottom of the specimen. This behavior is similar for the stress. Considering the accumulated plastic slip, it can be seen that a higher amount of plastic deformation occurs in the tensile regime. Since the temperature change in our model only depends on the evolution of the plastic deformations, the maximum temperature change in the specimen is directly related to the presence of the accumulated plastic slip. The microscopic results reveal that due to grain boundaries there are local peaks with values significantly higher than the average for strain, stress and accumulated plastic slip. Additionally, the correlation between plastic deformations and the temperature evolution is again clearly visible. Since the changes within the temperature field are rather small, only the fluctuating temperature field $\tilde{\theta} = \theta - \bar{\theta}$ is plotted. Hence, the field fluctuates around zero. This explains the negative values, which are not related to a cooling.

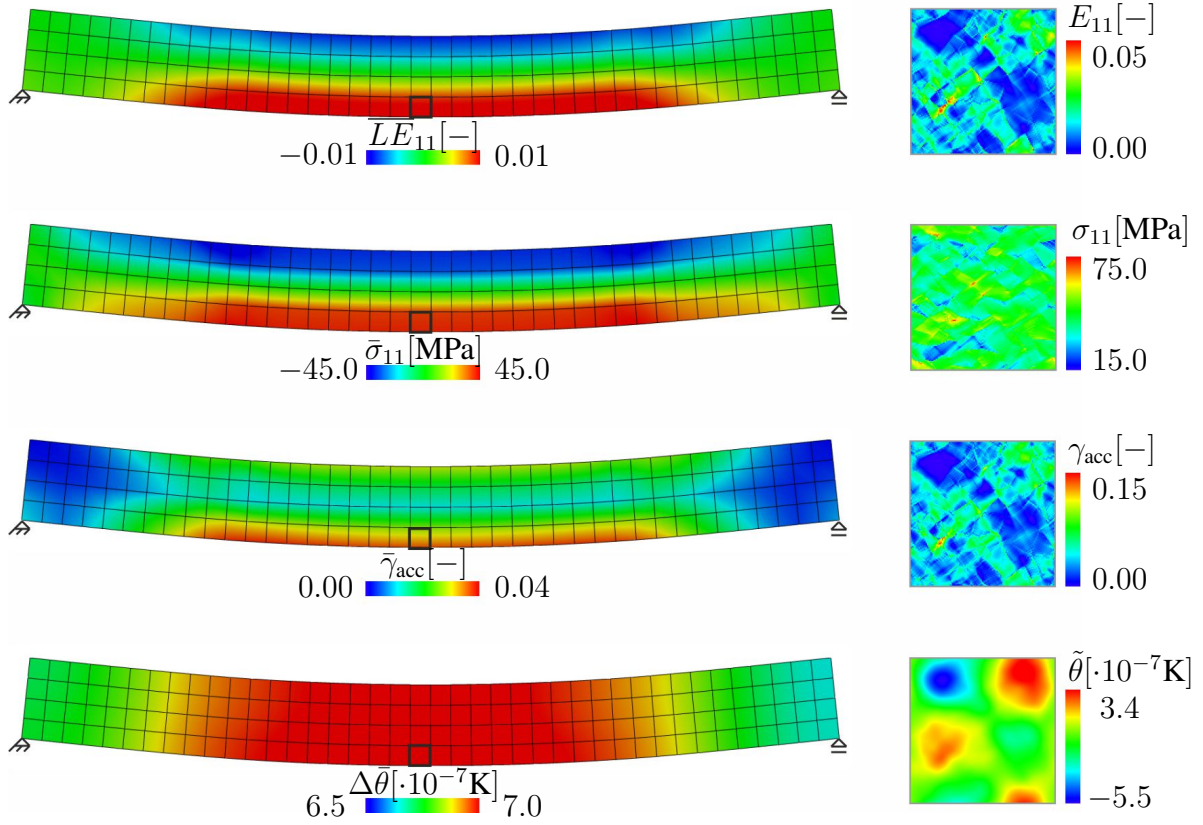


Figure 4.2: Macroscopic and microscopic results for the marked element of the strain, Cauchy stress, accumulated plastic slip as well as the change in the macroscopic temperature and microscopically fluctuating temperature field are shown for the maximum applied displacement.

4.7 Conclusion and outlook

In this work, we presented a thermomechanically coupled FE-FFT-based two-scale model for the simulation of polycrystalline microstructures. We considered not only fluctuating mechanical fields such as the strain, but also fluctuating thermal fields. The applicability of the model is demonstrated by considering the two-scale simulation of a four-point bending test of a copper specimen. It shows that due to plastic deformation, heat is generated in the specimen, which fluctuates as desired on the microscale.

However, the evolution of heat on the macroscale as well as the local fluctuations of the temperature on the microscale are rather small. Therefore, future work will deal with the investigation of different materials, such as shape memory alloys. In this context, microscopic phenomena such as martensitic phase transformations occur and will be modeled (e.g. shown for mechanically induced phase transformations in [355]). These martensitic phase transformations lead to an additional heat generation and therefore the temperature evolution is expected to be much

higher. Vice versa, phase transformations induced by the temperature will also occur in this context (see e.g. [356]) and have to be captured.

5 | Article 4:

A geometrically adapted reduced set of frequencies for a FFT-based microstructure simulation

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Disclosure of the individual authors’ contributions to the article:

C. Gierden reviewed the relevant existing literature and developed the idea of defining a geometrically adapted sampling pattern. Furthermore, he implemented the framework, performed the simulations, interpreted the results and wrote the article. J. Waimann, B. Svendsen and S. Reese gave conceptual advice, contributed to the discussion of the results, proofread the article and made valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

5.1 Abstract

We present a modified model order reduction (MOR) technique for the FFT-based simulation of composite microstructures. It utilizes the earlier introduced MOR technique ([17]), which is based on solving the Lippmann-Schwinger equation in Fourier space by a reduced set of frequencies. Crucial for the accuracy of this MOR technique is on the one hand the amount of used frequencies and on the other hand the choice of frequencies used within the simulation. Kochmann et al. [17] defined the reduced set of frequencies by using a fixed sampling pattern, which is most general but leads to poor microstructural results when considering only a few frequencies. Consequently, a reconstruction algorithm based on the TV_1 -algorithm [286] was used in a post-processing step to generate highly resolved micromechanical fields.

The present work deals with a modified sampling pattern generation for this MOR technique. Based on the idea, that the micromechanical material response strongly depends on the phase-wise material behavior, we propose the usage of sampling patterns adapted to the spatial arrangement of the individual phases. This leads to significantly improved microscopic and overall results. Hence, the time-consuming reconstruction in the post-processing step that was necessary in the earlier work is no longer required. To show the adaptability and robustness of this new choice of sampling patterns, several two dimensional examples are investigated. In addition, also the 3D extension of the algorithm is presented.

5.2 Introduction

To calculate spatial resolutions for complex microstructural material behaviors within structural finite element (FE) simulations, a two-scale full field simulation is necessary. To perform these highly resolved two-scale simulations, various methodologies have been established ([124]). Examples of these are the FE^2 method (e.g. [113, 123]) and the FE-FFT method (e.g. [13, 18]). In this context, we focus on the FE-FFT-based simulation approach, but restrict ourselves in this work exclusively to the FFT-based microstructure simulation. Such a microstructure may be given in terms of a representative volume element (RVE) or a unit cell (e.g. [161, 163]).

The FFT-based modelling of periodic microstructures was introduced by [11, 12]. Based on fixed-point iterations, it is used for the simulation of different microstructures, such as composites [190] and polycrystals [191]. In the last two decades improvements of the solution behavior of the FFT-based method were gained in various ways [14]. For example, by the development of more efficient solvers, which are numerically more robust and lead to better convergence behavior. Among these are polarization-based formulations [20, 198, 219], for-

mulations based on augmented Lagrangians [196, 201], or formulations based on conjugate gradients [195, 209, 215, 216]. In addition, numerical resolution problems related to the Gibbs phenomenon [19] have been addressed by using e.g. first- [30, 227] and higher-order [231] finite difference approximations of the differential operator. In summary, the FFT-based microstructure simulation is an accurate and efficient solution scheme, which is even more efficient than the common FE simulation as shown by [117] or [8]. Nevertheless, the computational effort especially in the context of a two-scale FE-FFT-based simulation is still extremely high. Hence, the development of even more efficient methods is necessary.

One possibility is to use hybrid homogenization methods, which combine numerical simulations and theoretical investigations, such as the uniform [114] or non-uniform [121, 122] transformation analysis or the clustering analysis [115, 357]. Concerning numerically efficient FE-FFT-based homogenization techniques a straight-forward ansatz is based on using a coarsely discretized microstructure. Consequently, this leads to coarse microstructural results so that a post-processing step is necessary to generate the required highly resolved microstructural fields [16, 319]. Other model order reduction techniques are for example based on a proper orthogonal decomposition (POD) [285] using the strain tensor in Fourier space $\hat{\epsilon}$ to compute the required projection tensor [234], low-rank approximations [236] or on computations using a reduced set of frequencies [17] in Fourier space.

The present paper deals with the model order reduction technique considering a reduced set of frequencies [17]. This technique reduces the computational effort of the spectral solver and is suitable for small [17] and finite strain kinematics [235]. The earlier proposed solution procedure uses a fixed sampling pattern to define the reduced set of frequencies. During the computations, this reduced set of frequencies is used to solve the Lippmann-Schwinger equation in Fourier space. Subsequently, in a post-processing step, a reconstruction and a compatibility step is performed to generate highly resolved microstructural fields. Since the selection of frequencies is crucial for the accuracy of the simulation in our current work, we propose to use a geometrically adapted sampling pattern instead, which incorporates the microstructural phase distribution. This leads to significantly better microstructural results, so that the time consuming reconstruction step using the TV_1 -algorithm proposed by [286] is not necessary anymore.

The paper is structured as follows. The microscopic boundary value problem (BVP) is reviewed in Section 5.3. The solution strategy to this microscopic BVP by using a spectral solver and fixed-point iterations is given in Section 5.4. Section 5.5 gives an overview of the recently introduced model order reduction technique based on a reduced set of frequencies with a fixed sampling pattern and the new technique based on using a geometrically adapted sampling

pattern. A comparison of the results of both methods is presented in Section 5.6. The paper ends with a conclusion and an outlook in Section 5.7.

Notation. A direct tensor notation is preferred throughout the text. Vectors and second-order tensors are represented by bold letters, e.g. $\mathbf{a}$ and $\mathbf{A}$, a tensor of fourth order by, e.g., $\mathbb{A}$. The linear mapping of a second-order tensor $\mathbf{B}$ by a fourth-order tensor $\mathbb{C}$ is denoted by $\mathbf{A} = \mathbb{C} : \mathbf{B}$. The scalar and dyadic products are denoted, e.g. by $\mathbf{a} \cdot \mathbf{b}$ as well as $\mathbf{A} : \mathbf{B}$, and $\mathbf{A} \otimes \mathbf{B}$, respectively. Furthermore, $\|\bullet\|$ represents the Frobenius norm and a bar over any quantity $\bar{A}$ always refers to a macroscopic quantity, while the absence of a bar is related to microscopic quantities. Additional notation is introduced when needed.

5.3 Microscopic boundary value problem (BVP)

Let us consider an inhomogeneous periodic microstructure $\Omega = \Omega_I \cup \Omega_M$ with inclusions Ω_I embedded in a softer matrix material Ω_M . One example is a microstructure with one centered spherical inclusion as shown in Figure 5.1.

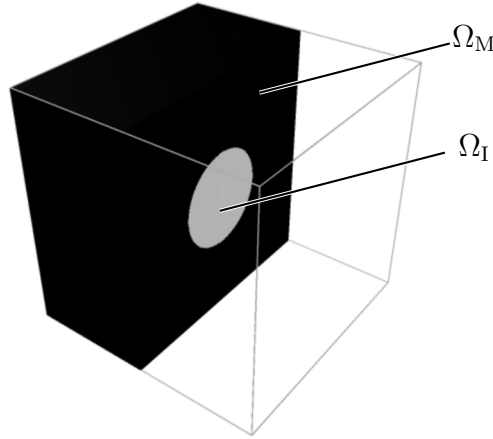


Figure 5.1: Microstructure with one centered spherical inclusion.

Considering small strain kinematics, the total strain $\boldsymbol{\varepsilon}(\bar{\mathbf{x}}, \mathbf{x}) = \bar{\boldsymbol{\varepsilon}}(\bar{\mathbf{x}}) + \tilde{\boldsymbol{\varepsilon}}(\mathbf{x})$ at the macroscopic position $\bar{\mathbf{x}}$ and the microscopic position $\mathbf{x}$ is additively split into the macroscopic part $\bar{\boldsymbol{\varepsilon}}(\bar{\mathbf{x}})$ and the microscopic fluctuating part $\tilde{\boldsymbol{\varepsilon}}(\mathbf{x})$, respectively. Subjecting the given microstructure to a macroscopic strain $\bar{\boldsymbol{\varepsilon}}(\bar{\mathbf{x}})$, the total stress $\boldsymbol{\sigma}(\bar{\mathbf{x}}, \mathbf{x})$ is computed by solving the

microscopic boundary value problem

$$\begin{aligned}\operatorname{div} \boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}) &= \mathbf{0} & \forall \boldsymbol{x} \in \Omega \\ \boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}) &= \boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}, \boldsymbol{\varepsilon}(\bar{\boldsymbol{x}}, \boldsymbol{x}), \boldsymbol{\alpha}(\boldsymbol{x})) \\ \boldsymbol{\varepsilon}(\bar{\boldsymbol{x}}, \boldsymbol{x}) &= \bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}}) + \nabla^S(\tilde{\boldsymbol{u}}(\boldsymbol{x}))\end{aligned}\tag{5.1}$$

for each macroscopic position $\bar{\boldsymbol{x}}$, while body forces are considered only on the macroscopic level and are thus neglected on the micro level. Within Equation (5.1), $\boldsymbol{\alpha}(\boldsymbol{x})$ describes a set of internal variables, $\tilde{\boldsymbol{u}}(\boldsymbol{x})$ is the microscopic fluctuating displacement field and ∇^S represents the symmetric gradient operator. In regard of comprehensibility, the dependence of all variable besides the macroscopic strains on the macroscopic position $\bar{\boldsymbol{x}}$ is not shown. The corresponding macroscopic stress $\bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{x}})$ and strain $\bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}})$ tensors are defined by the volume average of their local quantities:

$$\bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{x}}) := \frac{1}{V} \int_{\Omega} \boldsymbol{\sigma}(\boldsymbol{x}) \, d\Omega \quad \text{and} \quad \bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}}) := \frac{1}{V} \int_{\Omega} \boldsymbol{\varepsilon}(\boldsymbol{x}) \, d\Omega. \tag{5.2}$$

We restrict ourselves to microstructures consisting of two phases with linear elastic or linear elasto-plastic material behavior. Doing that, the total strain can be additively split into an elastic part $\boldsymbol{\varepsilon}_e(\boldsymbol{x})$ and a plastic part $\boldsymbol{\varepsilon}_p(\boldsymbol{x})$: $\boldsymbol{\varepsilon}(\boldsymbol{x}) = \boldsymbol{\varepsilon}_e(\boldsymbol{x}) + \boldsymbol{\varepsilon}_p(\boldsymbol{x})$. The linear-elastic stress-strain relation reads $\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbb{C}(\boldsymbol{x}) : \boldsymbol{\varepsilon}_e(\boldsymbol{x})$. The yield condition for the elasto-plastic behavior is defined as

$$\Phi(\boldsymbol{\sigma}(\boldsymbol{x}), \boldsymbol{\varepsilon}_p^{\text{acc}}(\boldsymbol{x}), \boldsymbol{x}) = \sigma^{\text{eq}}(\boldsymbol{x}) - [\sigma_y^0(\boldsymbol{x}) + H(\boldsymbol{x}) \boldsymbol{\varepsilon}_p^{\text{acc}}(\boldsymbol{x})] \tag{5.3}$$

which is the classical von Mises yield condition with an isotropic linear hardening. Here, $\sigma_y^0(\boldsymbol{x})$ is the initial yield stress, $\sigma^{\text{eq}}(\boldsymbol{x})$ is the von Mises equivalent stress, $H(\boldsymbol{x})$ is the hardening modulus, and $\boldsymbol{\varepsilon}_p^{\text{acc}}(\boldsymbol{x})$ is the accumulated plastic strain. In terms of an associative flow rule, the evolution of the plastic strain $\dot{\boldsymbol{\varepsilon}}_p$ is given by

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\gamma} \frac{\partial \Phi}{\partial \boldsymbol{\sigma}} \tag{5.4}$$

with the plastic multiplier $\dot{\gamma}$. Finally, the Karush-Kuhn-Tucker conditions $\Phi \leq 0$, $\dot{\gamma} \geq 0$ and $\Phi \dot{\gamma} = 0$ need to be fulfilled.

5.4 FFT-based microstructure simulation using the basic fixed-point scheme

To solve the inhomogeneous microscopic boundary value problem introduced in Equation 5.1, Hashin and Shtrikman [131] proposed to transfer it into an equivalent homogeneous representation

$$\begin{aligned} \operatorname{div} \mathbb{C}^0 : \varepsilon(\mathbf{x}) + \operatorname{div} \boldsymbol{\tau}(\mathbf{x}) &= \mathbf{0} & \forall \mathbf{x} \in \Omega \\ \boldsymbol{\tau}(\mathbf{x}) &:= \boldsymbol{\sigma}(\mathbf{x}, \varepsilon(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x})) - \mathbb{C}^0 : \varepsilon(\mathbf{x}) \\ \varepsilon(\mathbf{x}) &= \bar{\varepsilon}(\bar{\mathbf{x}}) + \nabla^S(\tilde{\mathbf{u}}(\mathbf{x})), \end{aligned} \quad (5.5)$$

by defining the polarization stress $\boldsymbol{\tau}(\mathbf{x})$. It describes the fluctuation of the microstructural stress around the stress of a homogeneous reference material with stiffness $\mathbb{C}^0$. Introducing Green's function $\mathbf{G}^0(\mathbf{x}, \mathbf{x}')$ and Green's operator $\mathbb{I}^{(0)}(\mathbf{x}, \mathbf{x}')$, respectively, the integral equation

$$\varepsilon(\mathbf{x}) = \bar{\varepsilon}(\bar{\mathbf{x}}) - \int_{\Omega} \mathbb{I}^{(0)}(\mathbf{x}, \mathbf{x}') : \boldsymbol{\tau}(\mathbf{x}') d\mathbf{x}' \quad (5.6)$$

enables the solution of Equation 5.5. Equation 5.6 is also known as Lippmann-Schwinger equation [Kröner [337], Willis [119]]. The present convolution integral is solved by transferring the Lippmann-Schwinger equation into Fourier space yielding

$$\hat{\varepsilon}(\boldsymbol{\xi}) = \begin{cases} -\hat{\mathbb{I}}^{(0)}(\boldsymbol{\xi}) \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) & \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\varepsilon} & \forall \boldsymbol{\xi} = \mathbf{0} \end{cases} \quad (5.7)$$

with the wave vector $\boldsymbol{\xi}$. In Fourier space, also Green's function and Green's operator

$$\hat{G}_{ik}^0(\boldsymbol{\xi}) = (\mathbb{C}_{ijkl}^0 \xi_j \xi_l)^{-1} \quad (5.8)$$

$$\text{and } \hat{\Gamma}_{ijkl}^0(\boldsymbol{\xi}) = \frac{1}{4} \left(\hat{G}_{jk,li}^0(\boldsymbol{\xi}) + \hat{G}_{ik,lj}^0(\boldsymbol{\xi}) + \hat{G}_{jl,ki}^0(\boldsymbol{\xi}) + \hat{G}_{il,kj}^0(\boldsymbol{\xi}) \right) \quad (5.9)$$

are explicitly known. An iterative solution scheme based on Equation 5.7 was first introduced by [11, 12]. The mechanical equilibrium is considered to be achieved when the convergence criterion

$$\frac{\|\varepsilon^{(i)}(\mathbf{x}) - \varepsilon^{(i-1)}(\mathbf{x})\|}{|\bar{\varepsilon}|} < \operatorname{tol}_{\varepsilon} \quad (5.10)$$

is fulfilled within iteration step i . Considering a fixed-point iteration scheme, the best convergence behavior is achieved by defining the homogeneous reference material behavior based on the arithmetic average of the spatially varying Lamé constants $\lambda(x)$ and $\mu(x)$ [12, 195]. This so-called basic fixed-point scheme is used within all following simulations. In addition we use a first-order central difference approximation of the differential operator in Equation 5.9 to avoid numerical resolution problems related to the Gibbs phenomenon, as proposed by [30].

5.5 Model order reduction technique based on a reduced set of frequencies

Recently, Kochmann et al. [17] proposed a model order reduction technique based on a reduced set of wave vectors ${}^R\xi$ to decrease the computational effort of the spectral solver. The general idea is that any function, such as the step function in Figure 5.2, may be approximated by a Fourier series. Using a reduced set of frequencies with only one or ten frequencies leads to a very coarse approximation (see Figure 5.2). Nevertheless, using 100 frequencies already yields an accurate approximation of the step function. More frequencies would lead to even better solutions, but the computational effort will also rise with more frequencies. Due to that, a reduced set of frequencies must be defined in a way, that leads to accurate results but also low computational costs.

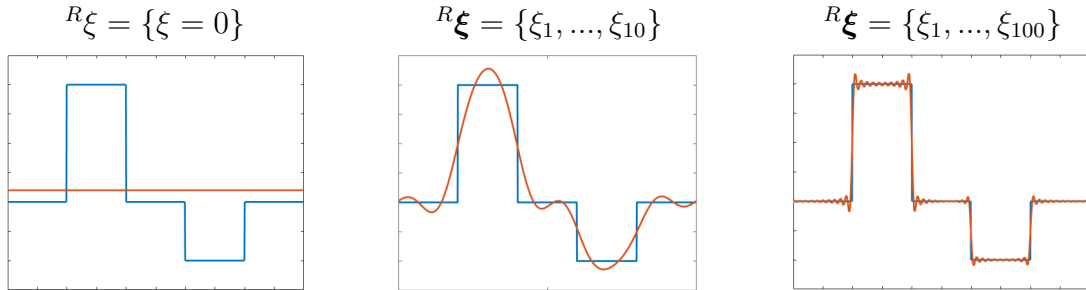


Figure 5.2: Approximating a step function with a Fourier series consisting of one, ten or 100 frequencies.

Using this idea in terms of the FFT-based method yields a reduced solution of the Lippmann-Schwinger equation in Fourier space. The resulting reduced fixed-point scheme is given in the following:

while $\frac{\|\boldsymbol{\varepsilon}^{(i+1)}(\boldsymbol{x}) - \boldsymbol{\varepsilon}^{(i)}(\boldsymbol{x})\|_{L_2}}{\|\bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}})\|_{L_2}} \leq \text{tol}_\varepsilon$ **do**

a) $\boldsymbol{\tau}^{(i)}(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{\varepsilon}^{(i)}(\boldsymbol{x})) - \mathbb{C}^0 : \boldsymbol{\varepsilon}^{(i)}(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Omega$

b) $\hat{\boldsymbol{\tau}}^{(i)}(\boldsymbol{\xi}) = \text{FFT} \{ \boldsymbol{\tau}^{(i)}(\boldsymbol{x}) \}$

c) ${}^R\hat{\boldsymbol{\varepsilon}}^{(i+1)}({}^R\boldsymbol{\xi}) = \begin{cases} - {}^R\hat{\mathbb{T}}^{(0)}({}^R\boldsymbol{\xi}) : {}^R\hat{\boldsymbol{\tau}}^{(i)}({}^R\boldsymbol{\xi}) & \text{for } {}^R\boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}}) & \text{for } {}^R\boldsymbol{\xi} = \mathbf{0} \end{cases}$

d) ${}^R\boldsymbol{\varepsilon}^{(i+1)}(\boldsymbol{x}) = \text{iFFT} \{ {}^R\hat{\boldsymbol{\varepsilon}}^{(i+1)}({}^R\boldsymbol{\xi}) \}$

end do

The speed-up in this algorithm is gained from step c) by solving the convolution integral in Fourier space using the reduced set of wave vectors. It is also possible to use the reduced set of frequencies and a discrete Fourier transformation (DFT) for the Fourier transformation in step b) and the inverse Fourier transformation in step d), but since the FFT with the full set of frequencies is even faster than the DFT with the reduced set of frequencies, the FFT is preferably used.

Crucial for the performance of this algorithm is the definition of the reduced set of frequencies. In the following, a short review of the recently proposed fixed sampling pattern for the choice of a reduced set of frequencies is given. Subsequently, a new method for the generation of sampling patterns based on the microstructural geometry is presented. For simplicity, both methods are presented for the 2D case.

5.5.1 Reduced set of frequencies based on a fixed sampling pattern

The proposed algorithm by Kochmann et al. [17] is based on the identification of a fixed sampling pattern, which is used to define the reduced set of wave vectors for the solution of the Lippmann-Schwinger equation. This sampling is always the same and therefore does not take the material behavior or the microstructural geometry into account. After performing the online computations with this reduced set of frequencies, a reconstruction based on the TV_1 -algorithm proposed by Candes et al. [286] is performed. Subsequently, a compatibility step is necessary to generate highly resolved micromechanical fields. To identify an appropriate set of wave vectors, a circular, a squared and a radial sampling pattern are investigated. The most general reduced set of frequencies, which is also most suitable for the reconstruction algorithm, is the radial sampling pattern, shown in Figure 5.3.

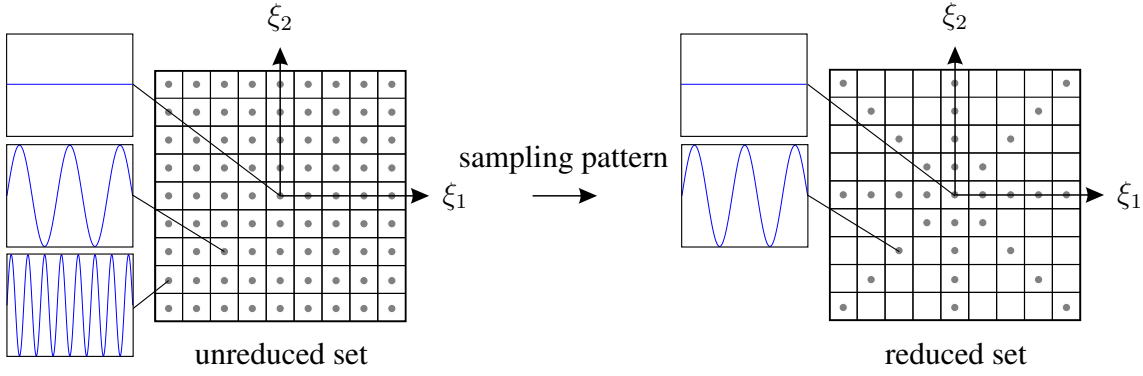


Figure 5.3: Unreduced set of frequencies (*left*) and a reduced set of frequencies based on a radial sampling pattern (*right*).

Figure 5.3 shows the full set of frequencies (*left*) as well as a reduced set of frequencies based on a radial sampling pattern (*right*) while the lowest frequencies are in the middle of the shown grid, beginning with the zeroth frequency, which is the mean of the approximated function.

If only a few percent of frequencies are considered, the usage of such a reduced set of frequencies leads to poor microstructural and overall results. Due to that, a post-processing step is used after the reduced simulation. This generates highly resolved data by using the TV_1 -algorithm proposed by Candes et al. [286]. In addition, thereafter, a compatibility step is needed to guarantee a compatible strain field.

5.5.2 A novel approach for a reduced set of frequencies based on a geometrically adapted sampling pattern

The mechanical behavior strongly depends on the geometrical representation of e.g. inclusions within the microstructure. As an example, smaller strains occur in stiffer inclusions and corresponding higher strains in softer matrix material. The idea of an adapted sampling pattern is to use the microstructural geometry to define the reduced set of frequencies. Therefore, the geometry of a two phase material is presented by a step function

$$g(\mathbf{x}) = \begin{cases} 0 & \text{for } \mathbf{x} \in \Omega_M \\ 1 & \text{for } \mathbf{x} \in \Omega_I, \end{cases} \quad (5.11)$$

in real space as shown in Figure 5.4 (*left*) (with 100×100 grid points). Transferring this representation of the microstructural geometry into Fourier space results in the plot given in

Figure 5.4 (*right*), in which the frequencies with the corresponding amplitudes are plotted. Again, the lowest frequencies are centered.

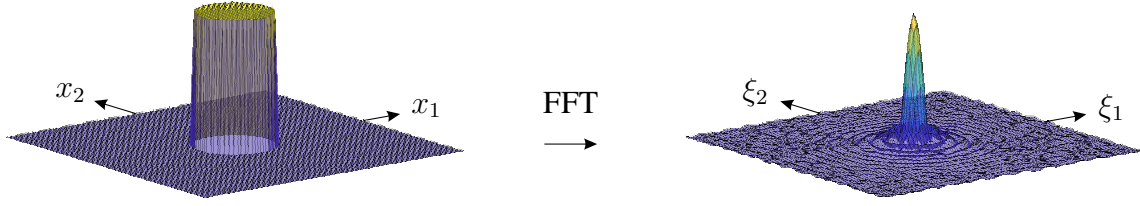


Figure 5.4: Geometry in real space $g(\mathbf{x})$ (*left*) and geometry transferred into Fourier space $\hat{g}(\boldsymbol{\xi})$ (*right*).

The highest amplitudes, given in this Fourier representation, correspond to the most needed frequencies for the approximation of the geometry. So, a reduced set of frequencies should be defined by taking into account a given percentage of frequencies with the highest amplitudes to obtain the best approximation. Using for example a reduced set of frequencies with $\mathcal{R} = 2\%$ of the highest frequencies leads to the sampling pattern given in Figure 5.5 (*left*), while $\mathcal{R}$ describes the percentage of used frequencies. The consideration of these frequencies for the approximation of the geometry in real space results in the approximated step function in Figure 5.5 (*right*).

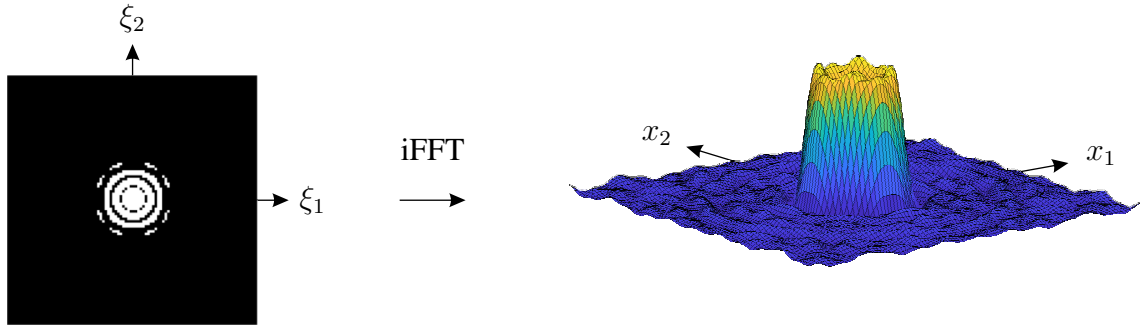


Figure 5.5: Geometrically adapted sampling pattern with $\mathcal{R} = 2\%$ of frequencies (*left*) and geometrical step function approximated by this reduced set of frequencies (*right*).

The idea of a geometrically adapted sampling pattern is to use the same sampling pattern as shown in Figure 5.5 (*left*) also for the approximation of the microstructural strains and therefore also for solving the Lippmann-Schwinger equation in Fourier space. Doing that, significantly better microscopic and overall results are achieved compared to the fixed radial sampling pattern (see Figure 5.3 (*right*)), as shown in Section 5.6. Due to that, the time consuming reconstruction algorithm which was necessary for the fixed sampling pattern is no longer needed.

5.6 Numerical examples and comparison of the results with fixed and adapted sampling patterns

To test the adaptivity and accuracy of a geometrically adapted sampling pattern, first, several 2D two phase microstructures with elastic material behavior and one centered inclusion are considered and compared to the results generated by the fixed sampling pattern in Section 5.6.1. This is followed by investigating the influence of the phase contrast on the accuracy and efficiency of the proposed method in Section 5.6.2, by considering a microstructure with several inclusions and an elastic or elasto-plastic material behavior in Section 5.6.3 and by the straight forward extension to the 3D case in Section 5.6.4.

All microstructures are assumed to be squared or cubic and discretized by $n = 256 \times 256$ and $n = 256 \times 256 \times 256$ equidistant grid points, respectively. The mechanical equilibrium is considered to be achieved for the tolerance $\text{tol}_\varepsilon < 10^{-8}$. To compare the results to the reference solution with the full set of frequencies, a macroscopic error $\bar{\mathcal{E}}$ and a microscopic error $\mathcal{E}$ is defined by:

$$\bar{\mathcal{E}} = \frac{\|\bar{\boldsymbol{\sigma}} - \bar{\boldsymbol{\sigma}}_{\text{ref}}\|}{\|\bar{\boldsymbol{\sigma}}_{\text{ref}}\|} \quad \text{and} \quad \mathcal{E} = \frac{1}{n} \sum_n \frac{\|\boldsymbol{\sigma}(n) - \boldsymbol{\sigma}_{\text{ref}}(n)\|}{\|\boldsymbol{\sigma}_{\text{ref}}(n)\|},$$

where n is the total number of grid points. All computations are performed using MATLAB with the build-in FFTW-library and pre-compiled material routines on a Dell notebook with a 2.80 GHz Intel *i7* quad-core processor and 32 GB of RAM.

5.6.1 Elastic 2D two phase materials with one inclusion

To illustrate the adaptivity of the newly introduced sampling pattern generation and the resulting microstructural fields compared to the results with the fixed sampling pattern, a two dimensional microstructure with different centered inclusions as shown in Figure 5.6 is investigated. Both, the inclusions and the matrix material are considered to be elastic with $\lambda_{\text{I}} = 2.0$ GPa and $\mu_{\text{I}} = 2.0$ GPa for the inclusion and $\lambda_{\text{M}} = 1.0$ GPa and $\mu_{\text{M}} = 1.0$ GPa for the matrix material, respectively. The applied macroscopic strain is set to $\bar{\varepsilon}_{11} = 0.01$ and $\bar{\varepsilon}_{22} = -0.01$.

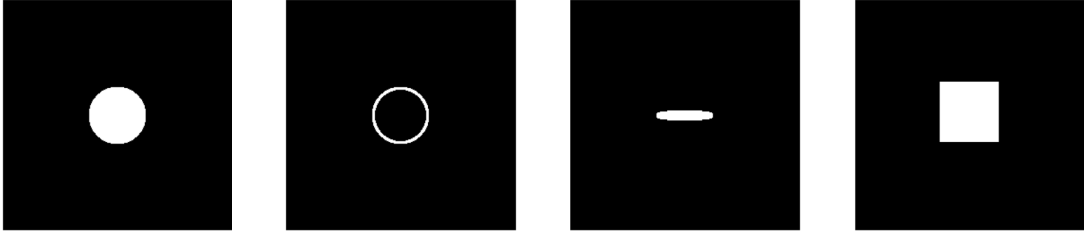


Figure 5.6: Microstructures with various kinds of central inclusions. The matrix material is colored black and the inclusion is colored white.

First, we investigate the microstructure with one circular inclusion. Note, that the following observations have been made for all stress and strain fields. The results related to the fixed and adapted sampling pattern are shown in Figure 5.7 and Figure 5.8, respectively.

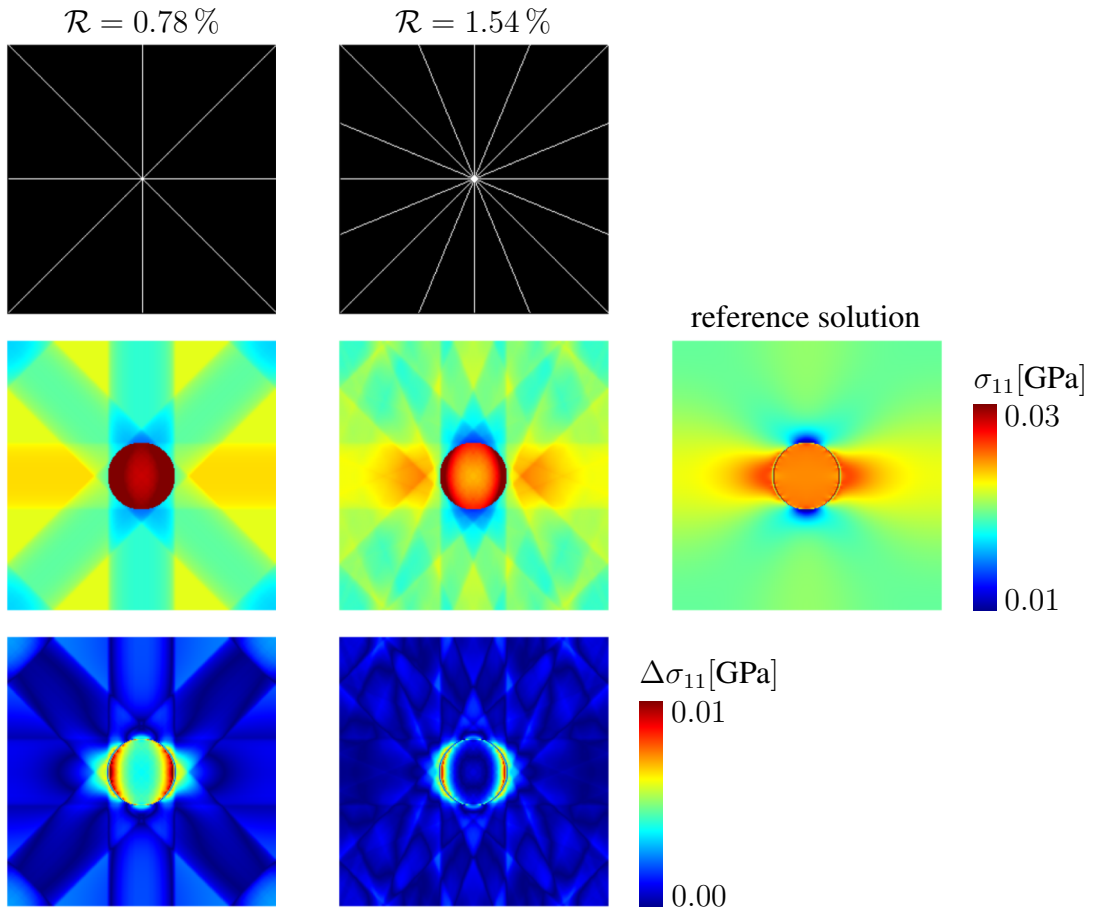


Figure 5.7: Microstructural fields for the 2D elastic microstructure with one circular inclusion. *Top row*: Fixed sampling pattern with two different numbers of wave vectors. *Middle row*: Corresponding microstructural stress field σ_{11} and reference stress field computed with the full set of frequencies. *Bottom row*: Absolute difference in the microstructural stress field $\Delta\sigma_{11}$.

In the top row, the sampling patterns for two reduced sets of frequencies ($\mathcal{R} = 0.78\%$ and $\mathcal{R} = 1.54\%$) are given. Subsequently, the corresponding stress fields σ_{11} and the reference solution incorporating the full set of frequencies are shown. In order to better recognize the difference between the results for the reduced sets of frequencies compared to the reference solution, the bottom row shows the point-wise absolute difference in the microstructural stress fields $\Delta\sigma_{11} = |\sigma_{11}^{\text{ref}} - \sigma_{11}|$.

As stated by [17] considering a fixed sampling pattern, the radial sampling pattern leads to good results in general since it considers a high amount of low frequencies, but also a certain amount of high frequencies. The low frequencies are necessary to capture the essential features of the microstructure, while the high frequencies are needed to capture for example

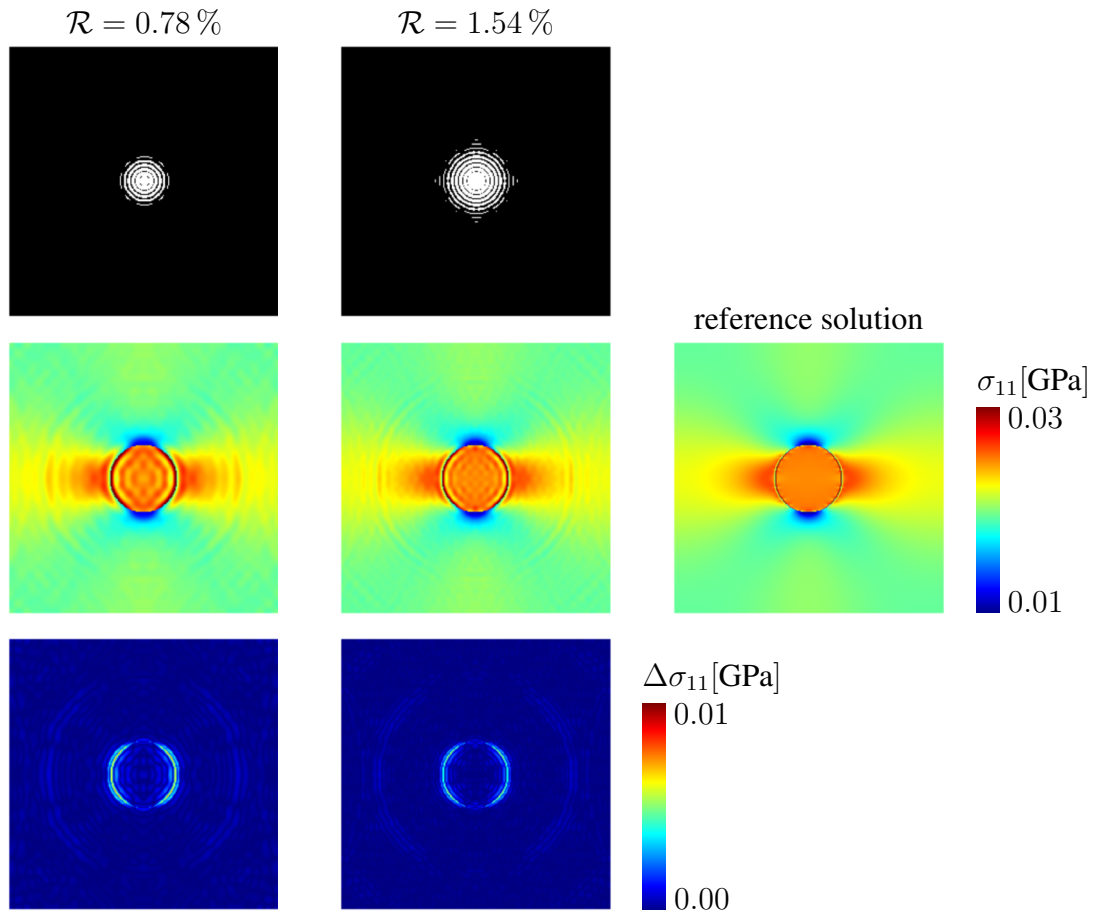


Figure 5.8: Microstructural fields for the 2D elastic microstructure with one circular inclusion. *Top row:* Adapted sampling pattern with two different numbers of wave vectors. *Middle row:* Corresponding microstructural stress field σ_{11} and reference stress field computed with the full set of frequencies. *Bottom row:* Absolute difference in the microstructural stress field $\Delta\sigma_{11}$.

microstructures with needle-like inclusions. Nevertheless, the radial sampling pattern leads to incoherent artifacts in the reduced solution, but which are needed in terms of the subsequent reconstruction algorithm. The difference in the microstructural stress fields compared to the reference solution is plotted in the last row of Figure 5.7, while no reconstruction is incorporated up to now. It can be seen, that this error goes up to 0.01 GPa in the area close to the edge of the inclusion, which is about one third compared to the maximum stress in the reference solution. Choosing the reduced set of frequencies based on the geometrically adapted sampling pattern and compared to the fixed sampling pattern, a higher amount of low frequencies is needed to capture the microstructural geometry (see Figure 5.8). Using this reduced set of frequencies also in terms of the microstructure simulation, more accurate results are generated. The highest error occurs in the transition from matrix to inclusion, which arises from the very high amount of frequencies which are necessary to capture such a sharp transition.

The macroscopic error $\bar{\mathcal{E}}$ and the microscopic error $\mathcal{E}$ are shown in Figure 5.9 depending on the reduced set of frequencies $\mathcal{R}$. Since a simple microstructure with only one centered circular inclusion is investigated in this example, the macroscopic (*left*) and the microscopic errors (*right*) are in both cases quite low. Nevertheless, the error corresponding to the adapted sampling pattern is always significantly smaller - especially, when the reduced set of frequencies consists only of few frequencies. For a higher number of frequencies, the errors of both solutions converge towards zero.

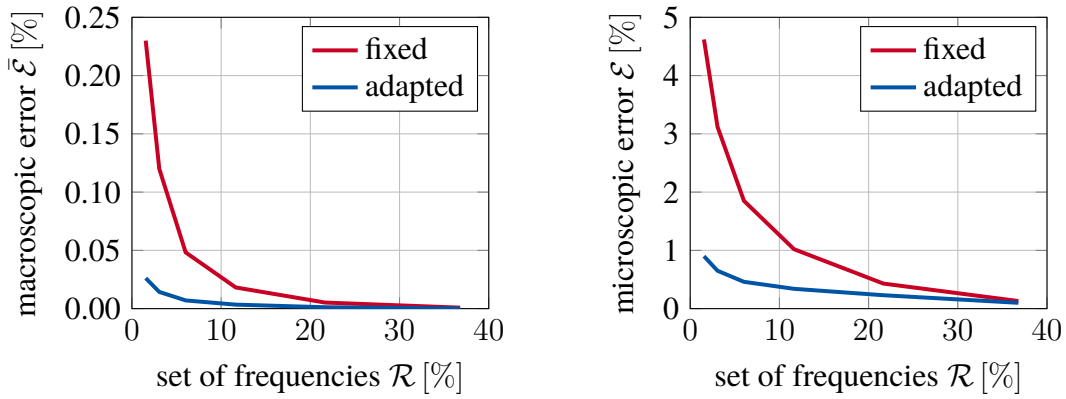


Figure 5.9: Macroscopic error $\bar{\mathcal{E}}$ (*left*) and microscopic error $\mathcal{E}$ (*right*) for the 2D elastic microstructure with one circular inclusion depending on the percentage of used frequencies $\mathcal{R}$ for the solution with the fixed and adapted sampling pattern.

Using the reconstruction algorithm and the compatibility step the solution for the fixed sampling pattern is improved as shown in Figure 5.10 in the left column. Since the microstructural fields related to the adapted sampling pattern do not have incoherent artifacts, the reconstruc-

tion algorithm does not yield any further improvement of the result and is therefore not needed. Instead, just the so-called compatibility step is applied. Thus, the Lippmann-Schwinger equation is solved once using the full set of frequencies based on the stress and the strain fields from the reduced simulation. It should be mentioned that in this context the earlier given name might be misleading, since the solutions are already compatible. The corresponding solutions are shown in Figure 5.10 in the centered column. It can be seen, that the micromechanical solution fields which are related to the adapted sampling pattern are still better compared to the solutions based on the fixed sampling pattern after the reconstruction.

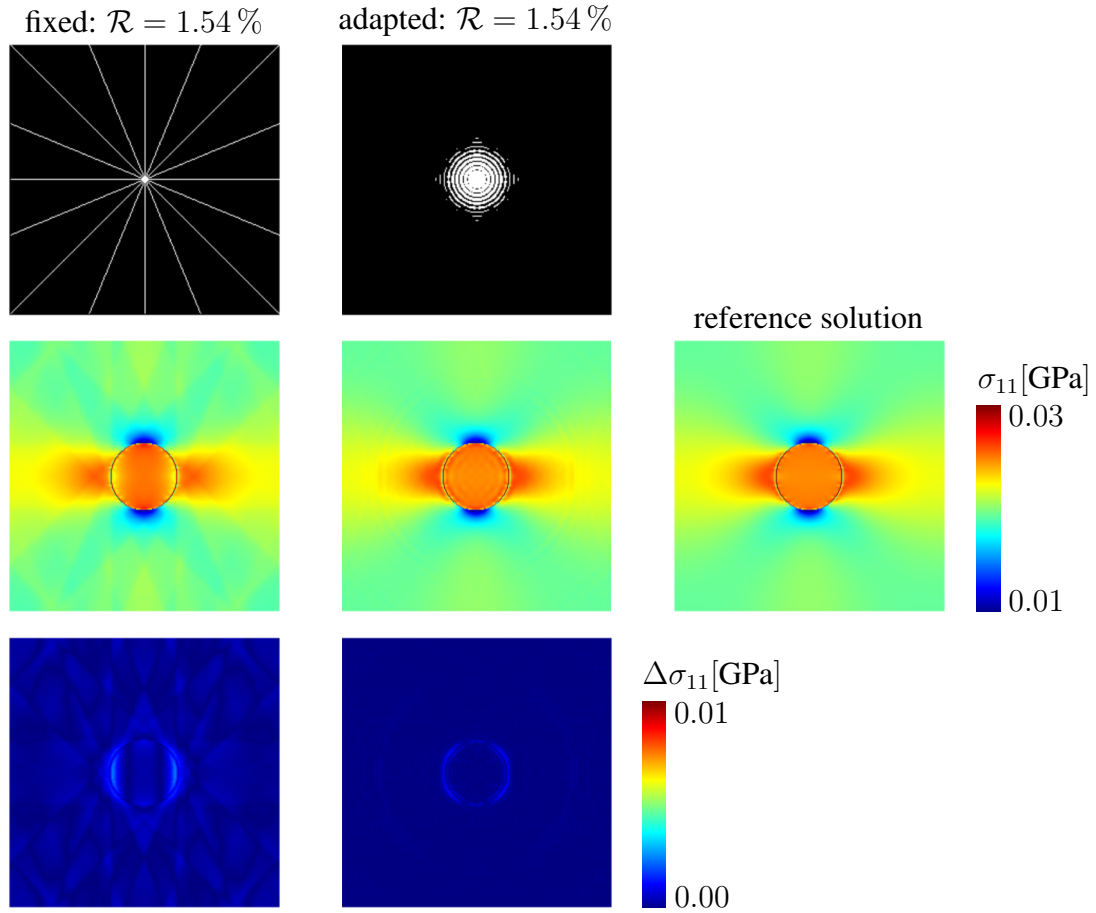


Figure 5.10: Microstructural fields for the 2D elastic microstructure with one circular inclusion. *Top row*: Fixed and adapted sampling pattern with the same number of wave vectors. *Middle row*: Corresponding microstructural stress field σ_{11} incorporating the reconstruction and compatibility step for the solution of the fixed sampling pattern and only the compatibility step for the solution of the adapted sampling pattern and reference stress field computed with the full set of frequencies. *Bottom row*: Absolute difference in the microstructural stress field $\Delta\sigma_{11}$.

Incorporating this post-processing step, the macroscopic error $\bar{\mathcal{E}}$ and microscopic error $\mathcal{E}$ are shown in Figure 5.11. For the fixed sampling pattern, the error refers to the solution after the reconstruction and the compatibility step. For the adapted sampling pattern, the error corresponds to the compatibility step, only. For both cases, Figure 5.11 shows the error depending on the percentage of used frequencies $\mathcal{R}$. The difference between the fixed and the adapted sampling pattern is rather small, while the error of the adapted sampling pattern is smaller for $\mathcal{R} < 6\%$ but larger for $\mathcal{R} \geq 6\%$. The range $\mathcal{R} < 6\%$ is of much larger interest, since the highest speed-up is gained by a set with a low number of frequencies.

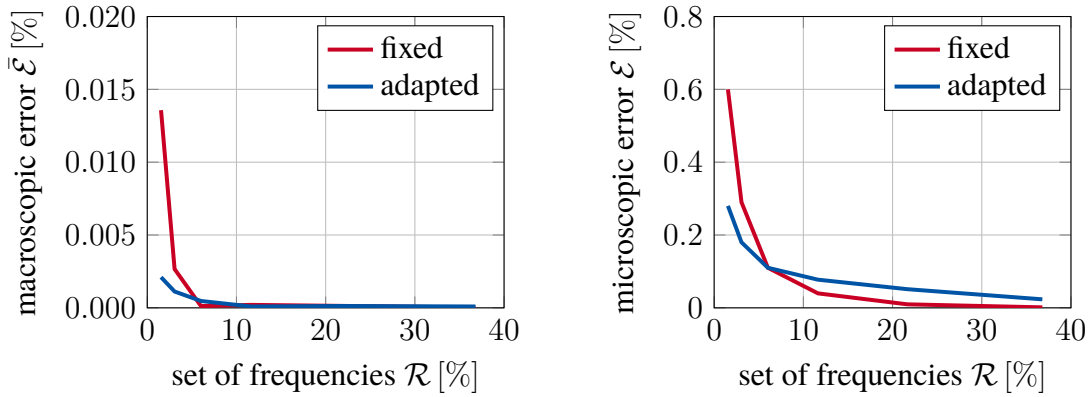


Figure 5.11: Macroscopic error $\bar{\mathcal{E}}$ (left) and microscopic error $\mathcal{E}$ (right) for the 2D elastic microstructure with one circular inclusion depending on the reduced set of frequencies $\mathcal{R}$ for the solution with the fixed sampling pattern with reconstruction and compatibility step and for the adapted sampling pattern only with the compatibility step.

Tables 5.1 and 5.2 present the total CPU times for the computations with the fixed and adapted sampling pattern, respectively. These CPU times are subdivided into the mean CPU time per iteration step for solving the convolution integral and the mean CPU time per iteration step for solving the constitutive law. The time for solving the constitutive law is almost independent of the number of considered frequencies. The speed up in the total CPU times is gained by solving the convolution integral in Fourier space with the reduced set of frequencies. Independent of the sampling pattern, the speed up factor for $\mathcal{R} = 1.54\%$ of frequencies is about 7-8, while the results with the adapted sampling pattern are more accurate. In addition, Table 5.1 shows the CPU times for the time consuming reconstruction step, which is not necessary for the adapted sampling pattern and the CPU time for the compatibility step, which is almost the same for the fixed and adapted sampling pattern (see Table 5.2).

elastic	CPU time [s] - fixed sampling pattern				
$\mathcal{R} [\%]$	total	$-\hat{\mathbb{I}}^{(0)} \hat{\tau}(\varepsilon)$ (mean)	$\sigma(\varepsilon)$ (mean)	reconstruction	compatibility
1.54	0.448	0.015	0.006	58.295	0.324
3.06	0.558	0.022	0.006	54.679	0.333
6.02	0.759	0.036	0.005	56.764	0.337
11.64	0.958	0.061	0.005	59.208	0.354
21.66	1.253	0.106	0.005	47.910	0.341
36.79	1.869	0.166	0.005	49.136	0.327
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
unreduced	3.196	0.302	0.004	-	-

Table 5.1: Total CPU time with mean CPU time per iteration step for solving the convolution integral and the constitutive law and CPU times for the reconstruction and the compatibility step of the simulation with the fixed sampling pattern for the 2D elastic microstructure with one circular inclusion.

elastic	CPU time [s] - adapted sampling pattern				
$\mathcal{R} [\%]$	total	$-\hat{\mathbb{I}}^{(0)} \hat{\tau}(\varepsilon)$ (mean)	$\sigma(\varepsilon)$ (mean)	reconstruction	compatibility
1.54	0.388	0.013	0.005	-	0.341
3.06	0.495	0.022	0.005	-	0.378
6.02	0.641	0.034	0.005	-	0.346
11.64	0.948	0.060	0.005	-	0.322
21.66	1.412	0.099	0.005	-	0.340
36.79	1.912	0.169	0.005	-	0.350
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
unreduced	3.196	0.302	0.004	-	-

Table 5.2: Total CPU time with mean CPU time per iteration step for solving the convolution integral and the constitutive law and CPU times for the reconstruction and the compatibility step of the simulation with the adapted sampling pattern for the 2D elastic microstructure with one circular inclusion.

The same investigations could be made using the microstructures with the annular, the elliptical, and the quadratic inclusion shown in Figure 5.6 and would lead to similar results. Due to that, we just show the sampling patterns and the corresponding microstructural stress fields σ_{11} for $\mathcal{R} = 1.54\%$ of frequencies considering these microstructures in Figures 5.12 -

5.14. The results show the relation between the arrangement of the considered frequencies in the adapted sampling pattern and the geometry of the inclusion within the matrix. Additionally it can be seen, that the results gained by the new approach are always closer to the reference solution than the solutions based on the fixed sampling pattern.

In Figure 5.12, the geometrically adapted sampling pattern of the microstructure with an annular inclusion is shown. This sampling pattern is similar to the adapted sampling corresponding to the circular inclusion; see Figure 5.8. Nevertheless, the amount of high frequencies is slightly higher. The adapted sampling pattern corresponding to the elliptical inclusion, shown in Figure 5.13, differs totally from that. It can be seen, that in direction of the major axis of the ellipse lower frequencies are needed and perpendicular to that higher frequencies are necessary, since a smaller distance needs to be bridged in this direction. As a last example, Figure 5.14 shows the microstructure with a quadratic inclusion. The sharp edges of this last examined type of inclusion again lead to a totally different set of frequencies.

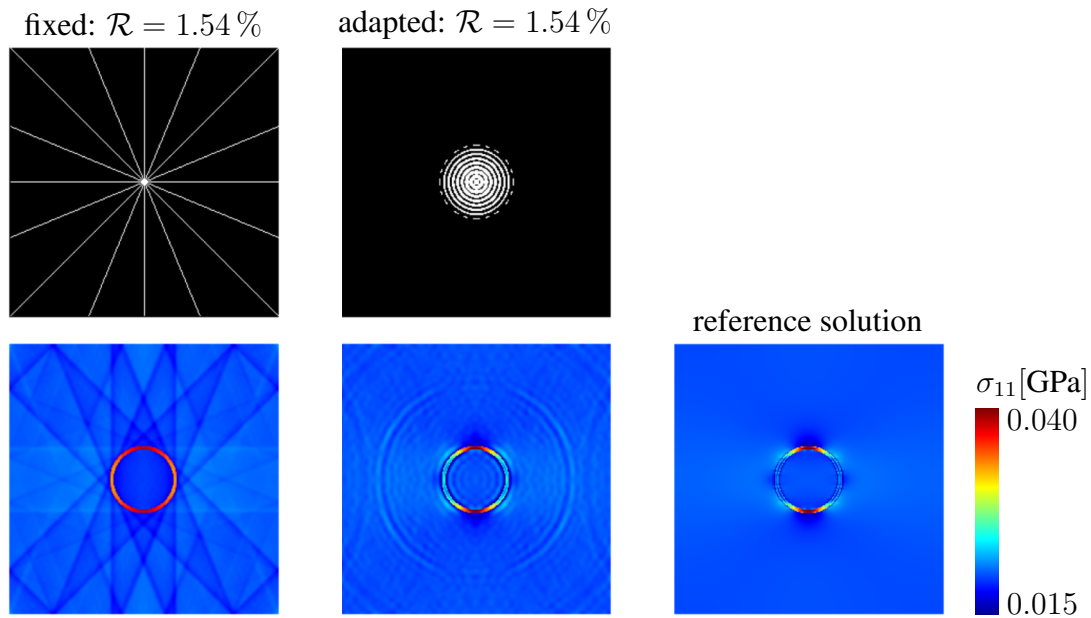


Figure 5.12: Microstructural fields for the 2D elastic microstructure with one annular inclusion. *Top row*: Fixed and adapted sampling pattern with the same number of wave vectors. *Bottom row*: Corresponding microstructural stress field σ_{11} and reference stress field computed with the full set of frequencies.

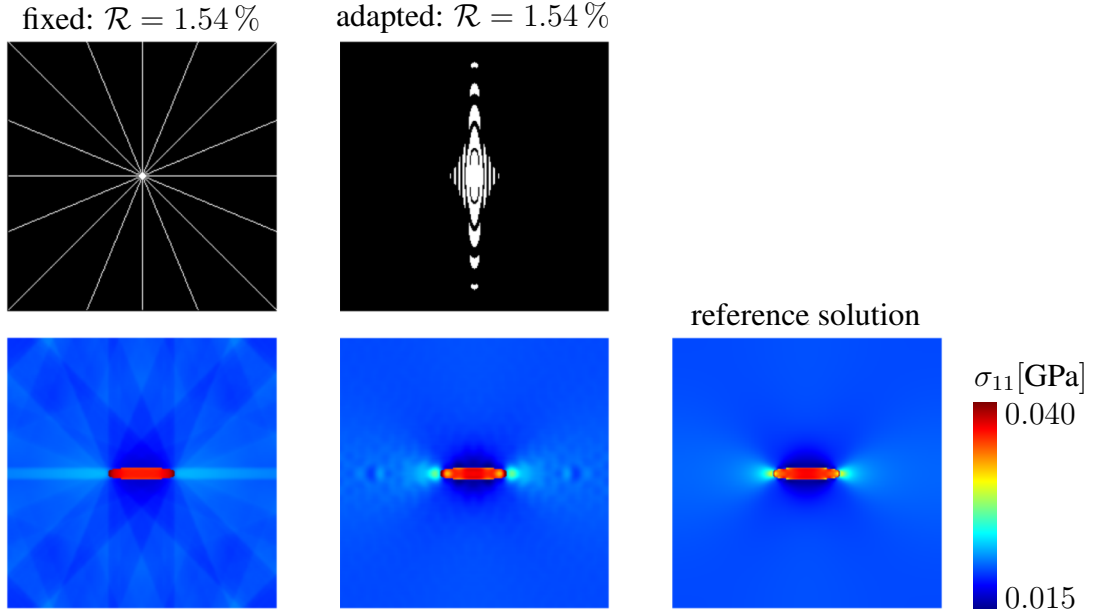


Figure 5.13: Microstructural fields for the 2D elastic microstructure with one elliptical inclusion. *Top row*: Fixed and adapted sampling pattern with the same number of wave vectors. *Bottom row*: Corresponding microstructural stress field σ_{11} and reference stress field computed with the full set of frequencies.

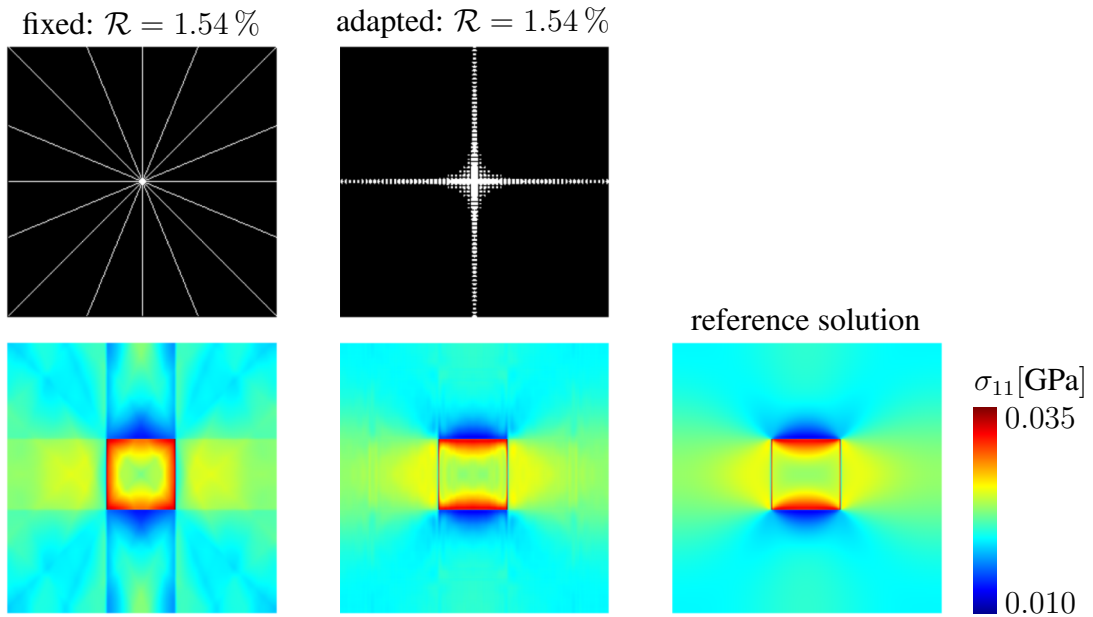


Figure 5.14: Microstructural fields for the 2D elastic microstructure with one quadratic inclusion. *Top row*: Fixed and adapted sampling pattern with the same number of wave vectors. *Bottom row*: Corresponding microstructural stress field σ_{11} and reference stress field computed with the full set of frequencies.

5.6.2 Elastic 2D two phase materials with one inclusion and different phase contrasts

After investigating the effect of different shaped inclusions on the sampling patterns and on the results, the focus is now on the influence of the phase contrast χ

$$\chi = \lambda_I/\lambda_M = \mu_I/\mu_M \quad (5.12)$$

on the solution behavior. Therefore, the microstructure with one circular inclusion (Figure 5.6, *left*) is considered with a phase contrast of $\chi = 2, 5, 10, 20, 50, 100$. Figure 5.15 shows the microscopic and macroscopic error for the fixed and adapted sampling pattern depending on the phase contrast. It can be seen, that these errors are barely influenced by different phase contrasts, while the error even decreases slightly for a higher phase contrast.

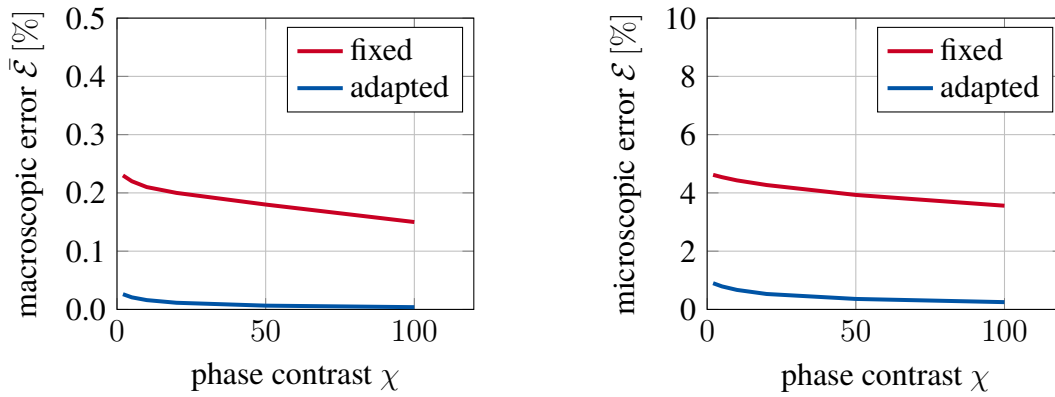


Figure 5.15: Macroscopic error $\bar{\mathcal{E}}$ (*left*) and microscopic error $\mathcal{E}$ (*right*) for the 2D elastic microstructure with one circular inclusion depending on the phase contrast χ for the solution with the fixed and adapted sampling pattern.

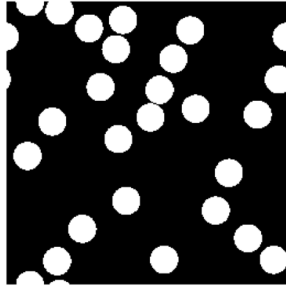
Table 5.3 shows the total CPU times for the fixed and adapted reduced simulation and the reference simulation, computed with the full set of frequencies. As expected, the CPU times increase with increasing phase contrast χ . Nevertheless, this behavior is similar for all three methods, so that the speed-up factor remains almost constant for the different phase contrasts. As shown by Figure 5.15 and Table 5.3, the accuracy and efficiency of the solution method is almost independent of χ . This is related to the fact, that the jump in the material constants is captured in a similar manner as the jump within the step function which is defined to capture the geometry (Equation 5.11). Therefore, always the same frequencies are needed just with different amplitudes, if the phase contrast changes.

	total CPU time [s] - depending on phase contrast χ					
	2	5	10	20	50	100
fixed	0.448	0.912	1.662	3.068	7.248	13.752
adapted	0.388	0.840	1.541	2.893	6.670	12.972
reference	3.196	8.625	16.356	31.411	75.708	144.809

Table 5.3: Total CPU time for the 2D elastic microstructure with one circular inclusion depending on the phase contrast χ for the solution with the fixed and adapted sampling pattern.

5.6.3 Elastic and elasto-plastic 2D two phase material with several inclusions

In the following, a composite with several circular inclusions is investigated. The elastic constants are the same as in the example before: $\lambda_I = 2.0$ GPa and $\mu_I = 2.0$ GPa for the inclusion and $\lambda_M = 1.0$ GPa and $\mu_M = 1.0$ GPa for the matrix material, respectively. Besides the elastic solution, also a simulation with an elasto-plastic matrix material behavior is performed. Considering an elasto-plastic material behavior of the matrix, the additional material parameters are set to $H_M = 0.01$ GPa as hardening modulus and $\sigma_{yM}^0 = 0.01$ GPa as initial yield stress. The investigated microstructure and the prescribed macroscopic strain is presented in Figure 5.16.



$$\bar{\epsilon} = \begin{pmatrix} 0.01 & 0.002 \\ 0.002 & -0.01 \end{pmatrix}$$

Figure 5.16: Composite with several circular inclusions and prescribed macroscopic strain.

For the fixed and the adapted sampling pattern the same amount of frequencies is used. Figure 5.17 shows the microstructural stress fields σ_{11} as well as the differences $\Delta\sigma_{11}$ to the reference solution for the pure elastic case. As already seen for one inclusion, the error in the solution based on the adapted reduced set of frequencies is significantly lower compared to the solution of the fixed sampling pattern. Regarding the solution with the adapted set of frequencies, the highest differences occur again in the transition from matrix to inclusion. Instead, for the fixed sampling pattern, the highest errors occur within the inclusions.

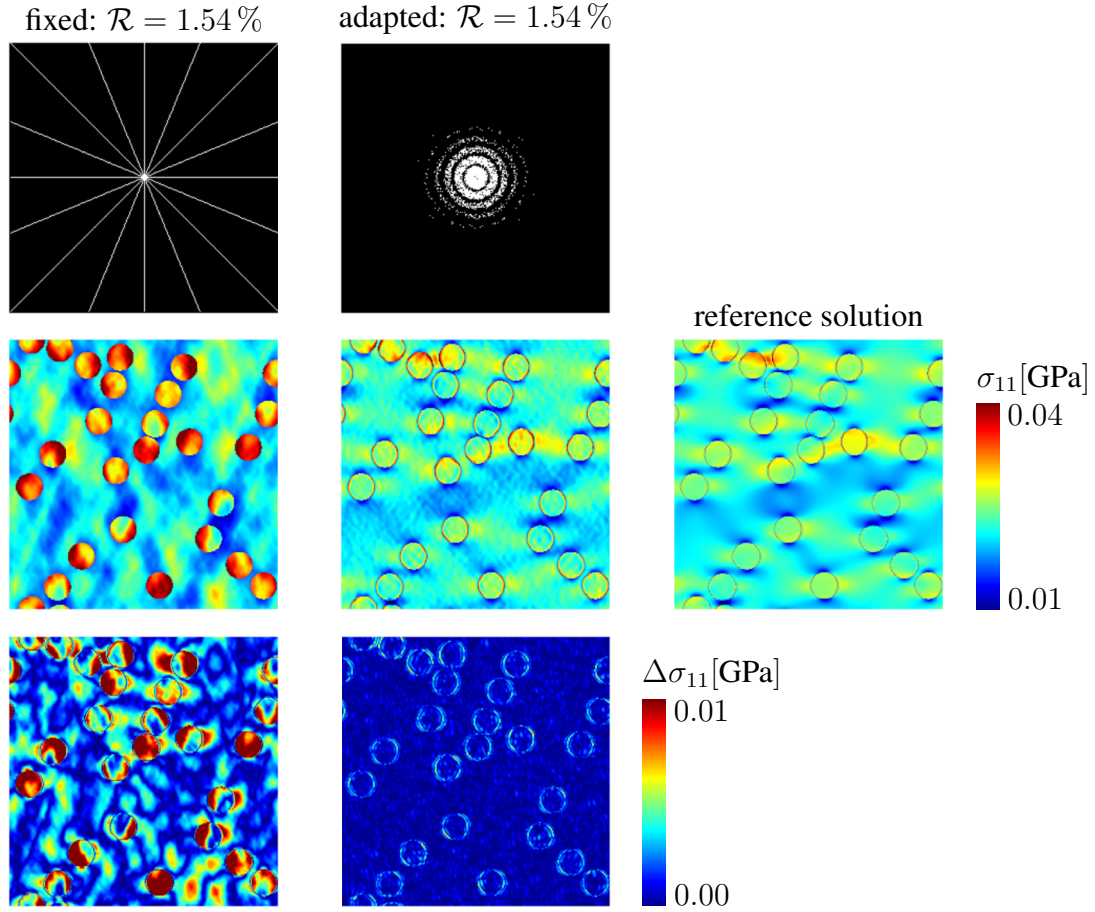


Figure 5.17: Microstructural fields for the 2D elastic microstructure with several circular inclusions. *Top row*: Fixed and adapted sampling pattern with the same number of wave vectors. *Middle row*: Corresponding microstructural stress field σ_{11} and reference stress field computed with the full set of frequencies. *Bottom row*: Absolute difference in the microstructural stress field $\Delta\sigma_{11}$.

Again, we perform the reconstruction and the compatibility step for the solution based on the fixed sampling pattern and only the compatibility step for the adapted sampling pattern. The corresponding microstructural fields are shown in Figure 5.18. Here, similar effects as described in Chapter 5.6.1 for a microstructure with only one inclusion occur: The solution with the adapted sampling pattern is more accurate.

Since the solution behavior of the elastic microstructures with one or several inclusions is similar, we do not present further results on that and focus in the following on the microstructure with elasto-plastic material behavior.

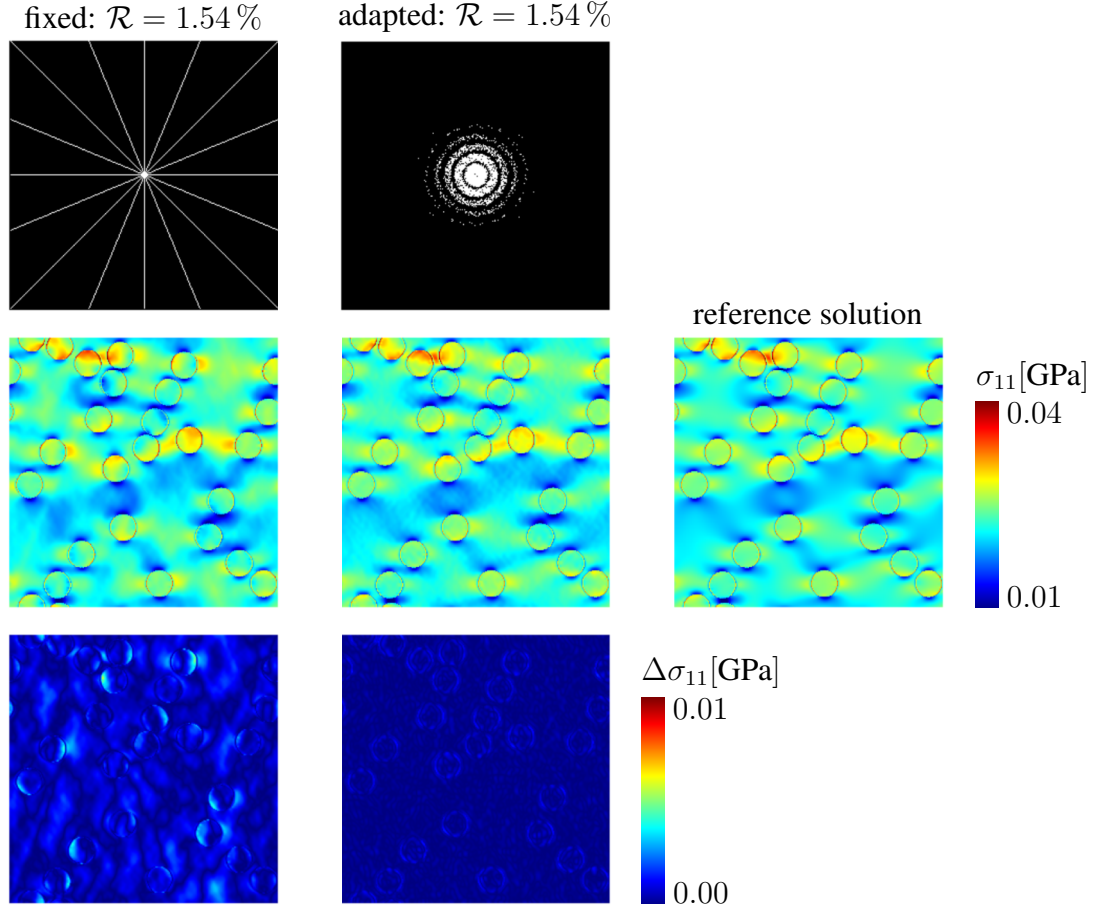


Figure 5.18: Microstructural fields for the 2D elastic microstructure with several circular inclusions. *Top row:* Fixed and adapted sampling pattern with the same number of wave vectors. *Middle row:* Corresponding microstructural stress field σ_{11} incorporating the reconstruction and compatibility step for the solution of the fixed sampling pattern and only the compatibility step for the solution of the adapted sampling pattern and reference stress field computed with the full set of frequencies. *Bottom row:* Absolute difference in the microstructural stress field $\Delta\sigma_{11}$.

The generation of a geometrically adapted sampling pattern does not depend on the material behavior itself, but only on the geometrical representation of the matrix and inclusions. Due to that, the geometrically adapted sampling pattern for the microstructure with several elastic inclusions and an elasto-plastic matrix material behavior is the same as for the microstructure with several inclusions and an overall elastic material behavior. Figure 5.19 shows the microscopic stress field σ_{11} corresponding to the fixed and adapted sampling pattern, the reference solution and the absolute difference in the reduced solution compared to the reference solution $\Delta\sigma_{11}$. It can be seen, that the stress difference for the fixed and the adapted sampling pattern

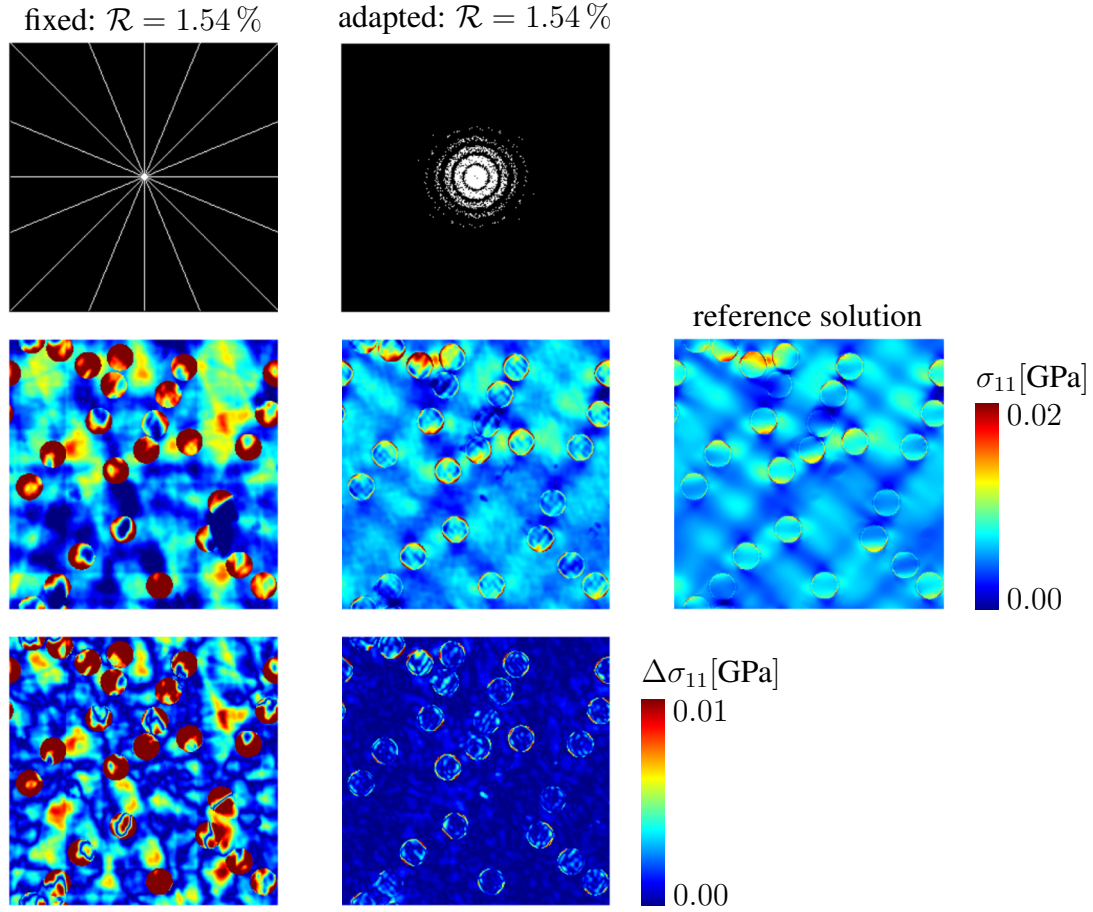


Figure 5.19: Microstructural fields for the 2D elasto-plastic microstructure with several circular inclusions. *Top row*: Fixed and adapted sampling pattern with the same number of wave vectors. *Middle row*: Corresponding microstructural stress field σ_{11} and reference stress field computed with the full set of frequencies. *Bottom row*: Absolute difference in the microstructural stress field $\Delta\sigma_{11}$.

is in general higher considering the nonlinear matrix material behavior instead of the purely linear material behavior shown in Figure 5.17. Nevertheless, the error in the solution with the adapted sampling pattern is again significantly lower than the error in the solution with the fixed sampling pattern. In addition, the error considering the adapted sampling pattern is still related to the transition from inclusion to matrix material, while the error for the fixed sampling pattern is again particularly high within the inclusions.

Figure 5.20 shows the macroscopic error $\bar{\mathcal{E}}$ (*left*) and the microscopic error $\mathcal{E}$ (*right*) again based on the reduced set of frequencies $\mathcal{R}$ for the solution with the fixed and adapted sampling pattern for the elasto-plastic composite. Incorporating $\mathcal{R} = 1.54\%$ and considering the fixed sampling pattern, these errors read $\bar{\mathcal{E}} \approx 34\%$ and $\mathcal{E} \approx 79\%$. Using the same amount of

frequencies and the adapted sampling pattern, the errors reduce to $\bar{\mathcal{E}} \approx 2\%$ and $\mathcal{E} \approx 14\%$, respectively. In addition, Figure 5.20 shows that at some point ($\mathcal{R} \approx 15\%$) the fixed sampling pattern leads to better results than the adapted sampling pattern. This might be related to the elasto-plastic material behavior of the matrix which results in a material behavior which is not that uniform within the matrix as the pure elastic material behavior. The adapted sampling pattern is only related to the geometrical representation of the matrix material and does not represent the different elasto-plastic material states. Due to that, the fixed sampling pattern, which is not bounded to the geometry, may lead to better results for a high amount of frequencies. Besides that, in the range of interest with a highly reduced set of frequencies, the adapted sampling pattern is performing significantly better than the fixed sampling pattern.

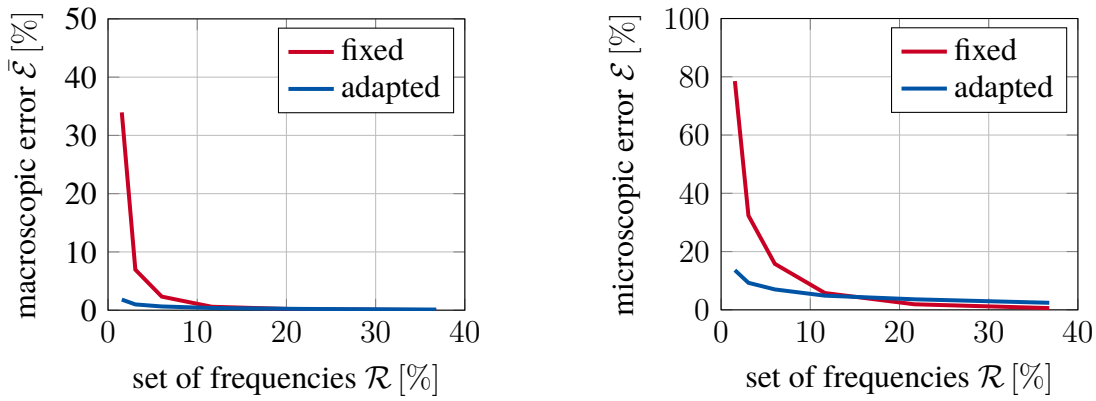


Figure 5.20: Macroscopic error $\bar{\mathcal{E}}$ (left) and microscopic error $\mathcal{E}$ (right) for the 2D elasto-plastic microstructure with several circular inclusions depending on the percentage of used frequencies $\mathcal{R}$ for the solution with the fixed and adapted sampling pattern.

In Figure 5.21 the accumulated plastic strain field ε_p^{acc} for $\mathcal{R} = 1.54\%$ of frequencies is shown. Also here, significant differences of the solution with the fixed sampling pattern compared to the reference solution are observed. For example, the accumulated plastic strain in the upper middle has a value of $\varepsilon_p^{acc} \approx 0.3$ in the reference solution, while the accumulated plastic strain in the reduced solution has a value of $\varepsilon_p^{acc} \approx 0$ at the same position. In contrast to that, the solution based on the adapted sampling pattern and the same amount of frequencies is quite similar to the reference solution.

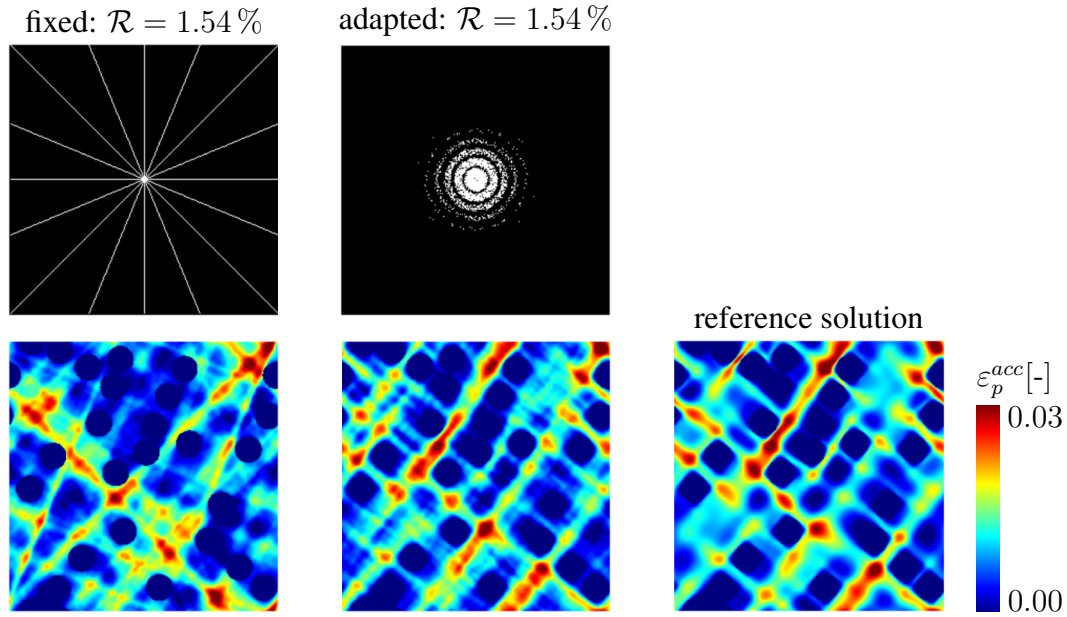


Figure 5.21: Microstructural fields for the 2D elasto-plastic microstructure with several circular inclusions. *Top row*: Fixed and adapted sampling pattern with the same number of wave vectors. *Bottom row*: Corresponding microstructural accumulated plastic strain field ε_p^{acc} and reference accumulated plastic strain field computed with the full set of frequencies.

Incorporating the reconstruction and compatibility step for the solution of the fixed sampling pattern and only the compatibility step for the solution of the adapted sampling pattern leads to the results given in Figures 5.22 and 5.23. Figure 5.22 shows the microstructural stress field σ_{11} and Figure 5.23 shows the accumulated plastic strain field ε_p^{acc} , respectively. Considering the fixed sampling pattern, it can be seen, that the calculated stress within the inclusions is improved by the reconstruction and the compatibility step, while the stress within the elasto-plastic matrix is not improved significantly. This is related to the accumulated plastic strain field, shown in Figure 5.23, which is also not improved by these post-processing steps. As shown in Figure 5.22, the microstructural stress field related to the solution with the adapted sampling pattern is slightly improved by solving the Lippmann-Schwinger equation once with the full set of frequencies.

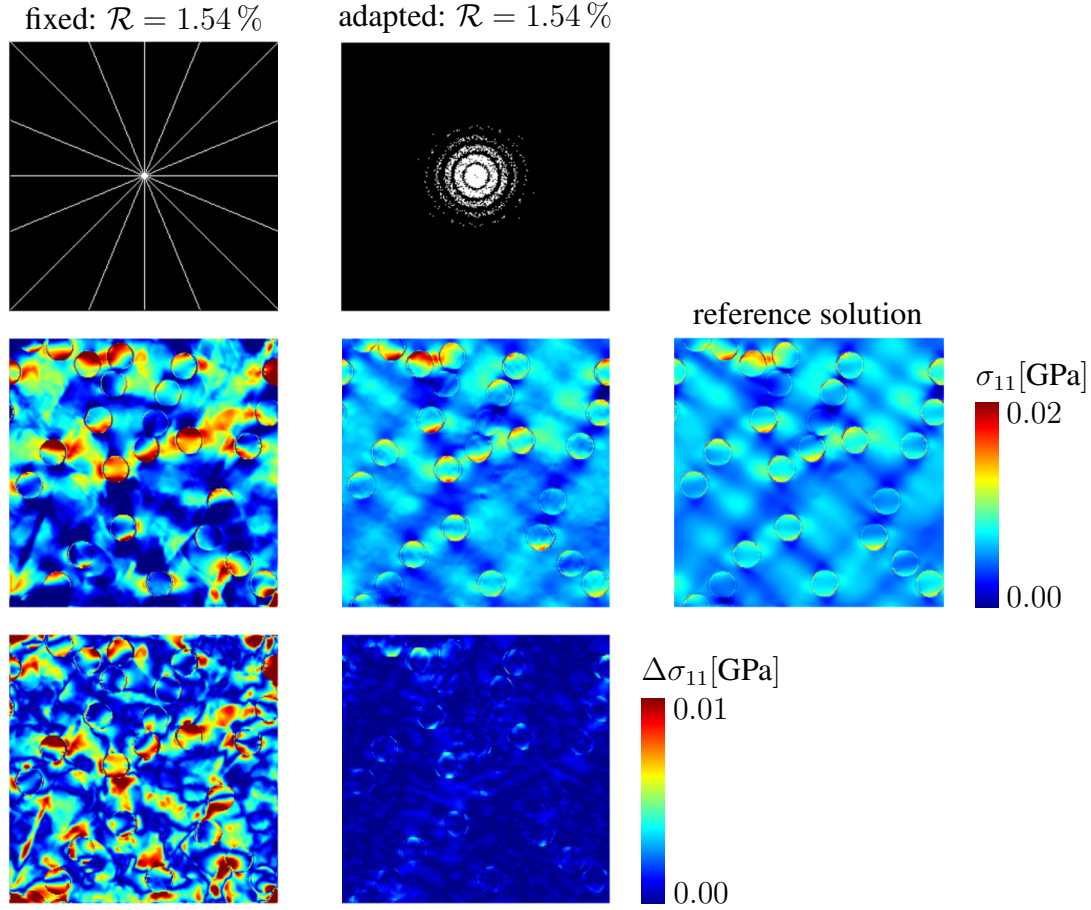


Figure 5.22: Microstructural fields for the 2D elasto-plastic microstructure with several circular inclusions. *Top row*: Fixed and adapted sampling pattern with the same number of wave vectors. *Middle row*: Corresponding microstructural stress field σ_{11} incorporating the reconstruction and compatibility step for the solution of the fixed sampling pattern and only the compatibility step for the solution of the adapted sampling pattern and reference stress field computed with the full set of frequencies. *Bottom row*: Absolute difference in the microstructural stress field $\Delta\sigma_{11}$.

The CPU times for both sampling patterns and the different amount of frequencies are given in Tables 5.4 and 5.5. The behavior of the CPU times is similar compared to the elastic case shown in Tables 5.1 and 5.2, while a speed-up factor of 5 - 6 is gained by considering a set of $\mathcal{R} = 1.54\%$ of frequencies in the nonlinear case.

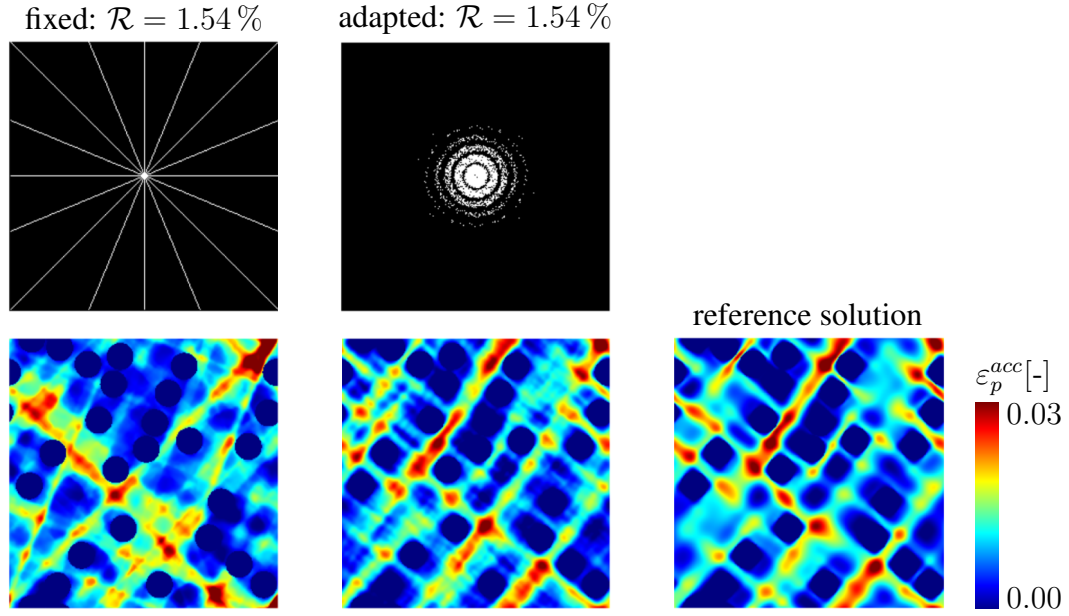


Figure 5.23: Microstructural fields for the 2D elasto-plastic microstructure with several circular inclusions. *Top row*: Fixed and adapted sampling pattern with the same number of wave vectors. *Bottom row*: Corresponding microstructural accumulated plastic strain field ε_p^{acc} incorporating the reconstruction and compatibility step for the solution of the fixed sampling pattern and only the compatibility step for the solution of the adapted sampling pattern and reference accumulated plastic strain field computed with the full set of frequencies.

elasto-plastic	CPU time [s] - fixed sampling pattern				
$\mathcal{R}$ [%]	total	$-\hat{\mathbb{T}}^{(0)} \hat{\boldsymbol{\tau}}(\boldsymbol{\varepsilon})$ (mean) $t = 100$	$\boldsymbol{\sigma}(\boldsymbol{\varepsilon})$ (mean) $t = 100$	reconstruction	compatibility
1.54	316.7	0.009	0.022	91.134	0.334
3.06	446.9	0.015	0.028	105.043	0.442
6.02	555.9	0.027	0.025	76.939	0.327
11.64	797.9	0.050	0.027	73.645	0.340
21.66	1139.4	0.087	0.024	65.870	0.339
36.79	1645.2	0.146	0.024	60.556	0.321
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
unreduced	1866.5	0.241	0.024	-	-

Table 5.4: Total CPU time with mean CPU time per iteration step for solving the convolution integral and the constitutive law and CPU times for the reconstruction and the compatibility step of the simulation with the fixed sampling pattern for the 2D elasto-plastic microstructure with several circular inclusions.

elasto-plastic	CPU time [s] - adapted sampling pattern				
$\mathcal{R}$ [%]	total	$-\hat{\mathbb{I}}^{(0)} \hat{\tau}(\varepsilon)$ (mean) $t = 100$	$\sigma(\varepsilon)$ (mean) $t = 100$	reconstruction	compatibility
1.54	366.7	0.008	0.025	-	0.323
3.06	431.0	0.015	0.020	-	0.342
6.02	533.8	0.026	0.021	-	0.334
11.64	744.4	0.050	0.023	-	0.338
21.66	1081.5	0.087	0.020	-	0.324
36.79	1637.3	0.149	0.023	-	0.342
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
unreduced	1866.5	0.241	0.024	-	-

Table 5.5: Total CPU time with mean CPU time per iteration step for solving the convolution integral and the constitutive law and CPU times for the reconstruction and the compatibility step of the simulation with the adapted sampling pattern for the 2D elasto-plastic microstructure with several circular inclusions.

5.6.4 Elastic 3D two phase material with one inclusion

Finally, a 3D microstructure with one centered spherical inclusion, as shown in Figure 5.24, is investigated. The inclusions and the matrix material are considered to be elastic again with $\lambda_I = 2.0$ GPa and $\mu_I = 2.0$ GPa for the inclusion and $\lambda_M = 1.0$ GPa and $\mu_M = 1.0$ GPa considering the matrix material, respectively. The applied macroscopic strain is set to $\bar{\varepsilon}_{11} = 0.01$.

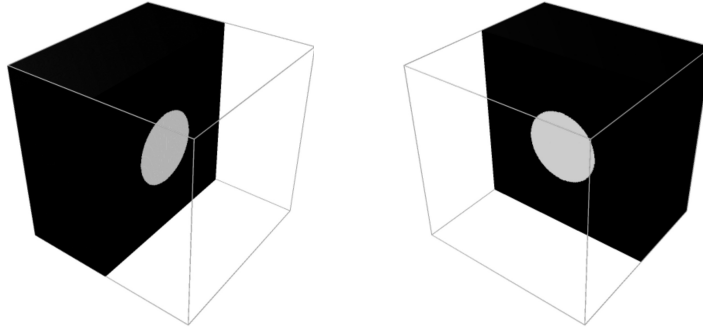


Figure 5.24: Two different intersections of the 3D microstructure with one spherical inclusion.

To generate the geometrically adapted sampling pattern in the 3D case, the same strategy as in the 2D case is used: First, the geometry is represented by a 3D step function. This

function is transferred into Fourier space. The set of frequencies with the highest amplitudes for the representation of the step function in Fourier space is used for the reduced simulation. The resulting adapted sampling pattern for $\mathcal{R} = 1.54\%$ of frequencies and the corresponding microstructural results are given in Figure 5.25. Since the 3D case with a spherical inclusion corresponds to the 2D case with a circular inclusion, the resulting sampling patterns are similar, see Figure 5.8. Also the behavior of the microstructural fields is similar to the 2D case described in Chapter 5.6.1. Using only $\mathcal{R} = 1.54\%$ of the frequencies, the micromechanical stress fields of the reduced simulation already match the reference solution very well. The highest errors are again within the transition from matrix to inclusion.

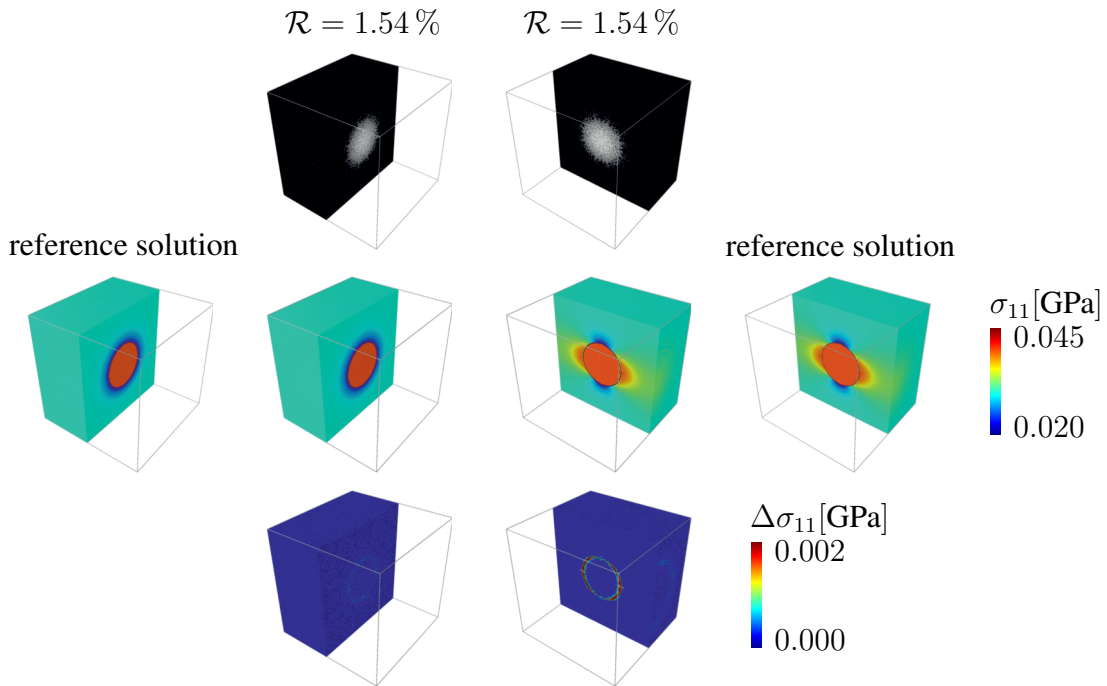


Figure 5.25: Microstructural fields of two different intersections for the 3D elastic microstructure with one circular inclusion. *Top row*: Adapted sampling pattern. *Middle row*: Corresponding microstructural stress field σ_{11} and reference stress field computed with the full set of frequencies. *Bottom row*: Absolute difference in the microstructural stress field $\Delta\sigma_{11}$.

The macroscopic error $\bar{\mathcal{E}}$ and the microscopic error $\mathcal{E}$ depending on the reduced set of frequencies $\mathcal{R}$ for the 3D case are plotted in Figure 5.26.

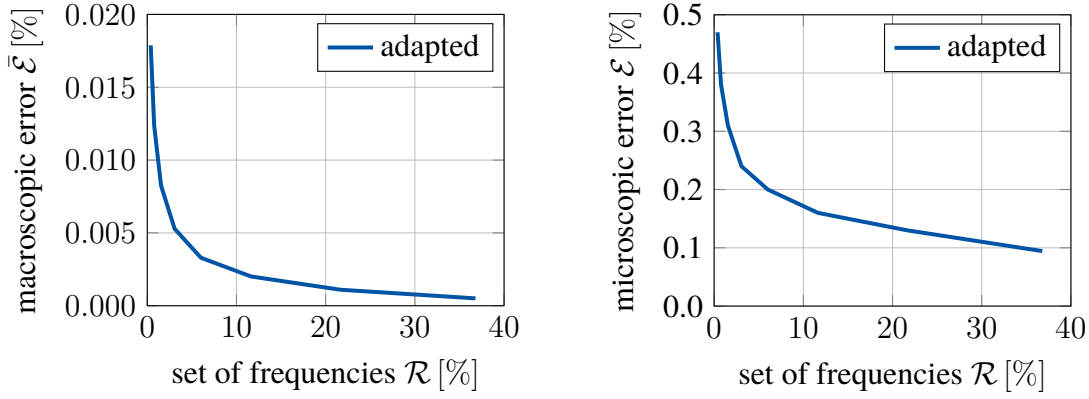


Figure 5.26: Macroscopic error $\bar{\mathcal{E}}$ (*left*) and microscopic error $\mathcal{E}$ (*right*) for the 3D elastic microstructure with one circular inclusion depending on the percentage of used frequencies $\mathcal{R}$ for the solution with the adapted sampling pattern.

Using the compatibility step, the microstructural stress field σ_{11} is again improved as shown in Figure 5.27.

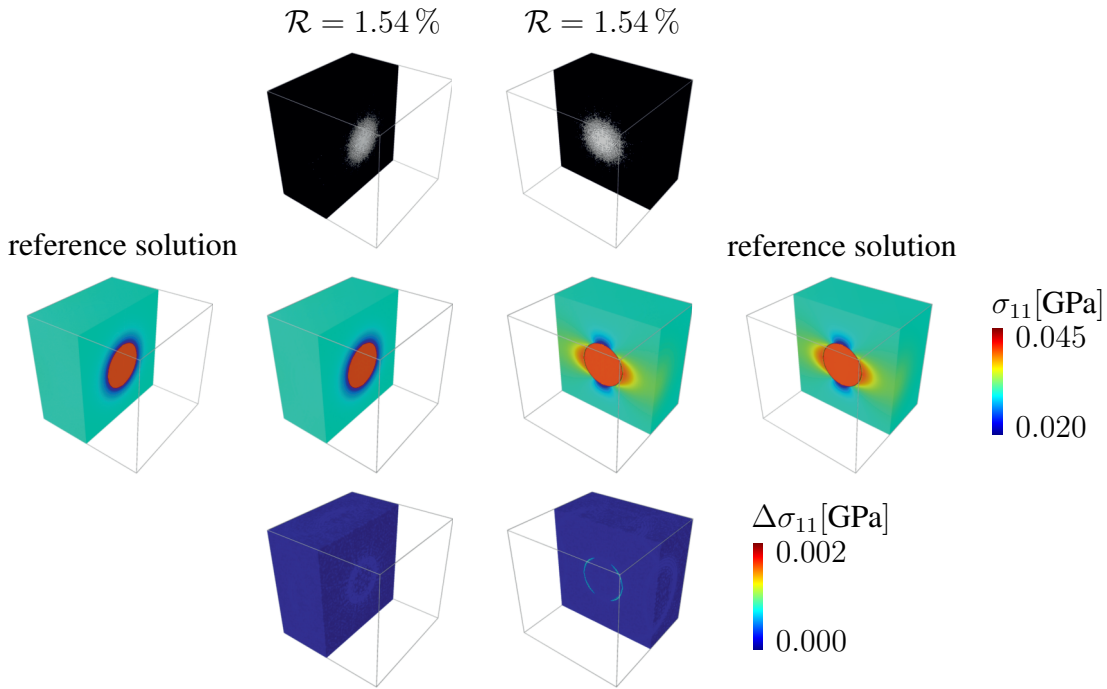


Figure 5.27: Microstructural fields of two different intersections for the 3D elastic microstructure with one circular inclusion. *Top row*: Adapted sampling pattern. *Middle row*: Corresponding microstructural stress field σ_{11} incorporating the compatibility step and reference stress field computed with the full set of frequencies. *Bottom row*: Absolute difference in the microstructural stress field $\Delta\sigma_{11}$.

Table 5.6 shows the CPU times for the reduced and reference solution in the 3D case. It can be seen, that a significant speed up factor of up to approximately 100 is gained by using the geometrically adapted reduced set of frequencies with $\mathcal{R} = 1.54\%$ of frequencies. This speed up is again only gained by solving the convolution integral in Fourier space with the reduced set of frequencies.

3D composite	CPU time [s] - adapted sampling pattern				
$\mathcal{R} [\%]$	total	$-\hat{\mathbb{I}}^{(0)} \hat{\tau}(\epsilon)$ (mean)	$\sigma(\epsilon)$ (mean)	reconstruction	compatibility
0.39	301.46	2.21	13.998	-	279.1
0.78	284.79	3.32	13.960	-	284.9
1.54	305.54	5.36	13.981	-	298.7
3.06	351.76	9.59	14.411	-	277.2
6.02	426.57	17.66	13.826	-	278.7
11.64	584.64	32.94	14.368	-	278.1
21.66	853.26	60.02	14.149	-	281.3
36.79	1260.20	100.94	13.920	-	279.8
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
unreduced	28188.0	2795.6	12.241	-	-

Table 5.6: Total CPU time with mean CPU time per iteration step for solving the convolution integral and the constitutive law and CPU times for the reconstruction and the compatibility step of the simulation with the adapted sampling pattern for the 3D elastic microstructure with one circular inclusion.

5.7 Conclusion and outlook

We presented a novel approach to identify a sampling pattern for a reduced set of frequencies which is used for the FFT-based microstructure simulation. The approach is based on transferring the microstructural phase distribution represented by a step function into Fourier space and identifying the corresponding frequencies with the highest amplitudes. A given percentage of these frequencies with the highest amplitudes is subsequently used to determine the reduced set of frequencies. As shown for several two and three dimensional examples, such an adapted sampling pattern leads to significant better microstructural and overall results compared to the earlier introduced fixed sampling pattern. Considering only a few frequencies in the reduced wave vector, the error compared to the reference solution is so small, that a reconstruction is not necessary anymore. Therefore, the solution algorithm is in addition much easier, especially

in the 3D case. Using the proposed solution strategy, a speed up factor of 5-8 in the 2D case and up to approximately 100 in the 3D case is obtained.

The proposed solution strategy is most accurate for the geometrically linear case. Nevertheless, it also improves the accuracy of the solution if a non-linear material behavior is considered, compared to the earlier proposed fixed sampling pattern. To further improve the accuracy of the model order reduction technique for nonlinear constitutive relations, a strain-based sampling pattern, as proposed by [38] may be used. In that case, the sampling pattern is adapted to the present strain field after each load step. In addition, the proposed solution strategy only reduces the computational effort of solving the convolution in Fourier space, so that the next step is the combination of the proposed MOR technique with e.g. a clustering analysis, since the most time consuming part for the simulation of a complex material behavior is the evaluation of the material law. Using such a microstructural clustering analysis the stress evaluation in each grid point is reduced to a stress evaluation in a defined number of clusters instead. Based on previous works [186, 187, 357] an additional significant speed-up is expected by combining both methods.

6 | Article 5:

FFT-based simulation using a reduced set of frequencies adapted to the underlying microstructure

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Disclosure of the individual authors’ contributions to the article:

C. Gierden reviewed the relevant existing literature and developed the idea of defining a strain-based sampling pattern. He implemented the framework, performed the simulations, interpreted the results and wrote the article. J. Waimann, B. Svendsen and S. Reese gave conceptual advice, contributed to the discussion of the results, proofread the article and made valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

6.1 Abstract

Instead of the classical finite element (FE) based microstructure simulation, a Fast Fourier transform (FFT) based microstructure simulation, introduced by Moulinec and Suquet [11, 12], also enables the computation of highly resolved microstructural fields. In this context, the microscopic boundary value problem is captured by the Lippmann-Schwinger equation and solved by using Fast Fourier transforms (FFT) and fixed-point iterations. To decrease the computational effort of the fixed-point solver, Kochmann et al. [17] introduced a model order reduction (MOR) technique based on solving the Lippmann-Schwinger equation in Fourier space with a reduced set of frequencies. Thereby, the accuracy of this MOR technique depends on the number of used frequencies and the choice of frequencies that are considered within the simulation. Instead of the earlier proposed fixed [17] or geometrically adapted [237] sampling patterns, we propose a sampling pattern which is updated after each load step based on the current strain. To show the precision of such a strain-based sampling pattern, an elasto-plastic two-phase composite microstructure is investigated.

6.2 Introduction

The classical numerical two-scale simulation approach considering a spatially resolved microstructure is the FE^2 method [113]. Within this simulation approach, the FE method is used to solve the macroscopic as well as the microscopic boundary value problem. Replacing the FE simulation on the microscale by a FFT-based simulation leads to the FE-FFT-based method [13, 18]. Under periodic boundary conditions, the FFT-based simulation approach has proven to be more efficient than the FE-based simulation [11, 12]. Thus, the FE-FFT-based method is a powerful alternative to the classical FE^2 method. Nevertheless, the high fidelity two-scale simulation of complex macroscopic boundary value problems is computationally very demanding for both methods.

To generate an efficient two-scale FE-FFT-based simulation approach for computing the overall material response, the microstructure might be coarsely discretized. Since this coarse discretization consequently only leads to inaccurate microstructural results, a subsequent post-processing step can be used to generate high fidelity microstructural fields. Therefore, the macroscopic strain/deformation gradient of any macroscopic point of interest is saved during the entire simulation and applied to a fine discretized microstructure in the post-processing step [16, 319]. Other recently developed MOR techniques deal with a more precise approximation of the microstructure during the entire FFT-based simulation. These methods are, for

example, based on a proper orthogonal decomposition [234], low-rank approximations [236] or a reduced set of frequencies [17].

The present paper concerns the MOR technique using a reduced set of frequencies. The accuracy of the applied MOR depends on the number and on the choice of considered frequencies. Therefore, Gierden et al. [237] presented a geometrically adapted sampling pattern to increase the precision of the initially introduced fixed, radial sampling pattern [17]. To generate even more precise results in terms of nonlinear material behavior, we introduce the utilization of a strain-based sampling pattern. Based on the microstructural strain, this sampling pattern is redefined after each load step.

After briefly reviewing the FFT-based method in Section 6.3, the MOR technique based on a reduced set of frequencies is summed up in Section 6.4. Thereafter, the focus of this section lies on the definition of the strain-based sampling pattern. Section 6.5 shows the numerical results using this sampling pattern and compares the results to the earlier introduced sampling patterns. The paper ends with a conclusion and an outlook in Section 6.6.

6.3 FFT-based microstructure simulation

Considering an inhomogeneous periodic microstructure Ω , the microscopic boundary value problem (BVP) considering small strain kinematics yields:

$$\begin{aligned} \operatorname{div} \boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}) &= \mathbf{0} & \forall \boldsymbol{x} \in \Omega \\ \boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}) &= \boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}, \boldsymbol{\varepsilon}(\bar{\boldsymbol{x}}, \boldsymbol{x}), \boldsymbol{\alpha}(\boldsymbol{x})) \\ \boldsymbol{\varepsilon}(\bar{\boldsymbol{x}}, \boldsymbol{x}) &= \bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}}) + \tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x}) \end{aligned} \quad (6.1)$$

Herein, the total microscopic strain $\boldsymbol{\varepsilon}(\bar{\boldsymbol{x}}, \boldsymbol{x})$ is additively split into a macroscopic part $\bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}})$ at the macroscopic position $\bar{\boldsymbol{x}}$ and a microscopically influenced part $\tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x})$ at the microscopic position $\boldsymbol{x}$. The total stress $\boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x})$ depends on the resulting total strain and some internal variables $\boldsymbol{\alpha}(\boldsymbol{x})$. In regard to comprehensibility, in the following, the dependence of all variables besides the macroscopic strains on the macroscopic position $\bar{\boldsymbol{x}}$ is not shown.

To capture an isotropic elasto-plastic material behavior, the total strain $\boldsymbol{\varepsilon}(\boldsymbol{x}) = \boldsymbol{\varepsilon}_e(\boldsymbol{x}) + \boldsymbol{\varepsilon}_p(\boldsymbol{x})$ is additively split into an elastic part $\boldsymbol{\varepsilon}_e(\boldsymbol{x})$ and a plastic part $\boldsymbol{\varepsilon}_p(\boldsymbol{x})$. The linear-elastic stress-strain relation reads $\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbb{C}(\boldsymbol{x}) : \boldsymbol{\varepsilon}_e(\boldsymbol{x})$ with the isotropic stiffness tensor $\mathbb{C}(\boldsymbol{x})$. In terms of the classical von Mises yield condition with isotropic linear hardening, the yield condition

has the form:

$$\Phi(\boldsymbol{\sigma}(\mathbf{x}), \boldsymbol{\varepsilon}_p^{\text{acc}}(\mathbf{x}), \mathbf{x}) = \sigma^{\text{eq}}(\mathbf{x}) - [\sigma_y^0(\mathbf{x}) + H(\mathbf{x}) \boldsymbol{\varepsilon}_p^{\text{acc}}(\mathbf{x})] \quad (6.2)$$

with the initial yield stress $\sigma_y^0(\mathbf{x})$, the von Mises equivalent stress $\sigma^{\text{eq}}(\mathbf{x})$, the hardening modulus $H(\mathbf{x})$ and the accumulated plastic strain $\boldsymbol{\varepsilon}_p^{\text{acc}}(\mathbf{x})$. The associative flow rule reads

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\gamma} \frac{\partial \Phi}{\partial \boldsymbol{\sigma}} \quad (6.3)$$

with the plastic multiplier $\dot{\gamma}$. Additionally, the Karush-Kuhn-Tucker conditions $\Phi \leq 0$, $\dot{\gamma} \geq 0$ and $\Phi \dot{\gamma} = 0$ need to be fulfilled.

Using the FFT-based method to solve the inhomogeneous BVP in Equation 6.1, this BVP is transferred into an equivalent homogeneous representation (Hashin & Shtrikman [131]) by defining a homogeneous reference material behavior $\mathbb{C}^0$ and the polarization stress $\boldsymbol{\tau}(\mathbf{x})$, which represents the inhomogeneities within the microstructural material behavior:

$$\begin{aligned} \text{div } \mathbb{C}^0 : \boldsymbol{\varepsilon}(\mathbf{x}) + \text{div } \boldsymbol{\tau}(\mathbf{x}) &= \mathbf{0} & \forall \mathbf{x} \in \Omega \\ \boldsymbol{\tau}(\mathbf{x}) &:= \boldsymbol{\sigma}(\mathbf{x}, \boldsymbol{\varepsilon}(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x})) - \mathbb{C}^0 : \boldsymbol{\varepsilon}(\mathbf{x}) \\ \boldsymbol{\varepsilon}(\mathbf{x}) &= \bar{\boldsymbol{\varepsilon}}(\bar{\mathbf{x}}) + \tilde{\boldsymbol{\varepsilon}}(\mathbf{x}) \end{aligned} \quad (6.4)$$

Using Green's function $\mathbf{G}^0(\mathbf{x}, \mathbf{x}')$ and thus the Lippmann-Schwinger operator $\Gamma^0(\mathbf{x}, \mathbf{x}')$ to solve the BVP yields the integral equation:

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}}(\bar{\mathbf{x}}) - \int \Gamma^0(\mathbf{x}, \mathbf{x}') : \boldsymbol{\tau}(\mathbf{x}') d\mathbf{x}' \quad (6.5)$$

which is known as the Lippmann-Schwinger equation [119, 337]. Its transfer into Fourier space enables the calculation of the strain in the Fourier space $\hat{\boldsymbol{\varepsilon}}(\boldsymbol{\xi})$, which is then depending on the frequencies:

$$\hat{\boldsymbol{\varepsilon}}(\boldsymbol{\xi}) = \begin{cases} -\hat{\Gamma}^0(\boldsymbol{\xi}) \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) & \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\boldsymbol{\varepsilon}} & \forall \boldsymbol{\xi} = \mathbf{0} \end{cases} \quad (6.6)$$

In Fourier space, Green's function $\hat{G}_{ik}^0(\boldsymbol{\xi})$ and the Lippmann-Schwinger operator $\hat{\Gamma}_{ijkl}^0(\boldsymbol{\xi})$ read:

$$\begin{aligned} \hat{G}_{ik}^0(\boldsymbol{\xi}) &= (C_{ijkl}^0 \xi_j \xi_l)^{-1} \\ \hat{\Gamma}_{ijkl}^0(\boldsymbol{\xi}) &= \frac{1}{4} (\hat{G}_{jk,li}^0(\boldsymbol{\xi}) + \hat{G}_{ik,lj}^0(\boldsymbol{\xi}) + \hat{G}_{jl,ki}^0(\boldsymbol{\xi}) \hat{G}_{il,kj}^0(\boldsymbol{\xi})) \end{aligned} \quad (6.7)$$

with the wave vector ξ gathering all the considered frequencies. To solve Equation 6.4 Moulinec and Suquet [11, 12] proposed an iterative solution procedure based on fixed point iterations computing $\tau(x)$ in real space and solving Equation 6.6 in Fourier space. The best convergence behavior in terms of this basic fixed-point scheme is achieved by defining the reference material behavior C^0 as arithmetic mean of the phase-wise material behavior. To avoid numerical resolution problems in this context, which are related to the Gibbs phenomenon [19], Willot [30] suggested using a first-order finite difference approximation of the differential operator in Equation 6.7.

6.4 Model order reduction technique based on a reduced set of frequencies

To reduce the computational effort of solving the Lippmann-Schwinger equation in Fourier space (Equation 6.6), Kochmann et al. [17] proposed a MOR technique, which only considers a reduced set of frequencies. This method utilizes the fact that Green's operator and the polarization stress in Equation 6.6 are given in terms of a Fourier series. The accuracy of this representation depends on the number of considered frequencies. While the exactness of the approximation decreases with a lower number of considered frequencies, also the computational effort of solving the Lippmann-Schwinger equation in Fourier space is reduced. Accordingly, a reduced set of frequencies should decrease this computational effort, but still lead to a desired quality of the solution.

Besides the dependence on the number of used frequencies, the accuracy of this MOR method also depends on their choice. While Kochmann et al. [17] suggested a fixed, radial sampling pattern, Gierden et al. [237] proposed to use a reduced set of frequencies adapted to the geometry of the microstructure. This new definition of sampling patterns significantly improves the quality of the results. Nevertheless, considering a nonlinear material behavior, the application of the strain-based sampling pattern $\mathcal{S}_\varepsilon$ leads to a further improvement of the calculated solution. In this context, the strain of the previous load step defines the sampling pattern for the next load step, as shown in Figure 6.1.

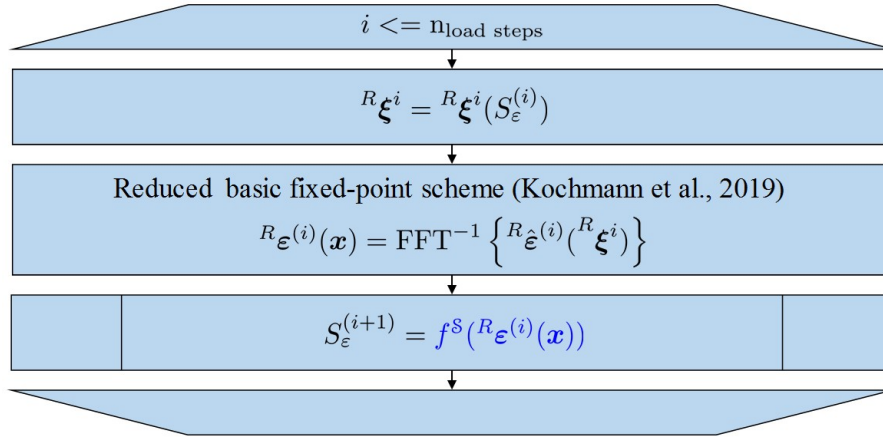


Figure 6.1: Algorithm for adapting the sampling pattern S_ϵ after each load step.

Therefore, the norm of the strain field ϵ is transferred into Fourier space. To achieve a good approximation of this strain using a reduced set of frequencies, the frequencies with the highest amplitudes must be used. Similar to the geometrically adapted sampling pattern by Gierden et al. [237], the sampling pattern is thereby defined as consisting of a prescribed percentage of frequencies with the highest amplitudes needed to capture the norm of the strain. To further improve the accurateness of this method, the strain is first computed once, using the full set of frequencies. Figure 6.2 summarizes this algorithm to define the strain-based sampling pattern.

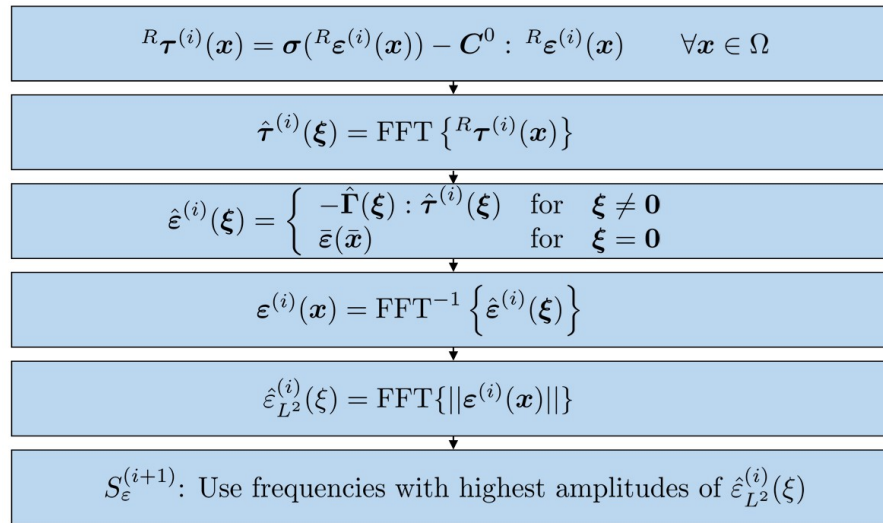
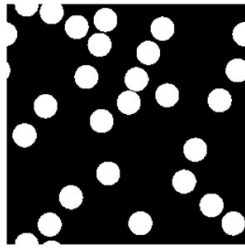


Figure 6.2: Algorithm $f^S(R\epsilon^{(i)}(x))$ to define the strain-based sampling pattern.

As shown in Section 6.5, such a strain-based sampling pattern leads to significantly more accurate results compared to the fixed, radial S_f and geometrically adapted S_g sampling patterns.

6.5 Results and discussion

To compare the results of the simulation with different sampling pattern definitions, we consider a two-phase microstructure with elastic inclusions embedded in an elasto-plastic matrix phase. Figure 6.3 shows the considered microstructure, material parameters, and prescribed macroscopic strain.



material constants

matrix

$$\mu_M = 1.0 \text{ GPa}, \lambda_M = 1.0 \text{ GPa}$$

$$\sigma_{y0,M} = 0.01 \text{ GPa}, H_M = 0.01 \text{ GPa}$$

inclusion

$$\mu_I = 2.0 \text{ GPa}, \lambda_I = 2.0 \text{ GPa}$$

macroscopic strain

$$\bar{\epsilon} = \begin{pmatrix} 0.01 & 0.002 \\ 0.002 & -0.01 \end{pmatrix}$$

Figure 6.3: Two-phase microstructure with several inclusions (white) embedded in a softer matrix material (black), material constants and prescribed macroscopic strain.

The prescribed strain is applied to the microstructure within 100 load steps. Figure 6.4 shows the resulting norm of the strain field and the related strain-based sampling pattern for four load steps. The strain field in the first load step is computed using the full set of frequencies. Considering the sampling patterns, the frequencies are rearranged on a squared grid with the lowest frequencies in the center and the highest frequencies at the edges. The frequencies highlighted in white correspond to the frequencies with the highest amplitudes in Fourier space needed to capture the norm of the strain field and are therefore taken into account within the simulation, while the frequencies highlighted in black are neglected.

The material behavior within the first 20 load steps is elastic. This results in a linear scaling of the present strain field within these load steps (see Figure 6.4, top row). Due to that, the sampling pattern does not change from load step 1 to 20 (see Figure 6.4, bottom row). After exceeding the yield stress within the matrix phase, the sampling pattern changes from step to step according to the elasto-plastic strain. Figure 6.4 shows for example norm of the elasto-plastic strain field and the sampling patterns for load step 30 and 100.

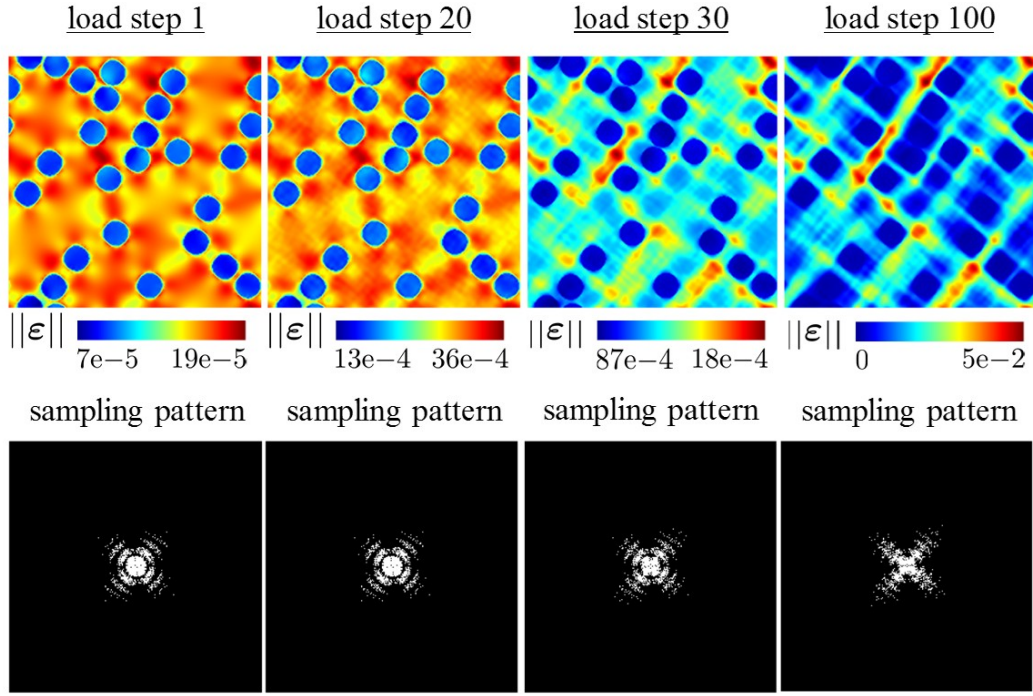


Figure 6.4: Norm of the strain field and sampling patterns with the considered frequencies highlighted in white for load steps 1, 20, 30 and 100.

The resulting stress field σ_{xx} computed with the strain-based sampling pattern $\mathcal{S}_\epsilon$ is presented and compared to the reference solution, computed with the full set of frequencies, in Figure 6.5. The difference $\Delta\sigma_{xx}$ in the resulting stress field is defined as follows:

$$\Delta\sigma_{xx} = |\sigma_{xx}^{\text{ref}} - \sigma_{xx}|$$

In addition, Figure 6.5 shows the results computed with the same number of frequencies but with the geometrically adapted sampling pattern $\mathcal{S}_g$. Considering $\mathcal{R} = 0.8\%$ of frequencies, the difference in the stress field compared to the reference solution is significantly smaller for the solution with the newly defined strain-based sampling pattern compared to the solution with the geometrically adapted sampling pattern. This improvement particularly holds in the transition zone from matrix material to inclusion.

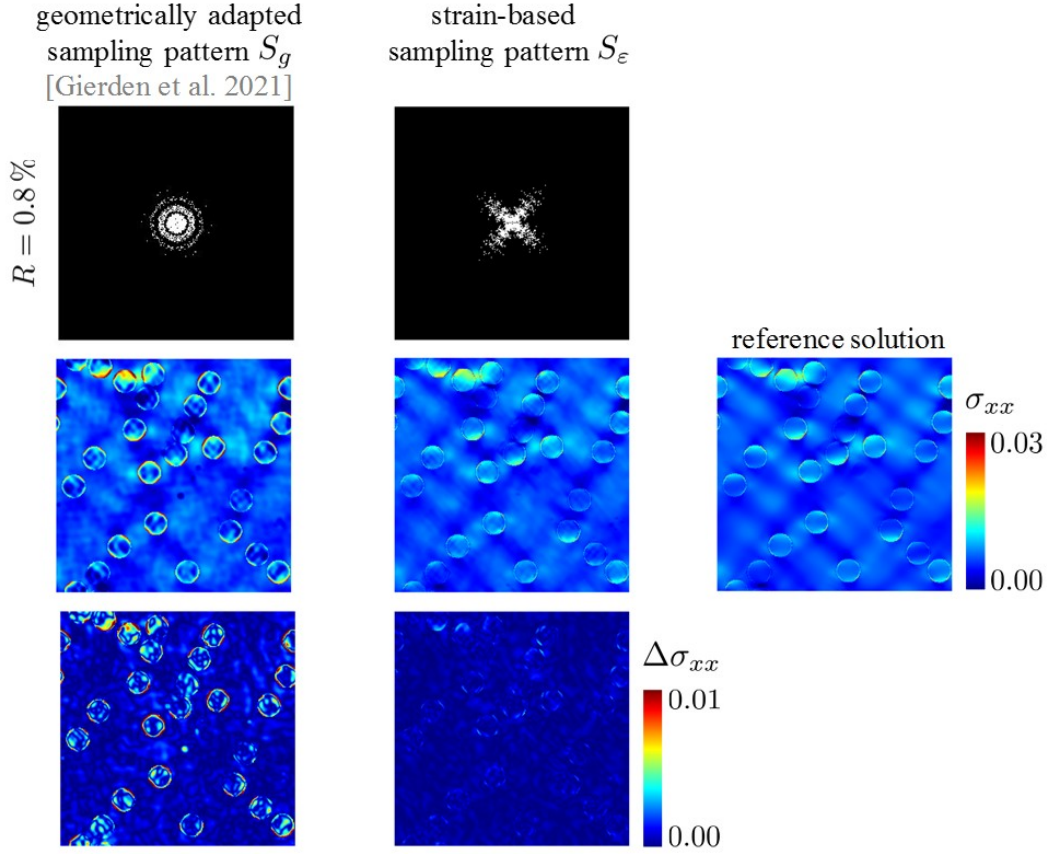


Figure 6.5: Geometrically adapted vs. strain-based sampling pattern of the last load step (*top*), corresponding stress fields and reference solution (*middle*), differences in the stress fields compared to the reference solution (*bottom*).

In addition, Figure 6.6 shows the relative macroscopic ($\bar{E}$) and microscopic error (E):

$$\bar{E} = \frac{\|\bar{\sigma} - \bar{\sigma}^{\text{ref}}\|}{\|\bar{\sigma}^{\text{ref}}\|}$$

$$E = \frac{1}{n} \sum_n \frac{\|\sigma(n) - \sigma^{\text{ref}}(n)\|}{\|\sigma^{\text{ref}}(n)\|}$$

for the fixed, the geometrically adapted, as well as the strain-based sampling pattern. Here, $\bar{\sigma}$ is the overall averaged stress, n is the number of grid points, and the superscript ref refers to the solution computed with the full set of frequencies. These errors are always the lowest for the strain-based sampling pattern. Considering a highly reduced set of frequencies, for example 1.5% of frequencies, the microscopic error for the fixed sampling pattern goes up to 80% , while this error is 14% for the geometrically adapted sampling pattern, but only 4% for the strain-based sampling pattern. Similar results are gained for the macroscopic error. For

the fixed sampling pattern, the error goes up to 34%, for the geometrically adapted sampling pattern the error is reduced to 1.8%, but for the strain-based sampling pattern, the error is even reduced to only 0.2%. The speed-up factor for all these simulations is about 5 compared to the simulation with the full set of frequencies and similar for all three different sampling patterns, see Figure 6.7. Even though the sampling pattern is redefined after each load step for the strain-based sampling pattern, the computational effort is not significantly higher since a better convergence behavior is observed for solving the Lippmann–Schwinger equation within one load step.

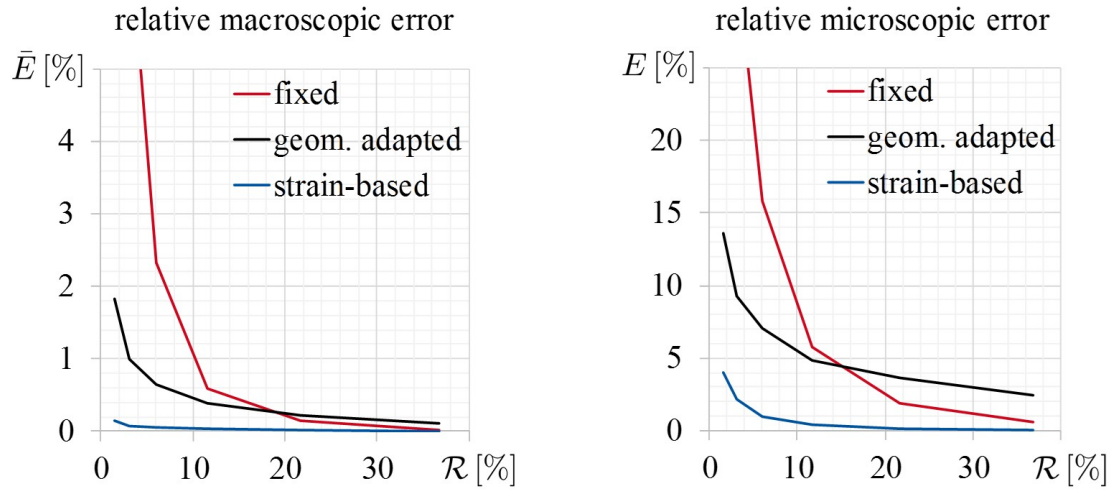


Figure 6.6: Relative macroscopic error $\bar{E}$ and relative microscopic error E for the solution with the fixed, geometrically adapted and strain-based sampling pattern.

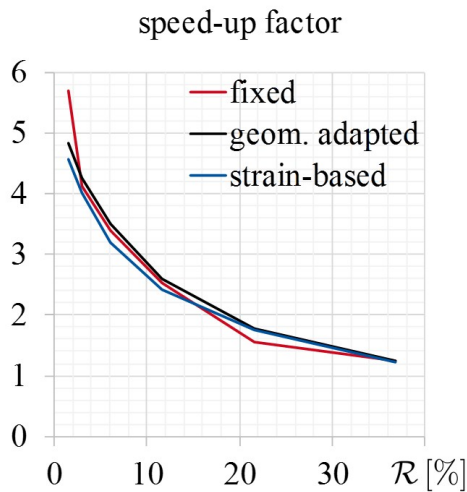


Figure 6.7: Speed-up factor for the simulation with the fixed, geometrically adapted and strain-based sampling pattern.

6.6 Conclusions and outlook

We presented a new approach to defining a strain-based reduced set of frequencies for a reduced FFT-based microstructure simulation. Considering a nonlinear material behavior, this approach utilizes the strain of the last load step to define the sampling pattern for the next load step. Compared to the results with the fixed and geometrically adapted sampling patterns, the new approach leads to more accurate results without increasing the computational effort of the reduced fixed-point scheme.

Since the MOR technique only reduces the computational costs for solving the Lippmann-Schwinger equation in Fourier space, there is no speed-up for the evaluation of the constitutive behavior. To decrease the related computational effort, a coupling of the MOR technique with a clustered microstructure [115, 128, 187] is currently under investigation. In further studies, the basic fixed-point scheme used will additionally be replaced by more efficient solvers, such as a Newton Krylov solver [209, 215], to further improve the computational performance.

7 | **Article 6:**

Using a reduced set of Fourier modes in terms of a FFT-based microstructure simulation

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Disclosure of the individual authors’ contributions to the article:

C. Gierden reviewed the relevant existing literature and developed the idea of defining a strain-based sampling pattern. Furthermore, he implemented the framework, performed the simulations, interpreted the results and wrote the article. J. Waimann, B. Svendsen and S. Reese gave conceptual advice, contributed to the discussion of the results, proofread the article and made valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

7.1 Abstract

Given a heterogeneous material, the mechanical behavior of its microstructure can be investigated by an algorithm that uses the Fourier representation of the Lippmann-Schwinger equation. Incorporating a model order reduction technique based on calculations with a reduced set of Fourier modes, the computational cost of this algorithm can be decreased. It was shown that the accuracy of this model order reduction technique strongly depends on the choice of Fourier modes by considering a geometrically adapted rather than a fixed sampling pattern to define the reduced set of Fourier modes. Since it is difficult to define a geometrically adapted sampling pattern for complex microstructures, additionally a strain-based sampling pattern was introduced. The accuracy and adaptability of this strain-based reduced set of Fourier modes is shown by incorporating a polycrystalline microstructure.

7.2 Introduction

Constitutive equations are usually based on a number of assumptions and even with a large number of material parameters, it is not always possible to fit the developed model to the actual material behavior. In contrast to that, multi-scale methods allow the consideration of physical and topological details of an evolving microstructure and thus an accurate representation of the resulting material behavior. In this context, a method using the finite element (FE) method on the macroscale and the fast Fourier transform (FFT) method on the microscale was introduced in [13] for the simulation of two-phase microstructures, while the FFT-based microstructure simulation was established by Moulinec and Suquet [11, 12]. An extension of the FFT-based microstructure simulation and FE-FFT-based two-scale simulation concerning polycrystalline materials was presented in [202, 350] and [18]. General reviews presenting the state of the art of the FFT-based and FE-FFT-based methods are given in [10, 14] and [15], respectively.

A drawback of such a highly resolved two-scale simulation is the extensive computational effort. Therefore, efficient two-scale solution strategies have been introduced using for example a coarse discretized microstructure for the entire simulation considering small [16] or finite [319] strains, or using a precomputed database in general and the highly resolved microstructure simulation only in macroscopic critical areas [254]. Other model order reduction (MOR) techniques are aiming exclusively at an efficient FFT-based microstructure simulation taking into account a proper orthogonal decomposition (POD) [234], low-rank tensor approximations [236] or a reduced set of Fourier modes [17].

The focus of the present paper lies on the FFT-based microstructure simulation based on a

reduced set of Fourier modes. This MOR technique was first introduced considering a fixed sampling pattern [17]. Since the accuracy of the method strongly depends on the choice of considered Fourier modes, an improvement in accuracy was achieved by using a geometrically adapted [237] or a strain-based [38] sampling pattern. In this work, we show how such a strain-based sampling pattern for the reduced FFT-based microstructure simulation is also suitable to capture the details of a complex microstructure, such as a polycrystal.

The paper is structured as follows: In Section 7.3 a brief review of the microstructural relations considering a polycrystalline microstructure is given. After presenting the approach for the reduced FFT-based microstructure simulation considering a strain-based sampling pattern in Section 7.4, the numerical results are discussed in Section 7.5. The paper ends with a conclusion and outlook in Section 7.6.

7.3 Microstructural boundary value problem

The quasi-static balance of linear momentum in absence of body forces on the microscale and taking into account small strain kinematics for a heterogeneous microstructure Ω yields

$$\operatorname{div} \boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}) = \mathbf{0} \quad \forall \boldsymbol{x} \in \Omega, \quad (7.1)$$

with the stress $\boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}) = \boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}, \boldsymbol{\varepsilon}(\bar{\boldsymbol{x}}, \boldsymbol{x}), \boldsymbol{\gamma}(\boldsymbol{x}))$ depending on the macroscopic and microscopic positions $\bar{\boldsymbol{x}}$ and $\boldsymbol{x}$, the total strain field $\boldsymbol{\varepsilon}(\bar{\boldsymbol{x}}, \boldsymbol{x})$ and internal variables $\boldsymbol{\gamma}(\boldsymbol{x})$. The total strain field $\boldsymbol{\varepsilon}(\bar{\boldsymbol{x}}, \boldsymbol{x}) = \bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}}) + \tilde{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}}, \boldsymbol{x})$ may additively be split into a constant macroscopic part $\bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}})$ and a microscopic fluctuating part $\tilde{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}}, \boldsymbol{x})$, while the macroscopic stress $\bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{x}})$ and strain $\bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}})$ are defined via the volume averages of their local fields:

$$\bar{\boldsymbol{\sigma}}(\bar{\boldsymbol{x}}) := \frac{1}{V} \int_{\Omega} \boldsymbol{\sigma}(\bar{\boldsymbol{x}}, \boldsymbol{x}) \, d\Omega \quad \text{and} \quad \bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}}) := \frac{1}{V} \int_{\Omega} \boldsymbol{\varepsilon}(\bar{\boldsymbol{x}}, \boldsymbol{x}) \, d\Omega. \quad (7.2)$$

Regarding the constitutive relations, a polycrystalline microstructure is taken into account. For the sake of clarity, the dependence of all variables on the macroscopic and microscopic positions $\bar{\boldsymbol{x}}$ and $\boldsymbol{x}$ are not shown in what follows. A general overview of constitutive laws and kinematics for crystal plasticity is given in [295]. Focusing on elasto-viscoplastic polycrystalline microstructures at small strains, the elastic stress-strain relation is defined by the linear relation $\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}_e$ with an additively split of the total strain $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p$ into an elastic part $\boldsymbol{\varepsilon}_e$ and a plastic part $\boldsymbol{\varepsilon}_p$ at each microscopic position $\boldsymbol{x} \in \Omega$. Considering only the dislocation slip as a plastic deformation process, it is assumed that the evolution of the plastic strain is the

sum of the contributions of the individual slip systems α :

$$\dot{\epsilon}_p = \sum_{\alpha=1}^{n_{slip}} \dot{\gamma}_\alpha \mathbf{m}_\alpha^s. \quad (7.3)$$

Here, $\dot{\gamma}_\alpha$ represents the plastic shear rate and $\mathbf{m}_\alpha^s = \frac{1}{2}(\mathbf{d}_\alpha \otimes \mathbf{n}_\alpha + \mathbf{n}_\alpha \otimes \mathbf{d}_\alpha)$ denotes the symmetric Schmid tensor with the slip direction $\mathbf{d}_\alpha$ and the slip plane normal $\mathbf{n}_\alpha$. The plastic shear rate is assumed to follow a Perzyna-type flow rule [342]

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \operatorname{sgn}(\tau_\alpha) \left\langle \frac{|\tau_\alpha| - \tau^c}{\tau^d} \right\rangle^p, \quad (7.4)$$

while $\tau_\alpha = \boldsymbol{\sigma} \cdot \mathbf{m}_\alpha^s$ is the resolved shear stress within slip system α , τ^c is the critical resolved shear stress and $\dot{\gamma}_0$, τ^d and p are the reference shear rate, drag stress and rate sensitivity parameter. The critical resolved shear stress $\tau^c = \tau^c(\gamma_{\text{acc}})$ is depending on the accumulated plastic slip $\gamma_{\text{acc}} = \sum_\alpha \int |\dot{\gamma}_\alpha| dt$ and it is assumed to follow the Voce-type isotropic hardening behavior

$$\tau^c(\gamma_{\text{acc}}) = \tau_0^c + (\tau_\infty - \tau_0^c) \tanh \left(\frac{(h_0 - h_\infty) \gamma_{\text{acc}}}{\tau_\infty - \tau_0^c} \right) + h_\infty \gamma_{\text{acc}}, \quad (7.5)$$

with τ_0^c , τ_∞ , h_0 and h_∞ as the initial critical resolved shear stress, the saturation shear stress, the initial hardening modulus and the saturation hardening modulus, respectively.

Regarding the numerical implementation, the flow rule (Equation (7.4)) is discretized using an implicit Euler scheme, while we use the enhanced power law subroutine introduced in [343]. The unknown stress $\boldsymbol{\sigma}$ and critical resolved shear stress τ_c are obtained by solving the local set of equilibrium equations

$$\begin{pmatrix} \mathbf{r}_\sigma \\ r_\tau \end{pmatrix} = \begin{pmatrix} \boldsymbol{\epsilon}_e^{i+1} - \mathbb{C}^{-1} : \boldsymbol{\sigma}^i \\ \tau_c^{i+1} - \tau_c^i \end{pmatrix} \stackrel{!}{=} \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix} \quad (7.6)$$

with i being the iteration number.

7.4 Reduced FFT-based microstructure simulation

To solve the microscopic balance of linear momentum (Equation (7.1)) for periodic microstructures, the FFT-based simulation approach [11, 12] may be used. Therefore, the polarization stress $\boldsymbol{\tau} = \boldsymbol{\sigma}(\boldsymbol{\epsilon}) - \mathbb{C}^0 : \boldsymbol{\epsilon}$, defined as the difference of the present stress and the stress within

an isotropic homogeneous reference material behavior $\mathbb{C}^0$, is introduced [131]. This leads to a reformulation of the balance of linear momentum as

$$\operatorname{div} [\boldsymbol{\tau} + \mathbb{C}^0 : \boldsymbol{\varepsilon}] = \mathbf{0} \quad \forall \mathbf{x} \in \Omega, \quad (7.7)$$

which may be solved using the Lippmann-Schwinger equation [118]:

$$\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \Gamma^0 * \boldsymbol{\tau} \quad \forall \mathbf{x} \in \Omega \quad (7.8)$$

Here, $*$ represents the convolution integral between the Lippmann-Schwinger operator Γ^0 and the polarization stress $\boldsymbol{\tau}$. To solve this equation, it is transferred into Fourier space

$$\hat{\boldsymbol{\varepsilon}}(\boldsymbol{\xi}) = \begin{cases} -\hat{\Gamma}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) & \text{for } \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\boldsymbol{\varepsilon}} & \text{for } \boldsymbol{\xi} = \mathbf{0} \end{cases} \quad (7.9)$$

with $(\hat{\cdot})$ referring to any quantity in Fourier space and $\boldsymbol{\xi}$ representing the wave vector, which gathers all the considered Fourier modes. The Lippmann-Schwinger operator in Fourier space is explicitly known as

$$\hat{\Gamma}^0(\boldsymbol{\xi}) = \frac{1}{2} \left(\hat{G}_{ik}^0 \xi_j + \hat{G}_{jk}^0 \xi_i \right) \xi_l \quad \text{with} \quad (\hat{G}_{jm}^0)^{-1} = \mathbb{C}_{jkmn}^0 \xi_k \xi_n \quad \text{for } \boldsymbol{\xi} \neq \mathbf{0}. \quad (7.10)$$

Moulinec and Suquet [11, 12] introduced a solution procedure, which makes use of this Fourier representation of the Lippmann-Schwinger equation and a fixed point solver. In order to decrease the computational effort of this simulation approach a MOR technique was introduced in [17] which reduces the computations in Fourier space by taking into account only a reduced set of Fourier modes. The accuracy of this technique directly depends on the number, but also on the choice of incorporated Fourier modes. Therefore, in [237] a choice of modes based on the representation of phases within a two-phase microstructure was introduced. This leads to an increase in accuracy, especially in the linear elastic case. To further improve the accuracy of the method for nonlinear material behavior a strain-based choice of Fourier modes was introduced in [38]. Therefore, the considered sampling pattern is updated after each load step by taking into account the norm of the strain field of the current load step and transferring it into Fourier space to define the sampling pattern $\mathcal{S}_\varepsilon$ for the next load step:

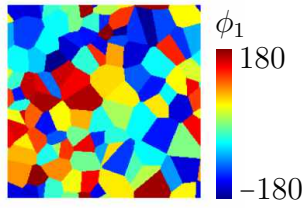
$$\mathcal{S}_\varepsilon^{i+1} : \text{Use Fourier modes with highest amplitudes of } \hat{\boldsymbol{\varepsilon}}_{L^2}^i(\boldsymbol{\xi}) = \text{FFT}\{||\boldsymbol{\varepsilon}^i(\mathbf{x})||\} \quad (7.11)$$

Such a strain-based sampling pattern also leads to accurate results when considering complex microstructures, such as polycrystals, which will be shown in the following section.

7.5 Numerical results

Let us consider a polycrystalline microstructure with 100 grains and the material parameters of copper for a reference shear rate of $\dot{\gamma}_0 = 10^{-3} \text{ 1/s}$ (cf. [202]) as shown in Figure 7.1, while the 12 slip systems of face-centered cubic (fcc) crystals are given by $\mathbf{d}_\alpha\{111\}$ and $\mathbf{n}_\alpha = [110]$.

Since we just considered the microscale simulation, we prescribed any macroscopic load,



Material parameters

$C_{11} = 170.2 \text{ GPa}$, $C_{12} = 114.9 \text{ GPa}$, $C_{44} = 61.0 \text{ GPa}$

$\tau_d = 10 \text{ MPa}$, $p = 20$

$\tau_0^c = 0.1 \text{ MPa}$, $\tau_\infty = 31 \text{ MPa}$, $h_0 = 51 \text{ MPa}$, $h_\infty = 1 \text{ MPa}$

Figure 7.1: Microstructure with the orientation of the first Eulerian angle ϕ_1 .

i.e. $\bar{\varepsilon}_{11} = 0.01$ and $\bar{\varepsilon}_{22} = -0.01$, but also any other macroscopic strain would be reasonable. The investigated microstructure is discretized by $n = 255 \times 255$ equidistant grid points and the results of the reduced FFT-based simulation are evaluated by considering the following microscopic and macroscopic error measurements:

$$\bar{\mathcal{E}} = \frac{\|\bar{\boldsymbol{\sigma}} - \bar{\boldsymbol{\sigma}}^{\text{ref}}\|}{\|\bar{\boldsymbol{\sigma}}^{\text{ref}}\|} \quad \text{and} \quad \mathcal{E} = \frac{1}{n} \sum_n \frac{\|\boldsymbol{\sigma}(n) - \boldsymbol{\sigma}^{\text{ref}}(n)\|}{\|\boldsymbol{\sigma}^{\text{ref}}(n)\|} \quad (7.12)$$

Here, $(\cdot)_{\text{ref}}$ refers to any quantity of the reference solution in which the full set of Fourier modes was utilized. In addition, the microstructural stress difference $\Delta\sigma_{11} = |\sigma_{11} - \sigma_{11}^{\text{ref}}|$, exemplarily for the 11-component, is investigated.

Figure 7.2 shows the evolution of the norm of the strain field $\|\boldsymbol{\varepsilon}\|$ and the identified strain-based sampling pattern for $\mathcal{R} \approx 0.8\%$ of considered Fourier modes for load steps 2, 20, 50 and 100 (from left to right). In the first load step, the full set of Fourier modes is used. In the beginning, the material behaves elastically until the critical resolved shear stress is exceeded. Therefore, the differences within the strain field and thus within the strain-based sampling pattern are most significant within the first load steps (cf. step 2 and 20). After that, only small differences occur.

The resulting stress fields σ_{11} and $\Delta\sigma_{11}$ of the reduced FFT-based microstructure simulation,

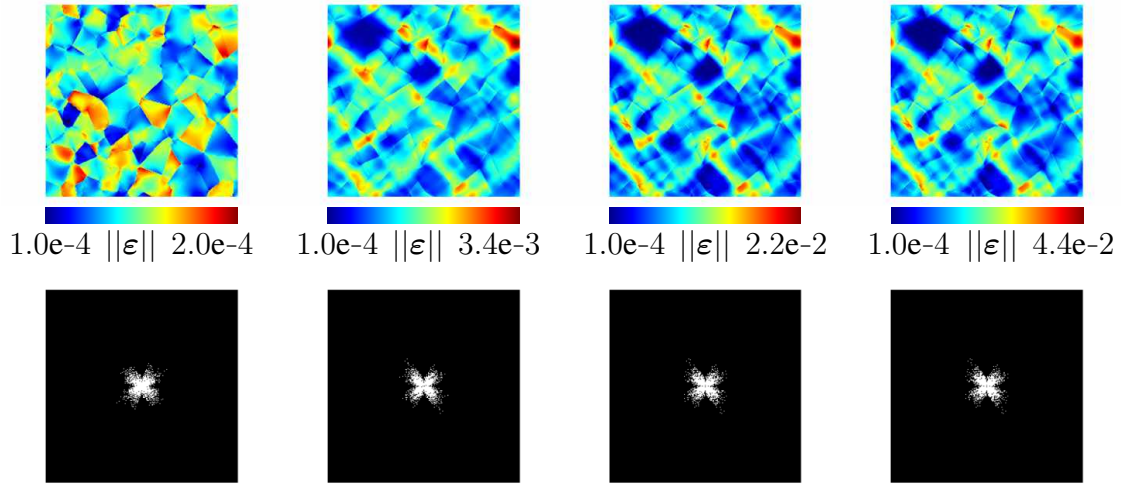


Figure 7.2: Norm of the strain field $||\epsilon||$ and corresponding strain-based sampling pattern with $\mathcal{R} \approx 0.8\%$ of considered Fourier modes for load steps 2, 20, 50 and 100 (from left to right).

considering $\mathcal{R} = 0.8\%$ and $\mathcal{R} = 11.6\%$ of Fourier modes and the reference solution are shown in Figure 7.3. It can be seen, that even by taking into account only $\mathcal{R} = 0.8\%$ of Fourier modes, the solution for the presented stress field σ_{11} is quite similar to the reference solution. This is confirmed by the differences within the microstructural stress field $\Delta\sigma_{11}$. As expected, by incorporating a larger amount of Fourier modes, such as $\mathcal{R} = 11.6\%$, these differences become even smaller.

Corresponding results can also be seen by looking at the overall macroscopic and microscopic errors $\mathcal{E}$ and $\bar{\mathcal{E}}$, shown in Figure 7.4. Both error measures decrease with higher number of Fourier modes. In addition Figure 7.4 shows the relative CPU time t . Utilizing $\mathcal{R} = 0.8\%$ of Fourier modes the CPU times may for example be decreased by 60 %.

7.6 Conclusion and outlook

We presented the application of the reduced FFT-based microstructure simulation utilizing a reduced set of Fourier modes for the simulation of complex microstructures, such as polycrystals. To bypass the difficulties of defining a geometrically adapted sampling pattern for a polycrystalline microstructure, we used a strain-based sampling pattern for the choice of considered Fourier modes. Doing that, a reduction of CPU time of up to 60 % was achieved, while the microscopic and macroscopic errors are reasonably low.

Up to now, we used the MOR technique only in terms of the basic fixed point scheme, intro-

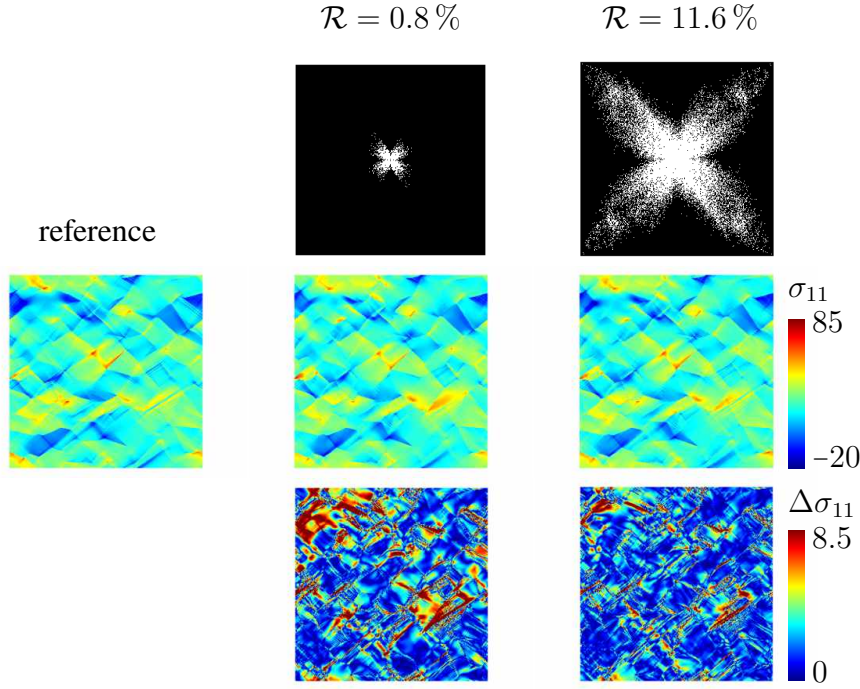


Figure 7.3: Microstructural fields: *Top row*: Strain-based sampling pattern for $\mathcal{R} = 0.8\%$ and $\mathcal{R} = 11.6\%$ of Fourier modes. *Middle row*: Corresponding and reference stress fields σ_{11} . *Bottom row*: Difference in the stress fields $\Delta\sigma_{11}$.

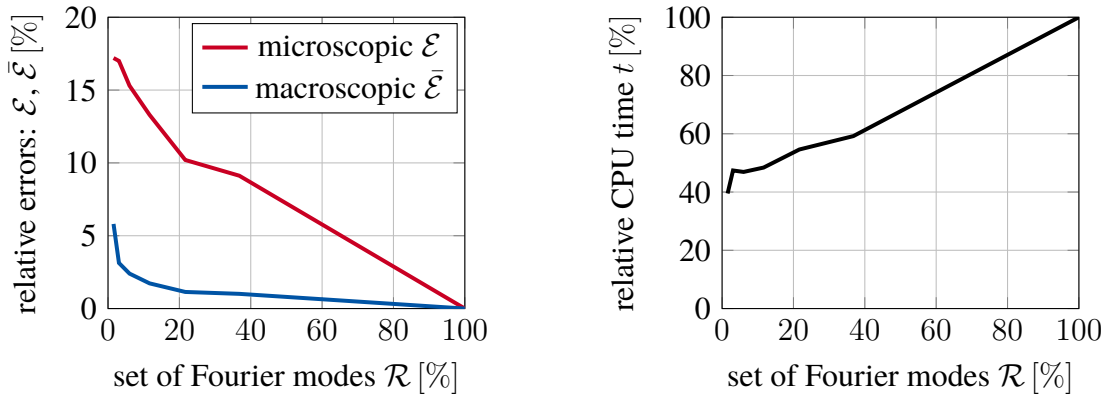


Figure 7.4: Macroscopic error $\bar{\mathcal{E}}$ (*left*) and microscopic error $\mathcal{E}$ (*right*) for the 2D elastic microstructure with one circular inclusion depending on the percentage of used Fourier modes $\mathcal{R}$ for the solution with the fixed and adapted sampling pattern.

duced by Moulinec and Suquet. Since much more efficient solvers are available nowadays, in future works we will consider the application of using a reduced set of Fourier modes with different solvers, such as fast gradient methods [217, 250] to reduce the computational costs in general. In addition, we will show the application of the MOR technique considering a strain-

based sampling pattern, which evolves with increasing loading, to evolving microstructures by considering for example polycrystals incorporating phase transformations [358]. Furthermore, to reduce the effect of Gibbs oscillations [19] on the convergence behavior, we will also consider first- [30, 227] and higher-order [231] finite difference approximations of the differential operators within the spectral solver.

8 | **Article 7:**

FFT-based simulation of evolving microstructures utilizing an adapting reduced set of Fourier modes

This article was published as:

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Disclosure of the individual authors’ contributions to the article:

C. Gierden reviewed the relevant existing literature and developed the idea of defining a strain-based sampling pattern. Furthermore, he implemented the framework, performed the simulations, interpreted the results and wrote the article. J. Waimann provided the variational material model to predict solid-solid phase transformations between austenite and martensite within a polycrystal. Moreover, she, B. Svendsen and S. Reese gave conceptual advice, contributed to the discussion of the results, proofread the article and made valuable suggestions for improvement. All authors approved the publication of the final version of the manuscript.

8.1 Abstract

The mechanical behavior of a periodic heterogeneous microstructure may be predicted by using a fast Fourier transform (FFT) based simulation approach. To reduce the computational effort of this method, we introduced a model order reduction (MOR) technique utilizing a reduced set of Fourier modes for the computations in Fourier space. To increase the accuracy of this MOR technique we developed a geometrically adapted sampling pattern for choosing the considered Fourier modes based on the representation of phases within the microstructure. Since the phase distribution of, for example, martensite and austenite in a polycrystalline microstructure evolves with increasing mechanical or thermal loads, the set of considered Fourier modes should also evolve according to the underlying micromechanical fields. We present the accuracy and the adaptability of this adaptive reduced set of Fourier modes by investigating the micromechanical fields of a polycrystal considering such phase transformations.

8.2 Introduction

Investigating the mechanical behavior of periodic microstructures, the FFT-based simulation method [11, 12] is an efficient and accurate alternative to classical FE-based simulations. This FFT-based microstructure simulation may also be used in terms of two-scale simulations resulting in a FE-FFT-based [13, 18] approach, which also serves as an efficient and accurate alternative to the common FE^2 method. Nevertheless, considering complex macroscopic boundary value problems and highly resolved microstructures, both, the FE^2 and FE-FFT-based method are computationally expensive. To reduce the computational effort in this context, different strategies have been developed.

Concerning efficient two-scale simulation approaches utilizing the FE-FFT-based approach, different methods may be used: For example, using a coarse discretized microstructure for the two-scale simulation followed by a post-processing step for the generation of highly resolved microstructural results for macroscopic integration points of interest [316, 319] or using a database base instead of the FE-FFT-based approach, while this FE-FFT-based approach is only used in macroscopic critical areas [254]. A general overview on FE-FFT-based two-scale methods is given in [39].

Instead of utilizing such solution strategies, model order reduction (MOR) techniques for the FFT-based microstructure simulation have been introduced. These MOR techniques are for example based on a proper orthogonal decomposition (POD) [234], low-rank tensor approximations [236] or utilizing a reduced set of Fourier modes [17]. In this paper, we show how

the concept of utilizing a reduced set of Fourier modes is used while accounting for evolving microstructures. A general overview on FFT-based methods for the simulation of periodic microstructures is given in [10, 14].

The FFT-based simulation using a reduced set of Fourier modes was introduced utilizing a fixed set of modes [17, 235]. In order to increase the accuracy of this MOR technique, a geometrically adapted selection of Fourier modes was developed in [237]. Since the geometry of a microstructure, such as the representation of phases within a microstructure, changes during different mechanical or thermal loading, an adaptively changing sampling pattern leads to even more accurate results throughout the simulation. In this context, a strain-based sampling pattern was introduced in [38], which adjusts the selection of Fourier modes to the strain field of the last load step. In the present paper, we show how this MOR technique performs investigating a polycrystalline microstructure incorporating solid-solid phase transformations between austenite and martensite.

The paper is structured as follows: In Section 8.3 the microstructural boundary value problem considering a polycrystalline microstructure with solid-solid phase transformations between austenite and martensite is briefly discussed. This is followed by introducing the reduced FFT-based microstructure simulation incorporating an adapting sampling pattern in Section 8.4. After discussing the numerical results in Section 8.5 the paper ends with a conclusion and outlook in Section 8.5.

8.3 Microstructural boundary value problem and material model

Considering inhomogeneous microstructures, the quasi-static balance of linear momentum reads

$$\operatorname{div} \boldsymbol{\sigma}(\boldsymbol{x}) = \mathbf{0} , \quad (8.1)$$

while body forces on the microscale are neglected and small strain kinematics are assumed. The stress $\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{x}), \boldsymbol{\alpha}(\boldsymbol{x}))$ depends on the microscopic position $\boldsymbol{x}$, the total strain $\boldsymbol{\varepsilon}(\boldsymbol{x})$ and the internal variables $\boldsymbol{\alpha}(\boldsymbol{x})$. The total strain $\boldsymbol{\varepsilon}(\boldsymbol{x}) = \bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x})$ is additively split into a macroscopic part $\bar{\boldsymbol{\varepsilon}}$ and a microscopically fluctuating part $\tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x})$. Finally, the overall

macroscopic stress $\bar{\sigma}$ and strain $\bar{\varepsilon}$ fields are defined as volume averages of their local fields:

$$\bar{\sigma} = \frac{1}{V} \int_{\Omega} \sigma(\mathbf{x}) \, d\Omega \quad \text{and} \quad \bar{\varepsilon} = \frac{1}{V} \int_{\Omega} \varepsilon(\mathbf{x}) \, d\Omega. \quad (8.2)$$

To account for solid-solid phase transformations between austenite and martensite within a polycrystalline microstructure, we used a variational material model [359]. This model is extended to take into account irreversible phase transformations in [358] and to predict transformation induced plasticity in steel in [360]. The individual phases within this model are represented by their volume fractions λ_i , with $\lambda_0 = \lambda_A$ the volume fraction of austenite and $\lambda_{i>0} = \lambda_{M_i}$ the volume fractions of different martensitic variants. Each phase is characterized by an elastic stiffness tensor C_i , a transformation strain η_i and a caloric part of the energy c_i . Taking into account the volume fractions of the individual phases, the corresponding effective quantities at one point j within the microstructure are given by:

$$\eta_{\text{eff}}^j = \sum_{i=0}^n \lambda_i^j \eta_i^j, \quad C_{\text{eff}}^j = \left(\sum_{i=0}^n \lambda_i^j (C_i^j)^{-1} \right)^{-1}, \quad c_{\text{eff}}^j = \sum_{i=0}^n \lambda_i^j c_i^j.$$

Using these effective quantities, the Helmholtz free energy Ψ^j within the point j in the microstructure is described as

$$\Psi^j = \frac{1}{2} (\varepsilon^j - \eta_{\text{eff}}^j) : C_{\text{eff}}^j : (\varepsilon^j - \eta_{\text{eff}}^j) + c_{\text{eff}}^j, \quad (8.3)$$

while the effective stiffness tensor C_{eff}^j and transformation strains η_{eff}^j need to be rotated corresponding to the crystal structure within the polycrystal. Finally, the point-wise energy needs to be summed up, to compute the total energy $\Psi(\varepsilon, \lambda)$.

To derive the material model, the principle of the minimum of dissipation potential is applied yielding

$$\mathcal{L} = \dot{\Psi}(\varepsilon, \lambda) + \mathcal{D}(\dot{\lambda}) + \text{cons} \rightarrow \min_{\dot{\lambda}}, \quad (8.4)$$

which is the minimization of a Lagrange function consisting of the rate of the Helmholtz free energy $\dot{\Psi}(\varepsilon, \lambda)$, a dissipation function $\mathcal{D}(\dot{\lambda})$ and constraints, in the examined case, the non-negativity of λ and the conservation of mass. The dissipation function $\mathcal{D} = r |\dot{\lambda}|$ is given by the material dependent dissipation parameter r and the norm of the rate of the volume fractions $|\dot{\lambda}|$. The minimization of Equation (8.4) leads to the evolution equation for the volume fraction

of the individual phases

$$\dot{\lambda}_i^j = \beta^j \operatorname{dev}_{\mathcal{A}^j} P_{Ti}^j \quad \forall i \in \mathcal{A}^j \quad (8.5)$$

with the consistency parameter β^j and the active deviator $\operatorname{dev}_{\mathcal{A}^j} P_{Ti}^j$, which holds for the active set $\mathcal{A}^j = \{i | \lambda_i^j > 0\} \cup \{i | \lambda_i^j = 0 \wedge \dot{\lambda}_i^j > 0\}$. The active deviator is computed as

$$\operatorname{dev}_{\mathcal{A}^j} P_{Ti}^j = P_{Ti}^j - \frac{1}{n_{\mathcal{A}}^j} \sum_{k \in \mathcal{A}^j} P_{Tk}^j \quad (8.6)$$

with the thermodynamic driving force P_{Ti}^j and the $n_{\mathcal{A}}^j$ active phases within $\mathcal{A}^j$. The thermodynamic driving force as well as the stress σ^j are defined as the partial derivatives of the energy (8.3) yielding

$$P_{Ti}^j = -\frac{\partial \Psi}{\partial \lambda_i^j} = \boldsymbol{\eta}^j : \boldsymbol{\sigma}^j + \frac{1}{2} \boldsymbol{\sigma}^j : (\mathbf{C}_i^j)^{-1} : \boldsymbol{\sigma}^j - c_i \quad (8.7)$$

$$\boldsymbol{\sigma}^j = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^j} = \mathbf{C}_{\text{eff}}^j : (\boldsymbol{\varepsilon}^j - \boldsymbol{\eta}_{\text{eff}}^j) . \quad (8.8)$$

Finally, the consistency parameter β^j is determined by the Karush-Kuhn-Tucker conditions

$$\Phi_T^j = \operatorname{dev}_{\mathcal{A}^j} \mathbf{P}_T^j \cdot \operatorname{dev}_{\mathcal{A}^j} \mathbf{P}_T^j - r^2 \leq 0, \quad \beta^j \geq 0, \quad \beta^j \Phi^j = 0. \quad (8.9)$$

These include the yield function Φ_T^j , which results from a Legendre transformation of the dissipation function $\mathcal{D}$.

8.4 Adaptively reduced FFT-based microstructure simulation

To solve the microscopic boundary value problem (BVP), the FFT-based fixed point solver [11, 12] is used incorporating a model order reduction technique based on a reduced set of Fourier modes. In order to use the spectral solver, the inhomogeneous BVP is transformed into an equivalent homogeneous BVP

$$\operatorname{div} [\mathbf{C}^0 : \boldsymbol{\varepsilon}(\mathbf{x})] + \operatorname{div} \boldsymbol{\tau}(\mathbf{x}) = \mathbf{0}, \quad (8.10)$$

by introducing the polarization stress $\boldsymbol{\tau}(\boldsymbol{x}) := \boldsymbol{\sigma}(\boldsymbol{x}) - \boldsymbol{C}^0 : \boldsymbol{\varepsilon}(\boldsymbol{x})$, which is the difference between the stress in the microstructure $\boldsymbol{\sigma}(\boldsymbol{x})$ and the stress in a homogeneous reference material $\boldsymbol{C}^0$ [131]. This equivalent homogeneous BVP may be solved using Green's function $\boldsymbol{G}^0(\boldsymbol{x}, \boldsymbol{x}')$ or Green's operator $\boldsymbol{\Gamma}^0(\boldsymbol{x}, \boldsymbol{x}')$ yielding the Lippmann-Schwinger equation [337]:

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \bar{\boldsymbol{\varepsilon}} - \int_{\Omega} \boldsymbol{\Gamma}^0(\boldsymbol{x}, \boldsymbol{x}') : \boldsymbol{\tau}(\boldsymbol{x}') d\boldsymbol{x}' . \quad (8.11)$$

In Fourier space this equation can directly be solved, since the occurring convolution integral ends up as simple multiplication

$$\hat{\boldsymbol{\varepsilon}}(\boldsymbol{\xi}) = \begin{cases} -\hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) & \forall \quad \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\boldsymbol{\varepsilon}} & \forall \quad \boldsymbol{\xi} = \mathbf{0} \end{cases} \quad (8.12)$$

and Green's function $G_{ik}^0(\boldsymbol{\xi}) = (C_{ijkl}^0 \xi_j \xi_l)^{-1}$ and Green's operator $\hat{\Gamma}_{ijkl}^0(\boldsymbol{\xi}) = \frac{1}{2} \left(\hat{G}_{ik}^0(\boldsymbol{\xi}) \xi_j \xi_l + \hat{G}_{jk}^0(\boldsymbol{\xi}) \xi_i \xi_l \right)$ are explicitly known and just depending on the homogeneous reference material behavior and the wave vector $\boldsymbol{\xi}$, that gathers all the Fourier modes considered within the simulation.

Moulinec and Suquet introduced a fixed point scheme computing the polarization stress in real space, which is then transferred into Fourier space and used to solve the Lippmann-Schwinger equation (8.12) in Fourier space to compute the strain for the next iteration [11, 12]. Considering polycrystalline microstructures, this FFT-based microstructure simulation was first used in [191, 202].

In order to reduce the computational effort of this spectral solver, a model order reduction technique utilizing just a reduced set of Fourier modes for solving the Lippmann-Schwinger equation in Fourier space was introduced in [17]. To increase the accuracy of this technique, we introduced a geometrically adapted sampling pattern [237]. This technique is based on a given and fixed representation of phases within the microstructure. Since the phases within a microstructure, for example in a polycrystal, may not be clearly defined and even evolve, we presented a strain-based sampling pattern in [38]. The idea of the strain-based sampling pattern is to consider the norm of the converged strain field of a given load step $\|\boldsymbol{\varepsilon}^i(\boldsymbol{x})\|$ for the definition of the reduced set of Fourier modes. This strain field is transferred into Fourier space and the sampling pattern for the next load step $\mathcal{S}_{\varepsilon}^{i+1}$ is defined by a given percentage $\mathcal{R}$ of Fourier modes with the highest amplitudes needed to capture the norm of the strain field in

Fourier space:

$$\mathcal{S}_\varepsilon^{i+1} : \text{Fourier modes with the highest amplitudes of } \mathcal{FFT} \{ ||\varepsilon^i(\mathbf{x})|| \}$$

This technique leads to an evolving sampling pattern that is always adapting to the strain within a microstructure and therefore to changes, such as solid-solid phase transformations between austenite and martensite, as can be seen in Section 8.5.

8.5 Numerical results

To show the adaptability and accuracy of the strain-based sampling pattern for evolving microstructures, we considered a polycrystalline nickel titanium (NiTi) alloy (known for the shape memory effect) incorporating phase transformations between austenite and twelve different martensitic variants. Figure 8.1 shows the polycrystalline microstructure, i.e. the orientation of the first Euler angle φ , and the lattice structure of the austenite and martensite.

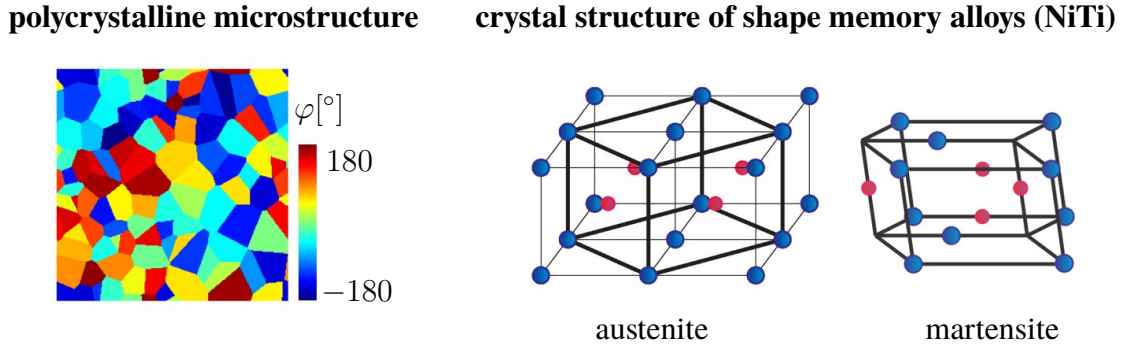


Figure 8.1: Left: Orientation of the first Euler angle φ of the polycrystal. Right: Crystal structure of austenite and martensite [361].

The following material parameters are considered for the simulation: The dissipation parameter is set to $r = 0.006$ GPa, the caloric energies read $c_A = -0.03$ GPa and $c_{M_i} = 0.0$ GPa and the stiffness tensors and transformation strains of the individual phases are taken from [362, 363]. For the simulations, we used a fine discretization with 255×255 grid points, while only $\mathcal{R} = 1\%$ of Fourier modes were utilized for the computations in Fourier space. Figure 8.2 shows the overall macroscopic and microstructural results and their differences from the reference solution computed with the full set of Fourier modes. Also shown is the stepwise changing sampling pattern for loading and unloading of the microstructure by $\bar{\varepsilon}_{xx} = 0.04$.

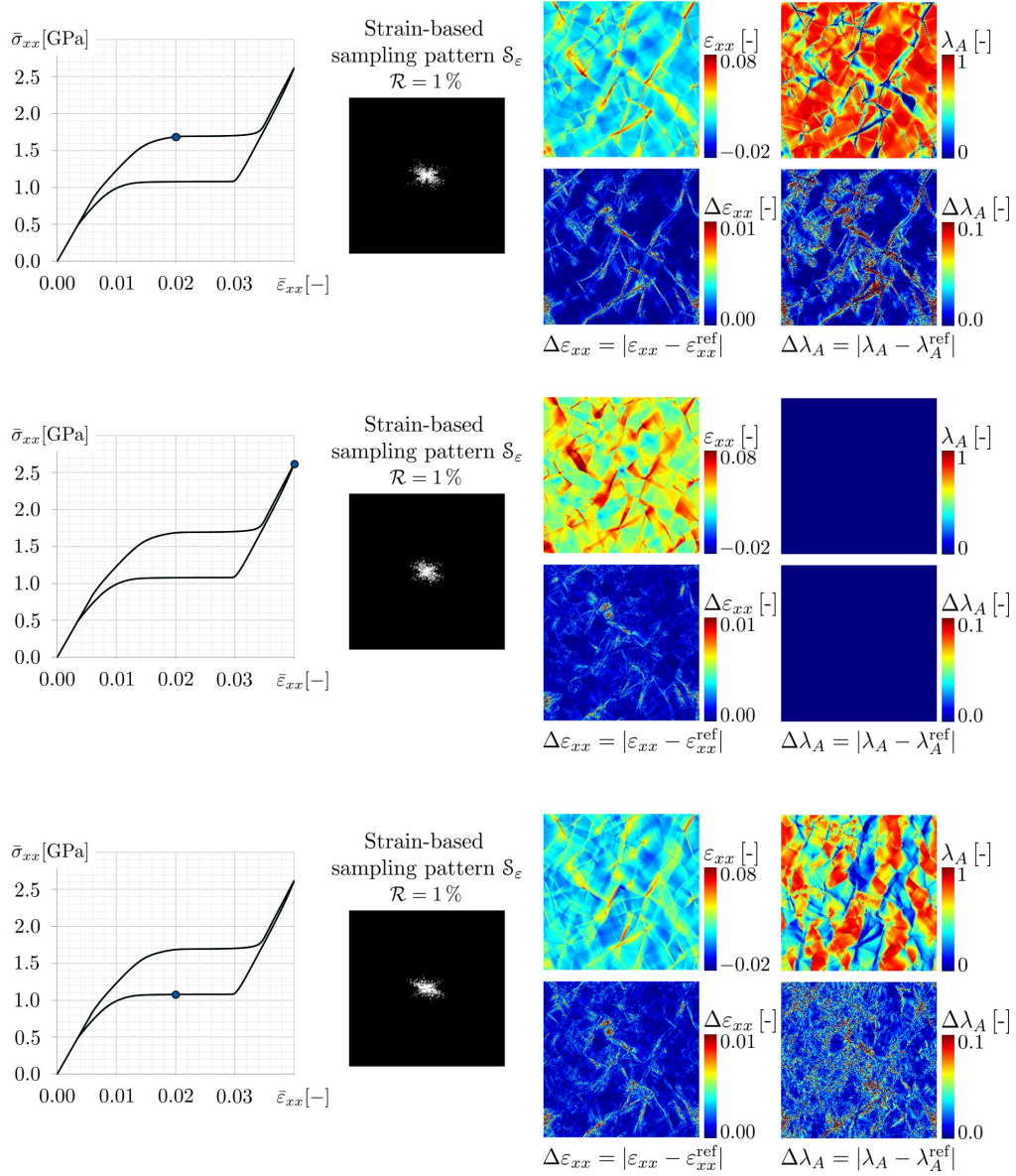


Figure 8.2: Overall stress-strain diagram, sampling pattern, microscopic strain ϵ_{xx} and volume fraction of the austenite λ_A and their differences compared to the reference solution for three different load steps of the loading/unloading paths.

The overall macroscopic stress-strain diagram shows the typical hysteresis curve for the pseudoelastic material behavior of a shape memory alloy. Starting with a pure austenitic microstructure and linear elastic material behavior, occurring phase transformations from austenite to martensite at certain points in the microstructure continuously lead to a plateau within the macroscopic stress-strain curve. After the transformation of the entire microstructure is completed, again a linear elastic material behavior, related to the material behavior of a pure martensitic microstructure, is observed. When the microstructure is unloaded, the same behavior occurs, but with a lower stress plateau, which refers to the back transformation from martensite to austenite.

Regarding the macroscopic material behavior, the total error associated with the model order reduction is extremely small. Therefore, the curves of the reduced and the unreduced solution overlap, and in Figure 8.2 on the left-hand side, only one macroscopic stress-strain curve can be seen.

Concerning the microstructural fields, in Figure 8.2 on the right side the strain ε_{xx} and the volume fraction of austenite λ_A as well as the corresponding absolute differences compared to the reference solution computed with the full set of Fourier modes are shown for three specific load steps. It can be seen, that the differences are the highest while phase transformations take place within the microstructure. Before and after the occurrence of these phase transformations, the error related to the volume fraction of austenite is zero, since a pure martensitic or austenitic microstructure is present without inhomogeneities related to the phase mixture of the microstructure. Accordingly, the error with respect to the microscopic strain field ε_{xx} is also lower when the phase transformations are completed.

In addition, the strain-based sampling pattern with 1% of Fourier modes for the three different load steps is shown as well. Since this sampling pattern is always adapted to the strain field of the last load step, it changes from load step to load step, whenever a nonlinear material behavior is present.

Although the results shown in Figure 8.2 are obtained by considering only 1% of Fourier modes for the computations in Fourier space, the maximum relative macroscopic and microscopic errors related to the stress fields that occur during the entire simulation (loading and unloading path) are as follows:

$$\bar{\mathcal{E}}_{\sigma} = \frac{\|\bar{\sigma} - \bar{\sigma}^{\text{ref}}\|}{\|\bar{\sigma}^{\text{ref}}\|} \leq 0.04\% \quad \text{and} \quad \mathcal{E}_{\sigma} = \frac{1}{n} \sum_n \frac{\|\sigma(n) - \sigma(n)^{\text{ref}}\|}{\|\sigma(n)^{\text{ref}}\|} \leq 0.25\%.$$

The accuracy and the reduction of the CPU time are influenced in an opposing way by the considered number of Fourier modes. The lower the number of used Fourier modes, the lower

is the CPU time, but the higher is the error. In the present case, the reduction to 1% of Fourier modes leads to the aforementioned accuracy, while a CPU time reduction of up to 20% is achieved.

8.6 Conclusion and outlook

We presented the application of the reduced FFT-based microstructure simulation with an adapting set of Fourier modes to an evolving microstructure with solid-solid phase transformations between austenite and martensite. Specifically, we investigated a nickel-titanium alloy (NiTi) known for its shape memory effect. Doing that and considering only 1% of Fourier modes, a CPU time reduction of up to 20 % can be achieved compared to calculations using the full set of Fourier modes. At the same time, the total macroscopic and microscopic errors related to the stress fields are below $\bar{\mathcal{E}}_\sigma \leq 0.04 \%$ and $\mathcal{E}_\sigma \leq 0.25 \%$, respectively, throughout the entire loading and unloading paths while the highest errors occur during the process of phase transformations.

Future works will address and further investigate various aspects of improving the FFT-based microstructure simulation with a reduced set of Fourier modes. In this context, interesting topics are related to decreasing the computational effort of the stress evaluations (e.g. by using a clustered microstructure [128, 364] for the stress evaluations in real space [351]), using more efficient solvers (e.g. Nesterov's fast gradient method [217] or the Heavy ball method [250]), or reducing the effect of Gibbs oscillations [19] on the convergence behavior (e.g. by using second [29, 229] or higher order [231] finite difference approximations of the Lippmann-Schwinger operator or the rotated scheme of Willot [30]).

9 | **Article 8:**

Reduced FFT-based numerical solution of mechanical equilibrium combined with finite-difference-based operator approximation for heterogeneous media

This article was published as:

Gierden, C., Waimann, J., Svendsen, B. and Reese, S. [2023], ‘Reduced FFT-based numerical solution of mechanical equilibrium combined with finite-difference-based operator approximation for heterogeneous media’ (working title), *in preparation*.

Disclosure of the individual authors’ contributions to the article:

C. Gierden reviewed the relevant existing literature and implemented the combination of the model order reduction technique with finite-difference-based operator approximations as well as fast gradient solvers. He performed the simulations, interpreted the results and wrote the preliminary version of the article. J. Waimann, B. Svendsen and S. Reese gave conceptual advice, contributed to the discussion of the results, proofread the preliminary version of the article and made valuable suggestions for improvement. All authors approved the publication of the preliminary version of the article in the present dissertation.

9.1 Abstract

In the current work, we introduce the straightforward combination of using a model order reduction technique based on a reduced set of Fourier modes for FFT-based microstructure simulations with modified Green's operators based on finite differences as well as fast gradient solvers. The model order reduction technique of using a reduced set of Fourier modes was introduced by Kochmann et al. [17] and first implemented in the context of the FFT-based basic scheme of Moulinec and Suquet [12]. In this context, the effect of different sampling schemes on the accuracy of the discretized Fourier series solution approximation was investigated. The advantage of the method is its independence from any pre-processing and its flexibility. Hence, methods to improve the accuracy and efficiency of the FFT-based microstructure simulation itself can easily be applied while working with a reduced set of Fourier modes. Here, we focus on optimized Green's operators based on finite differences to reduce the effect of Gibbs oscillations and on fast gradient solvers to improve the efficiency of the method. In any case, the momentum balance in the form of the Lippmann-Schwinger equation must be solved in Fourier space, where the before mentioned model order reduction technique is used. To demonstrate the feasibility of using a reduced set of Fourier modes with modified Green's operators and fast gradient solvers, several numerical examples are studied.

9.2 Introduction

When studying the overall material behavior of a structural component at the macroscale, the macroscopic behavior is directly influenced by the microstructural character of the considered material. Investigating different microstructures, one can distinguish, among others, between composite and polycrystalline microstructures, which are influenced, for example, by the volume fraction and distribution of different phases or by the size and orientation of grains, respectively. Several computational multiscale approaches [365] have been developed, in order to capture the overall mechanical behavior of structural components taking their microstructures and their characteristics in a highly resolved manner into account. The most common approach is the FE^2 -method [113, 123], which uses the finite element (FE) method at both scales, the macroscale and the microscale. Other computational two-scale methods are for example based on finite differences (FD) [175], virtual elements (VE) [177, 178], or fast Fourier transform (FFT)-based solvers [13, 18].

Focusing on the two-scale FE-FFT-based simulation approach, an efficient and accurate two-scale method can be generated either by developing a smart overall solution strategy or by

improving the efficiency of the simulations at the macro- and/or microscale. Smart solution strategies are based, for example, on performing a highly resolved two-scale simulation only at macroscopically critical integration points and otherwise using a purely macroscopic material model that was fitted to the present material model in a pre-processing step [246, 254]. Another strategy would be to define a numerically coarsely discretized microstructure, which is used for the two-scale simulation. In this case, the microstructure is modeled with as few grid points as possible to accurately capture the averaged material behavior. The detailed analysis of the quantities of interest at particular integration points is then performed in a post-processing step with a much finer discretization [16, 319]. A general and comprehensive review of the FE-FFT-based two-scale method is given in [15].

Concerning an efficient and accurate FE-simulation at the macroscale, one may consider different improvements such as mixed finite element methods, a reduced integration with a suitable hourglass stabilization [2, 366] or model order reduction techniques, such as the proper orthogonal decomposition (POD) method [5, 6]. However, the macroscopic FE-simulation and its improvements will not be further discussed in the following, but the characteristics and improvements of the FFT-based microstructure simulation are the scope of this work. This FFT-based microstructure simulation was introduced by Moulinec and Suquet [11, 12] to predict the mechanical fields in a composite periodic microstructure and adapted for predicting the mechanical fields in polycrystalline microstructures by Lebensohn [191]. In general, this method is an efficient and accurate alternative for an FE-based simulation of periodic microstructures, e.g. shown in [8, 9] for polycrystalline microstructures. A comprehensive overview of the state of the art regarding the FFT-based microstructure simulation is presented in [10, 14].

Reducing the effect of Gibbs oscillations. To reduce the effect of Gibbs oscillations [19], several methods have been developed. In [29, 229, 367] a method based on a finite difference approximation of the occurring derivatives was proposed. This method is related to an image filtering technique, in particular the Lanczos σ -approximation [368, 369]. In order to improve the accuracy of the finite difference approximation, the derivatives may also be approximated by higher-order finite differences [231, 232]. Furthermore, the accuracy and convergence behavior of the FFT-based solver can generally be increased using the finite difference discretization based on a rotated staggered grid [30, 227] as proposed by Willot and coworkers. In [230] also the application based on a standard staggered grid was introduced. Further finite difference based methods are presented in [228, 229]. Besides that, methods based on smoothing techniques [370], composite voxels [32], a discrete Green's operator [205, 209], a finite-element

discretization with reduced integration [217] (which is equivalent to the finite difference discretization based on a rotated staggered grid [30, 227]), or optimized projection operators [37] in the context of the FFT-based Galerkin method [23] have been investigated.

FFT-based solution methods. The FFT-based microstructure simulation [11, 12] was introduced utilizing a fixed point solver, which is referred to as basic scheme [196]. To improve the convergence behavior of the FFT-based algorithm, polarization-based schemes and schemes based on augmented Lagrangians [20, 196, 198] have been introduced. A comparison of these different schemes is given in [199, 200], where it was shown that all schemes are particular cases of a general polarization-based scheme. Other techniques to improve the convergence behavior of the FFT-based simulation are based on efficient solution methods. In this context, the basic scheme was interpreted as a gradient decent method minimizing the total energy in the unit cell in [195], which has been the basis for several more efficient solvers such as fast gradient methods [217, 250], Quasi-Newton methods [218, 222], Krylov subspace methods [209, 215] or particularly the Newton-Krylov method [195, 216].

Model order reduction techniques for FFT-based solvers. To further improve the efficiency of the FFT-based solvers, recently different model order reduction techniques have been applied to the method. In this context, methods are based for example on low-rank tensor approximations [236] where a POD of the strain field in Fourier space [234] is used or on a wavelet analysis with an adaptively refined grid in order to reduce the number of the material model evaluations [41]. Another, self-developed method is based on considering only a reduced set of Fourier modes for the computations in Fourier space [17]. First, the Fourier modes to be used were determined considering a fixed sampling pattern. To improve the accuracy of the method, a geometrically adapted [237] and a strain-based [38] sampling pattern have been developed. Using the strain-based sampling pattern, complex polycrystalline microstructures have been studied, taking into account crystal plasticity [39] or phase transformations [355]. The model order reduction technique is explicitly adapted to the spectral character of the solver and does not require any pre-calculations. Furthermore, the considered sampling pattern may be adapted after each load step in order to generate accurate results, which outlines the advantage of this method. To further reduce the computational effort of the method, also a clustered microstructure [115, 128] for the computations in real space may be considered [351].

Scope of this work. The model order reduction technique of using a reduced set of Fourier modes was initially introduced in the context of the basic scheme and without any technique

to reduce the effect of Gibbs oscillations. In this work we will present the application of the technique in terms of modern solvers, i.e. we consider fast gradient methods such as Nesterov's fast gradient method and the heavy ball scheme. In addition, we will apply different finite difference approximations to the occurring derivatives in order to reduce the effect of Gibbs oscillations, which are still present when taking into account a reduced set of Fourier modes.

In order to investigate the combination of the model order reduction technique with the different discretizations and modern solvers any microstructural material behavior might be considered. Nevertheless, we will focus on linear elastic two-phase composites and polycrystalline microstructures with an elasto-viscoplastic material behavior throughout this paper, which will be introduced in Section 9.3. This is followed by Section 9.4, in which the different discretizations leading to modified Green's operators and the fast gradient solvers considered in the studies are briefly discussed. After reviewing the underlying model order reduction technique and possible sampling patterns in Section 9.5, the numerical results are presented in Section 9.6. The paper ends with a conclusion and an outlook in Section 9.7.

9.3 Microstructure and material behavior

In the present study, we will consider two different microstructures, namely two-phase and polycrystalline unit cells. While the boundary value problem and the definition of the effective response, described in Section 9.3.1, are the same in both cases, the local constitutive equations, described in Section 9.3.2, will be different.

9.3.1 Boundary value problem and effective response

Let us consider an inhomogeneous unit cell Ω , which may be characterized either by two phases $n^{\text{pha}} = 2$ ($n^{\text{pha}} = 1 \rightarrow \Omega^{\text{Matrix}}$ and $n^{\text{pha}} = 2 \rightarrow \Omega^{\text{Inclusion}}$) with different elastic stiffnesses defined by the elasticity tensor $\mathbb{C}^{\text{pha}}$ or by a certain number of grains n^{grain} with different orientations, defined by the Eulerian angles $\{\phi_1, \phi_2, \phi_3\}$, see Figure 9.1.

Considering small strain kinematics, the strain $\varepsilon(\mathbf{x})$ at any microscopic position $\mathbf{x}$ within Ω is given by $\varepsilon(\mathbf{x}) = \bar{\varepsilon} + \tilde{\varepsilon}(\mathbf{x})$ with the homogeneous macroscopic strain $\bar{\varepsilon}$ and the local fluctuating strain field $\tilde{\varepsilon}(\mathbf{x}) = \nabla^s \tilde{\mathbf{u}}(\mathbf{x})$ defined as the symmetric gradient of the local fluctuating displacement field $\tilde{\mathbf{u}}$. Investigating purely mechanical and quasi-static processes, the

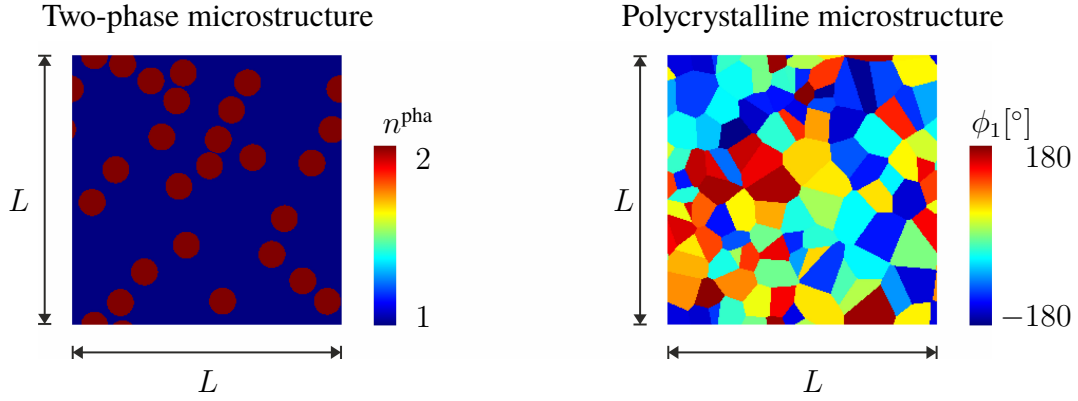


Figure 9.1: Left: Sketch of a microstructure with two different phases $n^{\text{pha}} = 2$. Right: Sketch of a polycrystalline microstructure with the orientation of the first Euler angle ϕ_1 .

microscopic balance of linear momentum reads:

$$\begin{aligned} \operatorname{div} \boldsymbol{\sigma}(\mathbf{x}) &= \mathbf{0} & \forall \mathbf{x} \in \Omega & \\ \boldsymbol{\sigma}(\mathbf{x}) &= \boldsymbol{\sigma}(\mathbf{x}, \boldsymbol{\varepsilon}(\mathbf{x}), \boldsymbol{\alpha}(\mathbf{x})) \\ \boldsymbol{\varepsilon}(\mathbf{x}) &= \bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}(\mathbf{x}). \end{aligned} \quad (9.1)$$

Herein, the stress $\boldsymbol{\sigma}(\mathbf{x})$ depends on the microscopic position, the strain and a set of internal variables $\boldsymbol{\alpha}(\mathbf{x})$, which will be specified in the context of the local constitutive equations in Section 9.3.2. Furthermore, potential body forces would be considered at the macroscale and are therefore neglected within the given microscopic balance equation. The microscopic boundary value problem is closed by assuming periodic boundary conditions.

The macroscopic strain $\bar{\boldsymbol{\varepsilon}}$ and stress $\bar{\boldsymbol{\sigma}}$ are finally defined as volume averages of their corresponding local fields:

$$\bar{\boldsymbol{\varepsilon}} := \frac{1}{V} \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{x}) \, dV \quad \text{and} \quad \bar{\boldsymbol{\sigma}} := \frac{1}{V} \int_{\Omega} \boldsymbol{\sigma}(\mathbf{x}) \, dV, \quad (9.2)$$

with V defining the volume of the considered unit cell.

9.3.2 Local constitutive equations

The previously introduced microstructures are assumed to follow different constitutive laws. While the two-phase microstructure is described by a linear elastic material behavior, given by $\boldsymbol{\sigma}(\mathbf{x}) = \mathbb{C}^{\text{pha}}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x})$, the polycrystalline microstructure is characterized by the constitutive framework of crystal plasticity. A general overview of constitutive laws and kinematics in

crystal plasticity is given in [295].

In this paper we focus on elasto-viscoplastic crystals (see eg. [301]). Thus, the total strain $\boldsymbol{\varepsilon}(\boldsymbol{x}) = \boldsymbol{\varepsilon}_e(\boldsymbol{x}) + \boldsymbol{\varepsilon}_p(\boldsymbol{x})$ is additively split into an elastic part $\boldsymbol{\varepsilon}_e(\boldsymbol{x})$ and a plastic part $\boldsymbol{\varepsilon}_p(\boldsymbol{x})$. For reasons of clarity, the dependence of all variables at the microscopic position $\boldsymbol{x}$ is not indicated in the following. Assuming dislocation slip as the only plastic deformation process, the plastic strain $\boldsymbol{\varepsilon}_p$ is defined as

$$\boldsymbol{\varepsilon}_p = \sum_{\alpha=1}^{n_{\text{slip}}} \gamma_{\alpha} \boldsymbol{m}_{\alpha}^s, \quad (9.3)$$

which is the sum of the plastic slips γ_{α} in a slip system α over all slip systems n_{slip} defined by the symmetric Schmid tensor $\boldsymbol{m}_{\alpha}^s = (\boldsymbol{d}_{\alpha} \otimes \boldsymbol{n}_{\alpha} + \boldsymbol{n}_{\alpha} \otimes \boldsymbol{d}_{\alpha})/2$ with the slip direction $\boldsymbol{d}_{\alpha}$ and the slip plane normal $\boldsymbol{n}_{\alpha}$.

The elasto-viscoplastic constitutive model is derived from the underlying free energy potential of the material, which is defined by the Helmholtz free energy $\psi = \psi_e(\boldsymbol{\varepsilon}_e) + \psi_p(\gamma_{\text{acc}})$, additively split into an elastic part $\psi_e(\boldsymbol{\varepsilon}_e)$ and a plastic part $\psi_p(\gamma_{\text{acc}})$. With the definition of the total strain, the elastic strain is given by $\boldsymbol{\varepsilon}_e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p$. The plastic part is depending on the accumulated plastic slip γ_{acc} , defined as $\gamma_{\text{acc}} = \sum_{\alpha} \int |\dot{\gamma}_{\alpha}| dt$. This leads to the set of internal variables $\boldsymbol{\alpha} = (\boldsymbol{\varepsilon}_p, \gamma_{\text{acc}})$. To derive the constitutive model in a thermodynamically consistent manner, the (isothermal) Clausius-Duhem inequality $-\dot{\psi} + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} \geq 0$ must be evaluated. Computing the time derivative of the Helmholtz free energy and rearranging the terms, the Clausius-Duhem inequality reads:

$$\left(\boldsymbol{\sigma} - \frac{\partial \psi_e(\boldsymbol{\varepsilon}_e)}{\partial \boldsymbol{\varepsilon}_e} \right) : \dot{\boldsymbol{\varepsilon}} + \frac{\partial \psi_e(\boldsymbol{\varepsilon}_e)}{\partial \boldsymbol{\varepsilon}_e} : \dot{\boldsymbol{\varepsilon}}_p - \frac{\partial \psi_p(\gamma_{\text{acc}})}{\partial \gamma_{\text{acc}}} : \dot{\gamma}_{\text{acc}} \geq 0. \quad (9.4)$$

Following the arguments of Coleman and Noll [371], the state law for the stress is given by

$$\boldsymbol{\sigma} := \frac{\partial \psi_e(\boldsymbol{\varepsilon}_e)}{\partial \boldsymbol{\varepsilon}_e}. \quad (9.5)$$

Defining the thermodynamic conjugate driving force of isotropic hardening

$$q_p := \frac{\partial \psi_p(\gamma_{\text{acc}})}{\partial \gamma_{\text{acc}}} \quad (9.6)$$

and exploiting the definition of the plastic strain (9.3), the reduced dissipation inequality yields

$$\mathcal{D}_{\text{red}} = \left(\sum_{\alpha=1}^{n_{\text{slip}}} \dot{\gamma}_{\alpha} \underbrace{\boldsymbol{\sigma} : \mathbf{m}_{\alpha}^s}_{\tau_{\alpha}} \right) - q_p \dot{\gamma}_{\text{acc}} \geq 0. \quad (9.7)$$

Here, τ_{α} represents the resolved shear stress of slip system α . In our case, a thermodynamically consistent viscoplastic evolution equation for the plastic shear rate $\dot{\gamma}_{\alpha}$ is defined by a Perzyna-type formulation (e.g. [342]), yielding

$$\dot{\gamma}_{\alpha} = \text{sgn}(\tau_{\alpha}) \dot{\gamma}_0 \left\langle \frac{|\tau_{\alpha}| - (\tau_0^c + q_p)}{\tau_D} \right\rangle^p \quad (9.8)$$

with the reference shear rate $\dot{\gamma}_0$, the initial critical resolved shear stress τ_0^c , the drag stress τ_D and the rate sensitivity parameter p .

For computing the examples in Section 9.6, the specific choices of the elastic and plastic energies are given by

$$\psi_e(\boldsymbol{\varepsilon}_e) = \frac{1}{2} \boldsymbol{\varepsilon}_e : \mathbb{C}^{\text{grain}} : \boldsymbol{\varepsilon}_e \quad (9.9)$$

with $\mathbb{C}^{\text{grain}}$ representing the rotated cubic anisotropic elasticity tensor depending on the orientation of the considered grain and

$$\psi_p(\gamma_{\text{acc}}) = \frac{(\tau_{\infty} - \tau_0^c)^2}{h_0} \ln \left(\cosh \left(\frac{h_0 \gamma_{\text{acc}}}{\tau_{\infty} - \tau_0^c} \right) \right) + \frac{1}{2} h_{\infty} \gamma_{\text{acc}}^2, \quad (9.10)$$

which describes a nonlinear isotropic hardening of Voce-type plus an additional linear hardening with the saturation stress τ_{∞} , the initial hardening rate h_0 and the linear hardening modulus h_{∞} (see e.g. [372, 373]). These definitions of the energies lead to the explicit forms of the stress

$$\boldsymbol{\sigma} = \mathbb{C}^{\text{grain}} : \boldsymbol{\varepsilon}_e \quad (9.11)$$

and the thermodynamic conjugated driving force of isotropic hardening

$$q_p = (\tau_{\infty} - \tau_0^c) \tanh \left(\frac{h_0 \gamma_{\text{acc}}}{\tau_{\infty} - \tau_0^c} \right) + h_{\infty} \gamma_{\text{acc}}. \quad (9.12)$$

With Equation (9.12) the critical resolved shear stress τ^c is defined as

$$\tau^c := \tau_0^c + q_p = \tau_0^c + (\tau_\infty - \tau_0^c) \tanh \left(\frac{h_0 \gamma_{\text{acc}}}{\tau_\infty - \tau_0^c} \right) + h_\infty \gamma_{\text{acc}}. \quad (9.13)$$

Time discretization and numerical solution

In order to solve Equations (9.11) and (9.13), the flow rule for $\dot{\epsilon}_p$ as well as the evolution equation for the shear rate $\dot{\gamma}_\alpha$ (9.8) are discretized by an implicit Euler scheme, yielding

$$\epsilon_p^{n+1} = \epsilon_p^n + \Delta \epsilon_p^{n+1} \quad \text{with} \quad \Delta \epsilon_p^{n+1} = \sum_{\alpha=1}^{n_{\text{slip}}} \Delta \gamma_\alpha^{n+1} \mathbf{m}_\alpha^s \quad (9.14)$$

and

$$\gamma_\alpha^{n+1} = \gamma_\alpha^n + \Delta \gamma_\alpha^{n+1} \quad \text{with} \quad \Delta \gamma_\alpha^{n+1} = \Delta t \operatorname{sgn}(\tau_\alpha^{n+1}) \dot{\gamma}_0 \left\langle \frac{|\tau_\alpha^{n+1}| - \tau^{c,n+1}}{\tau_D} \right\rangle^p, \quad (9.15)$$

respectively. The accumulated plastic slip rate $\dot{\gamma}_{\text{acc}}$ is discretized in the same way leading to

$$\gamma_{\text{acc}}^{n+1} = \gamma_{\text{acc}}^n + \Delta \gamma_{\text{acc}}^{n+1} \quad \text{with} \quad \Delta \gamma_{\text{acc}}^{n+1} = \sum_{\alpha}^{n_{\text{slip}}} |\Delta \gamma_\alpha^{n+1}|. \quad (9.16)$$

To improve the robustness of the numerical solution scheme the power-type creep law is regularized using the regularization scheme described in [343]. Choosing $(\boldsymbol{\sigma}, \tau^c)$ as primary unknowns, the set of nonlinear equations, which needs to be solved on material point level, is given by Equation (9.11) with the definition of the total strain and Equation (9.13) with the definition of the thermodynamic conjugate driving force of isotropic hardening:

$$\begin{pmatrix} \mathbf{r}_\sigma \\ r_{\tau^c} \end{pmatrix} := \begin{pmatrix} (\mathbb{C}^{\text{grain}})^{-1} : \boldsymbol{\sigma}^{n+1} - \boldsymbol{\epsilon}^{n+1} + \boldsymbol{\epsilon}_p^{n+1} \\ \left(\tau_0^c + (\tau_\infty - \tau_0^c) \tanh \left(\frac{h_0 \gamma_{\text{acc}}^{n+1}}{\tau_\infty - \tau_0^c} \right) + h_\infty \gamma_{\text{acc}}^{n+1} - \tau^{c,n+1} \right) / \tau_0 \end{pmatrix} = \mathbf{0}, \quad (9.17)$$

where the parameter τ_0 is introduced to obtain a unit-free residual vector. The given set of nonlinear equations is solved using Newton's method.

9.4 FFT-based microstructure simulation

To solve the microscopic balance of linear momentum (9.1), we use the FFT-based method [11, 12]. Therefore, a homogeneous reference material, defined by the isotropic elasticity tensor $\mathbb{C}^0$ is introduced [125, 131], which is used to transfer the balance equation for the inhomogeneous

microstructure into a balance equation for an equivalent homogeneous microstructure yielding

$$\begin{aligned}\operatorname{div}(\mathbb{C}^0 : \varepsilon) + \operatorname{div}(\boldsymbol{\tau}) &= \mathbf{0} & \forall \mathbf{x} \in \Omega \\ \boldsymbol{\tau} &= \boldsymbol{\sigma} - \mathbb{C}^0 : \varepsilon \\ \varepsilon &= \bar{\varepsilon} + \tilde{\varepsilon}.\end{aligned}\tag{9.18}$$

Here, the homogeneous reference material is subjected to the polarization stress $\boldsymbol{\tau}$, which describes the difference between the stress in the real microstructure and the stress in the homogeneous reference material. The microscopic boundary value problem is again closed, by considering the aforementioned periodic boundary conditions. To solve this auxiliary problem, its Fourier transformation can be used [151]. The general definitions of the discrete Fourier transform and its inverse for an arbitrary field, such as the displacement field u_k , are given by

$$\hat{u}_k(\boldsymbol{\xi}) = \frac{1}{n} \sum_{\mathbf{x} \in \mathcal{R}} u_k(\mathbf{x}) \exp(-\boldsymbol{\xi} \cdot \mathbf{x}) \tag{9.19}$$

$$\text{and } u_k(\mathbf{x}) = \sum_{\boldsymbol{\xi} \in \mathcal{T}} \hat{u}_k(\boldsymbol{\xi}) \exp(\boldsymbol{\xi} \cdot \mathbf{x}) \tag{9.20}$$

with $(\hat{\cdot})$ defining the Fourier representation of the corresponding field depending on the set of Fourier modes $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^T$ with

$$\xi_j(k) = \imath \frac{2\pi}{L_j} k \quad \text{and} \quad -\frac{N_j}{2} < k < \frac{N_j}{2} - 1 \tag{9.21}$$

for a unit cell with a side length L_j discretized by an odd number of grid points N_j in the j -th direction and a total number of grid points n . Considering a quadratic unit cell the angular wave number is given by $h = 2\pi/L$. Furthermore, $\imath = \sqrt{-1}$ represents the imaginary unit and τ is the chosen set of wave vectors. For the auxiliary problem (9.18), this leads to

$$\hat{\varepsilon}(\boldsymbol{\xi}) = \begin{cases} -\hat{\Gamma}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}(\boldsymbol{\xi}) & \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\varepsilon} & \forall \boldsymbol{\xi} = \mathbf{0} \end{cases}, \tag{9.22}$$

which is known as Lippmann-Schwinger equation in Fourier space [118]. The Green's operator in Fourier space $\hat{\Gamma}^0(\boldsymbol{\xi})$ is explicitly known and defined as

$$\hat{\Gamma}_{ijkl}^0(\boldsymbol{\xi}) = \frac{1}{2} \left(\hat{A}_{ik}^{-1}(\boldsymbol{\xi}) \xi_l \xi_j + \hat{A}_{il}^{-1}(\boldsymbol{\xi}) \xi_k \xi_j \right) \tag{9.23}$$

for small strains, where $\hat{A}_{ik}(\boldsymbol{\xi}) = \mathbb{C}_{ijkl}^0 \xi_j \xi_l$ represents the acoustic tensor and $\hat{G}_{ik}(\boldsymbol{\xi}) = \hat{A}_{ik}^{-1}(\boldsymbol{\xi})$ is Green's function in Fourier space.

The solution of the Lippmann-Schwinger equation in Fourier space 9.22 is accompanied by numerical artifacts (known as Gibbs oscillations [19]), which is discussed in Subsection 9.4.1. Furthermore, in Subsection 9.4.2 the basic scheme of Moulinec and Suquet [11, 12] and two fast gradient solvers used to solve the auxiliary problem (9.18) are reviewed.

9.4.1 Finite-difference approximations of Green's operator

A well-known numerical artifact of a Fourier approximation of any function $f(\boldsymbol{x})$ relies on considering only a finite set of Fourier modes for the computation of the Fourier series, which leads to ringing artifacts (known as Gibbs oscillations [19]) in the case of sharp contrasts in any local property. While the displacement fields within the microstructure are continuous (if no microstructural cracks are considered), this is not the case for the microstructural stress and strain fields. To smooth the jumps within these fields, the derivatives may be computed using finite difference based approximations. In the following, we briefly discuss the application of second and higher order central difference approximations in this context [29, 231] and the rotated discretization of Willot [30], which is equivalent to an averaged forward-backward difference approximation [207].

9.4.1.1 Second and higher order central difference approximation

The analytic gradient of the inverse Fourier transform of any field, such as the displacement field u_k , can be easily computed by

$$u_{k,l}(\boldsymbol{x}) = \frac{\partial u_k}{\partial x_l} = \sum_{\boldsymbol{\xi} \in \mathcal{T}} \xi_l \hat{u}_k(\boldsymbol{\xi}) \exp(\boldsymbol{\xi} \cdot \boldsymbol{x}). \quad (9.24)$$

Considering a second order central difference approximation for the gradient operator

$$u_{k,l}(\boldsymbol{x}) \approx \frac{u_k(\boldsymbol{x} + \Delta x_l \boldsymbol{e}_l) - u_k(\boldsymbol{x} - \Delta x_l \boldsymbol{e}_l)}{2\Delta x_l} + \mathcal{O}(\Delta x_l^2), \quad (9.25)$$

where higher order terms $\mathcal{O}(\Delta x_l^2)$ are neglected, the second order central difference approximation of the inverse Fourier transform reads

$$\begin{aligned} u_{k,l}(\mathbf{x}) &\approx \sum_{\boldsymbol{\xi} \in \mathcal{T}} \hat{u}_k(\boldsymbol{\xi}) \frac{\exp(\boldsymbol{\xi} \cdot (\mathbf{x} + \Delta x_l \mathbf{e}_l)) - \exp(\boldsymbol{\xi} \cdot (\mathbf{x} - \Delta x_l \mathbf{e}_l))}{2\Delta x_l} \\ &\approx \sum_{\boldsymbol{\xi} \in \mathcal{T}} \underbrace{i \frac{\sin(hK_l \Delta x_l)}{\Delta x_l}}_{\xi_l^c} \hat{u}_k(\boldsymbol{\xi}) \exp(\boldsymbol{\xi} \cdot \mathbf{x}) \end{aligned} \quad (9.26)$$

with the modified Fourier modes ξ_l^c . Considering the same approximation for the divergence operator, this leads to a modified Green's operator in Fourier space $\hat{\Gamma}_{ijkl}^0(\boldsymbol{\xi}^c)$ yielding

$$\hat{\Gamma}_{ijkl}^0(\boldsymbol{\xi}^c) = \frac{1}{2} \left(\hat{A}_{ik}^{-1}(\boldsymbol{\xi}^c) \xi_l^c \xi_j^c + \hat{A}_{il}^{-1}(\boldsymbol{\xi}^c) \xi_k^c \xi_j^c \right). \quad (9.27)$$

The modified Green's operator can be used in Equation (9.22) to reduce the effect of Gibbs oscillations for the FFT-based microstructure simulation.

To increase the accuracy of the central difference approximation, higher order approximations can be used [231]. The corresponding modified Fourier modes ξ_l^c are shown below for three different orders:

$$\text{fourth order: } \xi_l^c = i \left[\frac{8 \sin(hK_l \Delta x_l)}{6\Delta x_l} - \frac{\sin(2hK_l \Delta x_l)}{6\Delta x_l} \right]$$

$$\text{sixth order: } \xi_l^c = i \left[\frac{9 \sin(hK_l \Delta x_l)}{6\Delta x_l} - \frac{3 \sin(2hK_l \Delta x_l)}{10\Delta x_l} + \frac{\sin(3hK_l \Delta x_l)}{30\Delta x_l} \right]$$

$$\text{eighth order: } \xi_l^c = i \left[\frac{8 \sin(hK_l \Delta x_l)}{5\Delta x_l} - \frac{2 \sin(2hK_l \Delta x_l)}{5\Delta x_l} + \frac{8 \sin(3hK_l \Delta x_l)}{105\Delta x_l} - \frac{\sin(4hK_l \Delta x_l)}{140\Delta x_l} \right]$$

9.4.1.2 Averaged forward-backward difference approximation

Instead of using a central difference approximation a forward and backward difference approximation was used in [30, 227] for the gradient and the divergence operator, respectively. Then, the gradient of the displacements and the divergence of the stress yield

$$u_{k,l}(\mathbf{x}) \approx \frac{u_k(\mathbf{x} + \Delta x_l \mathbf{e}_l) - u_k(\mathbf{x})}{\Delta x_l} + \mathcal{O}(\Delta x_l^2) \quad (9.28)$$

$$\sigma_{ij,j}(\mathbf{x}) \approx \frac{\sigma_{ij}(\mathbf{x}) - \sigma_{ij}(\mathbf{x} - \Delta x_j \mathbf{e}_j)}{\Delta x_j} + \mathcal{O}(\Delta x_j^2) \quad (9.29)$$

Neglecting again the higher order terms $\mathcal{O}(\Delta x_l^2)$, the corresponding difference approximations of the inverse Fourier transform read

$$\begin{aligned} u_{k,l}(\mathbf{x}) &\approx \sum_{\boldsymbol{\xi} \in \mathcal{T}} \hat{u}_k(\boldsymbol{\xi}) \frac{\exp(\boldsymbol{\xi} \cdot (\mathbf{x} + \Delta x_l \mathbf{e}_l)) - \exp(\boldsymbol{\xi} \cdot \mathbf{x})}{\Delta x_l} \\ &\approx \sum_{\boldsymbol{\xi} \in \mathcal{T}} \underbrace{\frac{\exp(\boldsymbol{\xi} \cdot \Delta x_l \mathbf{e}_l) - 1}{\Delta x_l}}_{\xi_l^{\text{fw}}} \hat{u}_k(\boldsymbol{\xi}) \exp(\boldsymbol{\xi} \cdot \mathbf{x}) \end{aligned} \quad (9.30)$$

$$\begin{aligned} \sigma_{ij,j}(\mathbf{x}) &\approx \sum_{\boldsymbol{\xi} \in \mathcal{T}} \hat{\sigma}_{ij}(\boldsymbol{\xi}) \frac{\exp(\boldsymbol{\xi} \cdot \mathbf{x}) - \exp(\boldsymbol{\xi} \cdot (\mathbf{x} - \Delta x_j \mathbf{e}_j))}{\Delta x_j} \\ &\approx \sum_{\boldsymbol{\xi} \in \mathcal{T}} \underbrace{\frac{1 - \exp(-\boldsymbol{\xi} \cdot \Delta x_j \mathbf{e}_j)}{\Delta x_j}}_{\xi_j^{\text{bw}}} \hat{\sigma}_{ij}(\boldsymbol{\xi}) \exp(\boldsymbol{\xi} \cdot \mathbf{x}) \\ &\approx \sum_{\boldsymbol{\xi} \in \mathcal{T}} -\xi_j^{\text{fw},*} \hat{\sigma}_{ij}(\boldsymbol{\xi}) \exp(\boldsymbol{\xi} \cdot \mathbf{x}) \end{aligned} \quad (9.31)$$

with $*$ denoting the complex conjugate. Unlike the central difference approximation discussed in Section 9.4.1.1, this forward-backward approximation breaks symmetry, such that the computed local fields for a symmetric unit cell will not be symmetric. To solve this problem, also an approximation based on a rotated grid was proposed in [30, 227]. This formulation is equivalent to an averaged forward-backward approximation [207], which is explained below for the 2D case. Considering the averaged forward finite difference approximation for the gradient operator, the finite difference approximation is evaluated at $u_k(x_1, x_2)$ and $u_k(x_1, x_2 + \Delta x_2)$ as well as at $u_k(x_1, x_2)$ and $u_k(x_1 + \Delta x_1, x_2)$ and then averaged for the 1-direction and 2-direction, respectively, while higher order terms are again neglected:

$$\begin{aligned} u_{k,1}(x_1, x_2) &\approx \frac{1}{2} \left(\frac{u_k(x_1 + \Delta x_1, x_2) - u_k(x_1, x_2)}{\Delta x_1} \right. \\ &\quad \left. + \frac{u_k(x_1 + \Delta x_1, x_2 + \Delta x_2) - u_k(x_1, x_2 + \Delta x_2)}{\Delta x_1} \right) \end{aligned} \quad (9.32)$$

$$\begin{aligned} u_{k,2}(x_1, x_2) &\approx \frac{1}{2} \left(\frac{u_k(x_1, x_2 + \Delta x_2) - u_k(x_1, x_2)}{\Delta x_2} \right. \\ &\quad \left. + \frac{u_k(x_1 + \Delta x_1, x_2 + \Delta x_2) - u_k(x_1 + \Delta x_1, x_2)}{\Delta x_2} \right). \end{aligned} \quad (9.33)$$

The corresponding difference approximations of the inverse Fourier transform read

$$\begin{aligned}
 u_{k,1}(x_1, x_2) &\approx \sum_{\xi \in \mathcal{T}} \frac{\hat{u}_k(\xi_1, \xi_2)}{2 \Delta x_1} \left(\exp(\xi_1 x_1) \exp(\xi_1 \Delta x_1) \exp(\xi_2 x_2) - \exp(\xi_1 x_1) \exp(\xi_2 x_2) \right. \\
 &\quad \left. + \exp(\xi_1 x_1) \exp(\xi_1 \Delta x_1) \exp(\xi_2 x_2) \exp(\xi_2 \Delta x_2) - \exp(\xi_1 x_1) \exp(\xi_2 x_2) \exp(\xi_2 \Delta x_2) \right) \\
 &\approx \sum_{\xi \in \mathcal{T}} \frac{\hat{u}_k(\xi_1, \xi_2)}{2 \Delta x_1} \exp(\xi_1 x_1) \exp(\xi_2 x_2) \left((\exp(\xi_1 \Delta x_1) - 1)(\exp(\xi_2 \Delta x_2) + 1) \right) \quad (9.34)
 \end{aligned}$$

$$\begin{aligned}
 u_{k,2}(x_1, x_2) &\approx \sum_{\xi \in \mathcal{T}} \frac{\hat{u}_k(\xi_1, \xi_2)}{2 \Delta x_2} \left(\exp(\xi_1 x_1) \exp(\xi_2 x_2) \exp(\xi_2 \Delta x_2) - \exp(\xi_1 x_1) \exp(\xi_2 x_2) \right. \\
 &\quad \left. + \exp(\xi_1 x_1) \exp(\xi_1 \Delta x_1) \exp(\xi_2 x_2) \exp(\xi_2 \Delta x_2) - \exp(\xi_1 x_1) \exp(\xi_1 \Delta x_1) \exp(\xi_2 x_2) \right) \\
 &\approx \sum_{\xi \in \mathcal{T}} \frac{\hat{u}_k(\xi_1, \xi_2)}{2 \Delta x_2} \exp(\xi_1 x_1) \exp(\xi_2 x_2) \left((\exp(\xi_1 \Delta x_1) + 1)(\exp(\xi_2 \Delta x_2) - 1) \right) \quad (9.35)
 \end{aligned}$$

$$\Rightarrow u_{k,l}(\xi) \approx \sum_{\xi \in \mathcal{T}} \underbrace{\left[\frac{1}{2 \Delta x_1} (\exp(\xi_1 \Delta x_1) - 1)(\exp(\xi_2 \Delta x_2) + 1) \right]}_{\xi_l^{\text{afw}}} \hat{u}_k(\xi) \exp(\xi \cdot x). \quad (9.36)$$

Considering the averaged backward finite difference approximation for the divergence operator, the finite difference approximation is evaluated at $u_k(x_1, x_2)$ and $u_k(x_1, x_2 - \Delta x_2)$ as well as at $u_k(x_1, x_2)$ and $u_k(x_1 - \Delta x_1, x_2)$ and then averaged for the 1-direction and 2-direction, respectively. Using the same ideas as above, this leads to:

$$\sigma_{ij,j}(\xi) \approx \sum_{\xi \in \mathcal{T}} \underbrace{-\xi_j^{\text{afw},*}}_{\xi_j^{\text{abw}}} \hat{\sigma}_{ij}(\xi) \exp(\xi \cdot x). \quad (9.37)$$

Utilizing the modified Fourier modes ξ^{afw} and ξ^{abw} , the modified Green's operator in Fourier space $\hat{\Gamma}_{ijkl}^0(\xi^{\text{afw/abw}})$ considering the averaged forward-backward finite difference approximation yields

$$\hat{\Gamma}_{ijkl}^0(\xi^{\text{afb}}) = \frac{1}{2} \left((\mathbb{C}_{ijkl}^0 \xi_j^{\text{afw}} \xi_l^{\text{abw}})^{-1} \xi_l^{\text{afw}} \xi_j^{\text{abw}} + (\mathbb{C}_{ijkl}^0 \xi_j^{\text{afw}} \xi_k^{\text{abw}})^{-1} \xi_k^{\text{afw}} \xi_j^{\text{abw}} \right). \quad (9.38)$$

This modified Green's operator does not break symmetry and can therefore also be used to reduce the effect of Gibbs oscillations for the FFT-based microstructure simulation.

9.4.2 Spectral solution schemes

To solve the auxiliary problem described in Equation (9.18), Moulinec and Suquet proposed to use a fixed point iteration scheme, known as the basic scheme, and summarized in Subsection 9.4.2.1. This scheme can be interpreted as gradient decent method, which minimizes the total energy in the unit cell. To improve the efficiency of this scheme, several methods have been proposed. In this work we will focus on fast gradient methods (Subsection 9.4.2.2 and 9.4.2.3), which additionally consider a momentum term within the iteration.

9.4.2.1 Basic fixed point scheme

In [195] it was shown, that solving the microscopic balance of linear momentum (Equation (9.1) with the definition of the stress in Equation (9.5))

$$\operatorname{div} \left[\frac{\partial \psi_e(\boldsymbol{\varepsilon}_e)}{\partial \boldsymbol{\varepsilon}_e} \right] = \mathbf{0} \quad \forall \mathbf{x} \in \Omega \quad (9.39)$$

is equivalent to minimizing the elastic energy within the considered unit cell

$$\bar{\psi}(\boldsymbol{\varepsilon}_e) = \int_{\Omega} \psi(\boldsymbol{\varepsilon}_e) \, dV \rightarrow \min_{\boldsymbol{\varepsilon}_e}. \quad (9.40)$$

This energy minimum can be found by using a gradient decent method yielding:

$$\boldsymbol{\varepsilon}^{i+1} = \boldsymbol{\varepsilon}^i - \alpha^i \operatorname{grad} [\bar{\psi}(\boldsymbol{\varepsilon}_e^i)] \quad (9.41)$$

$$= \boldsymbol{\varepsilon}^i - \alpha^i \boldsymbol{\Gamma} * \left[\frac{\partial \psi_e(\boldsymbol{\varepsilon}_e^i)}{\partial \boldsymbol{\varepsilon}_e} \right], \quad (9.42)$$

in which α^i denotes the step size, $\boldsymbol{\Gamma}$ indicates the Green's operator and $*$ represents the convolution integral. Using the equality $\boldsymbol{\varepsilon}^i = \bar{\boldsymbol{\varepsilon}} + \boldsymbol{\Gamma} * \boldsymbol{\varepsilon}^i$ the equation above can be rewritten as

$$\boldsymbol{\varepsilon}^{i+1} = \bar{\boldsymbol{\varepsilon}} - \alpha^i \boldsymbol{\Gamma} * \left[\frac{\partial \psi_e(\boldsymbol{\varepsilon}_e^i)}{\partial \boldsymbol{\varepsilon}_e} - \frac{1}{\alpha^i} \boldsymbol{\varepsilon}^i \right]. \quad (9.43)$$

Finally, by defining the elasticity tensor of the homogeneous reference material as $\mathbb{C}^0 = \frac{1}{\alpha^i} \mathbb{I}$ with $\mathbb{I}$ being the fourth order identity tensor and $\frac{1}{\alpha^i} = \frac{c_-^i + c_+^i}{2}$ while c_-^i , c_+^i are the minimal and maximal eigenvalues of the material tangent as well as defining the Green's operator for the

strain as $\Gamma^0 = \alpha^i \Gamma$, the aforementioned equation yields

$$\epsilon^{i+1} = \bar{\epsilon} - \Gamma^0 * \underbrace{\left[\frac{\partial \psi_e(\epsilon_e^i)}{\partial \epsilon_e} - \mathbb{C}^0 : \epsilon^i \right]}_{\tau^i} \quad (9.44)$$

and is equivalent to the basic scheme of Moulinec and Suquet [12], which is summarized in Algorithm 2.

Set: $i = 0, \epsilon^i(x) = \bar{\epsilon}$
do while $\sum_{x \in \Omega} \|\epsilon^{i+1}(x) - \epsilon^i(x)\| / \|\bar{\epsilon}\| > tol$
 Set: $i = i + 1$
 Calc:
 a) $\sigma^i(x) = \sigma(x, \epsilon^i(x), \alpha^i(x))$
 b) $\tau^i(x) = \sigma^i(x) - \mathbb{C}^0 : \epsilon^i(x)$
 c) $\hat{\tau}^i(\xi) = \mathcal{FFT}\{\tau^i(x)\}$
 d) $\hat{\epsilon}^{i+1}(\xi) = \begin{cases} -\hat{\Gamma}^0(\xi) : \hat{\tau}^i(\xi) & \forall \xi \neq 0 \\ \bar{\epsilon} & \forall \xi = 0 \end{cases}$
 e) $\epsilon^{i+1}(x) = \mathcal{FFT}^{-1}\{\hat{\epsilon}^{i+1}(\xi)\}$
end

Algorithm 2: FFT-based basic scheme [12].

9.4.2.2 Nesterov's fast gradient method

In context of the FFT-based microstructure simulation Nesterov's fast gradient method was introduced in [217]. Therefore, the strain-like field $e^i = \epsilon^i + \beta^i (\epsilon^i - \epsilon^{i-1})$ is introduced, where additionally to the current strain, also the strain of the last iteration is involved. This momentum term leads to an accelerated convergence behavior, while its influence is scaled by the momentum coefficient $\beta^{i+1} = \frac{i-1}{i+2}$. This leads to the following recursion for computing the microstructural strain field (cf. (9.43)):

$$\epsilon^{i+1} = \bar{\epsilon} - \alpha^i \Gamma * \left[\frac{\partial \psi_e(e_e^i)}{\partial \epsilon_e} - \frac{1}{\alpha^i} e^i \right], \quad (9.45)$$

while $\frac{1}{\alpha^i} = c_+^i$ is chosen. To increase the convergence speed of the method, a speed restart can be performed, i.e. the value for the momentum coefficient β^{i+1} is reset when the speed $s^i = \|\epsilon^i - \epsilon^{i-1}\|^2$ decreases. This results in Algorithm 2, while $i_{\min}$ is the minimal number of steps before a restart is performed.

```

Set:  $i = 0, s^i = 0, \boldsymbol{\varepsilon}^i(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}}, \mathbf{e}^i(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}}$ 
do while  $\sum_{\mathbf{x} \in \Omega} \|\boldsymbol{\varepsilon}^{i+1}(\mathbf{x}) - \boldsymbol{\varepsilon}^i(\mathbf{x})\| / \|\bar{\boldsymbol{\varepsilon}}\| > tol$ 
    Set:  $i = i + 1$ 
    Calc:
    a)  $\boldsymbol{\sigma}^i(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{x}, \mathbf{e}^i(\mathbf{x}), \boldsymbol{\alpha}^i(\mathbf{x}))$ 
    b)  $\boldsymbol{\tau}^i(\mathbf{x}) = \boldsymbol{\sigma}^i(\mathbf{x}) - \frac{1}{\alpha^i} \mathbf{e}^i(\mathbf{x})$ 
    c)  $\hat{\boldsymbol{\tau}}^i(\boldsymbol{\xi}) = \mathcal{FFT}\{\boldsymbol{\tau}^i(\mathbf{x})\}$ 
    d)  $\hat{\boldsymbol{\varepsilon}}^{i+1}(\boldsymbol{\xi}) = \begin{cases} -\alpha^i \hat{\boldsymbol{\Gamma}}(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}^i(\boldsymbol{\xi}) & \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\boldsymbol{\varepsilon}} & \forall \boldsymbol{\xi} = \mathbf{0} \end{cases}$ 
    e)  $\boldsymbol{\varepsilon}^{i+1}(\mathbf{x}) = \mathcal{FFT}^{-1}\{\hat{\boldsymbol{\varepsilon}}^{i+1}(\boldsymbol{\xi})\}$ 
    Calc:  $s^{i+1} = \|\boldsymbol{\varepsilon}^{i+1} - \boldsymbol{\varepsilon}^i\|^2$ 
    if  $\frac{s^{i+1}}{s^i} < s^i$  and  $i > i_{\min}$  then
        Set:  $\mathbf{e}^{i+1} = \boldsymbol{\varepsilon}^{i+1}$ 
        Set:  $i = 0$ 
    else
        Calc:  $\mathbf{e}^{i+1} = \boldsymbol{\varepsilon}^{i+1} + \frac{i-1}{i+2} (\boldsymbol{\varepsilon}^{i+1} - \boldsymbol{\varepsilon}^i)$ 
    end
end

```

Algorithm 3: FFT-based fast gradient method [217].

9.4.2.3 Heavy ball scheme

Next, let us consider the heavy ball scheme which has been introduced in [250] for the FFT-based microstructure simulation. Here, the strain of the last iteration $\boldsymbol{\varepsilon}^{i-1}$ is also involved in the recursion (cf. Equation (9.43)), and again weighted by a momentum coefficient β^i , yielding

$$\begin{aligned}
 \boldsymbol{\varepsilon}^{i+1} &= \bar{\boldsymbol{\varepsilon}} - \alpha^i \boldsymbol{\Gamma} * \left[\frac{\partial \psi_e(\boldsymbol{\varepsilon}_e^i)}{\partial \boldsymbol{\varepsilon}_e} - \frac{1}{\alpha^i} \boldsymbol{\varepsilon}^i \right] + \beta^i (\boldsymbol{\varepsilon}^i - \boldsymbol{\varepsilon}^{i-1}) \\
 \Leftrightarrow \boldsymbol{\varepsilon}^{i+1} &= \bar{\boldsymbol{\varepsilon}} - \alpha^i \boldsymbol{\Gamma} * \left[\frac{\partial \psi_e(\boldsymbol{\varepsilon}_e^i)}{\partial \boldsymbol{\varepsilon}_e} - \frac{1}{\alpha^i} \boldsymbol{\varepsilon}^i - \frac{\beta^i}{\alpha^i} (\boldsymbol{\varepsilon}^i - \boldsymbol{\varepsilon}^{i-1}) \right].
 \end{aligned} \tag{9.46}$$

The parameters α^i and β^i are chosen according to the formulae of Polyak [374]

$$\frac{1}{\alpha^i} = \left(\frac{\sqrt{c_-^i} + \sqrt{c_+^i}}{2} \right)^2 \quad \text{and} \quad \beta^i = \left(\frac{\sqrt{c_+^i} - \sqrt{c_-^i}}{\sqrt{c_+^i} + \sqrt{c_-^i}} \right)^2,$$

which leads to the following algorithm in the context of an FFT-based microstructure simulation:

```

Set:  $i = 0, \boldsymbol{\varepsilon}^i(\boldsymbol{x}) = \bar{\boldsymbol{\varepsilon}}$ 
do while  $\sum_{\boldsymbol{x} \in \Omega} \|\boldsymbol{\varepsilon}^{i+1}(\boldsymbol{x}) - \boldsymbol{\varepsilon}^i(\boldsymbol{x})\| / \|\bar{\boldsymbol{\varepsilon}}\| > tol$ 
    Set:  $i = i + 1$ 
    Calc:
    a)  $\boldsymbol{\sigma}^i(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{x}, \boldsymbol{\varepsilon}^i(\boldsymbol{x}), \boldsymbol{\alpha}^i(\boldsymbol{x}))$ 
    b)  $\boldsymbol{\tau}^i(\boldsymbol{x}) = \boldsymbol{\sigma}^i(\boldsymbol{x}) - \frac{1}{\alpha^i} \boldsymbol{\varepsilon}^i(\boldsymbol{x}) - \frac{\beta^i}{\alpha^i} (\boldsymbol{\varepsilon}^i - \boldsymbol{\varepsilon}^{i-1})$ 
    c)  $\hat{\boldsymbol{\tau}}^i(\boldsymbol{\xi}) = \mathcal{FFT}\{\boldsymbol{\tau}^i(\boldsymbol{x})\}$ 
    d)  $\hat{\boldsymbol{\varepsilon}}^{i+1}(\boldsymbol{\xi}) = \begin{cases} -\alpha^i \hat{\boldsymbol{\Gamma}}(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}^i(\boldsymbol{\xi}) & \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\boldsymbol{\varepsilon}} & \forall \boldsymbol{\xi} = \mathbf{0} \end{cases}$ 
    e)  $\boldsymbol{\varepsilon}^{i+1}(\boldsymbol{x}) = \mathcal{FFT}^{-1}\{\hat{\boldsymbol{\varepsilon}}^{i+1}(\boldsymbol{\xi})\}$ 
end

```

Algorithm 4: FFT-based heavy ball scheme [250].

9.5 Model order reduction using a reduced set of Fourier modes

The idea of the considered model order reduction technique is based on using only a reduced set of Fourier modes $\boldsymbol{\xi}_R$ to solve the convolution integral in Fourier space in terms of the FFT-based basic scheme. In this case, the strains in Fourier space are computed based on the reduced set of Fourier modes such that item d) in Algorithm 2 reads:

$$\hat{\boldsymbol{\varepsilon}}^{i+1}(\boldsymbol{\xi}_R) = \begin{cases} -\hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}_R) : \hat{\boldsymbol{\tau}}^i(\boldsymbol{\xi}_R) & \forall \boldsymbol{\xi} \neq \mathbf{0} \\ \bar{\boldsymbol{\varepsilon}} & \forall \boldsymbol{\xi} = \mathbf{0} \end{cases}. \quad (9.47)$$

Since this model order reduction technique is only concerned with solving the convolution integral in Fourier space, it is straightforward to combine it with the modified Green's operators and fast gradient solvers presented in Sections 9.4.1 and 9.4.2, respectively. Using the modified Green's operators, the modified Fourier modes are selected according to the considered sampling pattern and using the different fast gradient solvers, the Lippmann-Schwinger equation must be solved in Fourier space anyway (item d) for each solver).

The accuracy of this model order reduction technique strongly depends on the number, but also on the choice of the considered Fourier modes. Starting with a fixed sampling pattern [17], subsequently also a geometrically adapted sampling pattern [237] and a strain-based sampling pattern [38] were proposed to identify the Fourier modes. In the following subsections, the definitions of these sampling patterns are briefly discussed. In general the Fourier modes are arranged in a way, that the mean value is in the center and the higher modes are at the edge of the grid. The ideas of the sampling patterns are explained considering the 2D case, while a

3D extension is easily possible as shown in [237].

9.5.1 Fixed sampling pattern

The fixed sampling pattern is independent of the characteristics of the underlying microstructure or the microstructural evolution of the strain field, and is therefore defined before the simulation. Investigating different shapes for the sampling pattern, i.e. a circular, a squared or a star-shaped pattern, the most reliable choice was found to be the star-shaped sampling pattern [17]. Using this pattern, a high amount of low Fourier modes (near the center) are considered, which are needed to capture the general behavior of the microstructure, but also some higher Fourier modes are utilized, which are for example needed to capture local stress and strain peaks. In Figure 9.2 a sketch for defining the star-shaped sampling pattern is given.

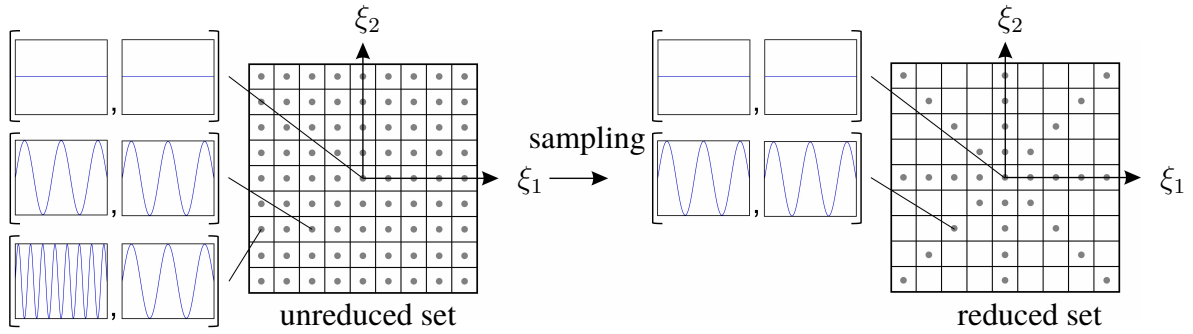


Figure 9.2: Idea of the fixed star-shaped sampling pattern [17].

9.5.2 Geometrically adapted sampling pattern

The hypothesis behind the geometrically adapted sampling pattern is that the microstructural mechanical fields, such as the strain or stress field, are strongly related to the distribution of phases within a microstructure, at least when considering elastic material behavior [237]. Using this sampling pattern and examining, for example, a two-phase microstructure, the representation of the phases within this microstructure is captured by the characteristic function

$$g(\mathbf{x}) = \begin{cases} 0 & \forall \mathbf{x} \in \Omega_{\text{Matrix}} \\ 1 & \forall \mathbf{x} \in \Omega_{\text{Inclusion}} \end{cases}. \quad (9.48)$$

This function is transformed into Fourier space. To obtain the best approximation of the function using only a reduced set of Fourier modes, the Fourier modes with the highest amplitudes $\hat{A}(\xi_1, \xi_2)$ must be used, which then define the sampling pattern, see Figure 9.3.

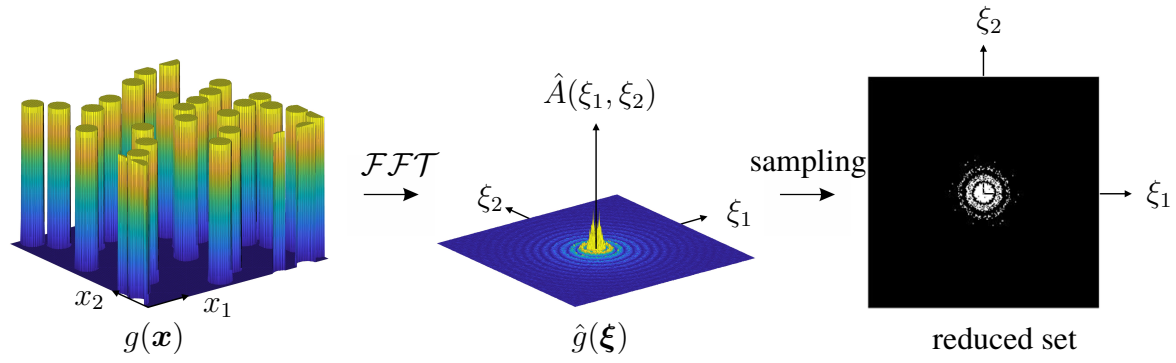


Figure 9.3: Idea of the geometrically adapted sampling pattern [237].

9.5.3 Strain-based sampling pattern

Since it is not trivial to define the geometrically adapted sampling for complex microstructures such as polycrystalline microstructures, or even for microstructures with evolving phases (e.g. considering solid-solid phase transformations), we introduced a strain-based sampling pattern in [38]. In this case, the sampling pattern is redefined after each load step depending on the norm of the microstructural strain field. As shown in Figure 9.4, the adaption procedure is similar to the one of the geometrically adapted sampling pattern. After computing the norm of the strain field in real space, it is transferred into Fourier space and the most accurate approximation is again reached by using the Fourier modes with the highest amplitudes $\hat{A}(\xi_1, \xi_2)$, which then define the strain-based sampling pattern.

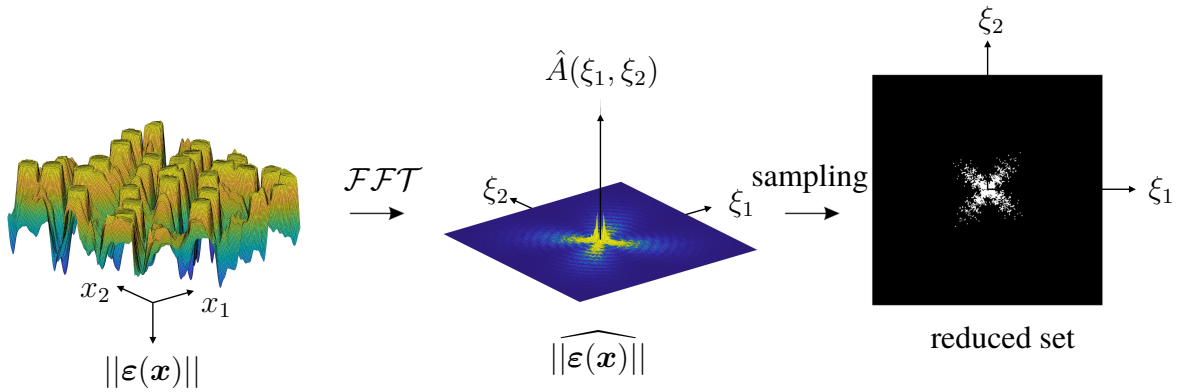


Figure 9.4: Idea of the strain-based sampling pattern after one specific load step [38].

9.6 Numerical examples

Several numerical examples are given below to explore the combination of using a reduced set of Fourier modes with modified Green's operators and fast gradient solvers. For each example, we consider a 2D plain strain setting, while we generally use the strain-based sampling pattern,

which was found to be the most accurate in [237]. To compare the performance of the model order reduction technique, the relative macroscopic and microscopic errors $\bar{\mathcal{E}}$ [%] and $\mathcal{E}$ [%] as well as the relative CPU times (using Fortran) for solving the Lippmann-Schwinger equation in Fourier space $t_{\text{LippEq}}^{\text{rel}}$ [%] and for computing one iteration in the context of the introduced solvers $t_{\text{Iter}}^{\text{rel}}$ [%] are defined as follows:

$$\bar{\mathcal{E}} = \frac{\|\bar{\boldsymbol{\sigma}} - \bar{\boldsymbol{\sigma}}^{\text{ref}}\|}{\|\bar{\boldsymbol{\sigma}}^{\text{ref}}\|}, \quad \mathcal{E} = \frac{1}{n} \sum_n \frac{\|\boldsymbol{\sigma}(n) - \boldsymbol{\sigma}(n)^{\text{ref}}\|}{\|\boldsymbol{\sigma}(n)^{\text{ref}}\|}, \quad t_{\text{LippEq}}^{\text{rel}} = \frac{t_{\text{LippEq}}}{t_{\text{LippEq}}^{\text{ref}}}, \quad t_{\text{Iter}}^{\text{rel}} = \frac{t_{\text{Iter}}}{t_{\text{Iter}}^{\text{ref}}},$$

where the index $(\cdot)^{\text{ref}}$ refers to computations performed using all Fourier modes ($\mathcal{R} = 100\%$).

9.6.1 Investigation on different discretizations

To investigate the effect of the modified Green's operators in the context of using a reduced set of Fourier modes, we consider three different examples: A microstructure with a circular inclusion with a small phase contrast (9.6.1.1), a microstructure with a squared inclusion with a high phase contrast (9.6.1.2), and a polycrystalline microstructure (9.6.1.3). In each case, we consider a linear elastic material behavior and use the basic fixed point scheme. The different solvers are compared in Section 9.6.2.

9.6.1.1 Circular inclusion with small phase contrast

In the first example, we study a microstructure with a centered circular inclusion of radius $r = 0.25L$, similar to the studies in [231], which is discretized by 255×255 grid points. The Lamé parameters of the matrix and inclusion are set to $\lambda^{\text{M}} = 0.6 \text{ MPa}$ and $\mu^{\text{M}} = 0.6 \text{ MPa}$ and $\lambda^{\text{I}} = 1.0 \text{ MPa}$ and $\mu^{\text{I}} = 1.0 \text{ MPa}$, respectively, and a macroscopic biaxial tension

$$\bar{\boldsymbol{\varepsilon}} = \begin{bmatrix} 0.01 & 0 \\ 0 & 0.01 \end{bmatrix}$$

is applied. In order to use a strain-based sampling pattern, this macroscopic strain is artificially prescribed within two load steps, such that the strain of the first load step is used to define the sampling pattern for the second load step. The results for the second load step of the stress

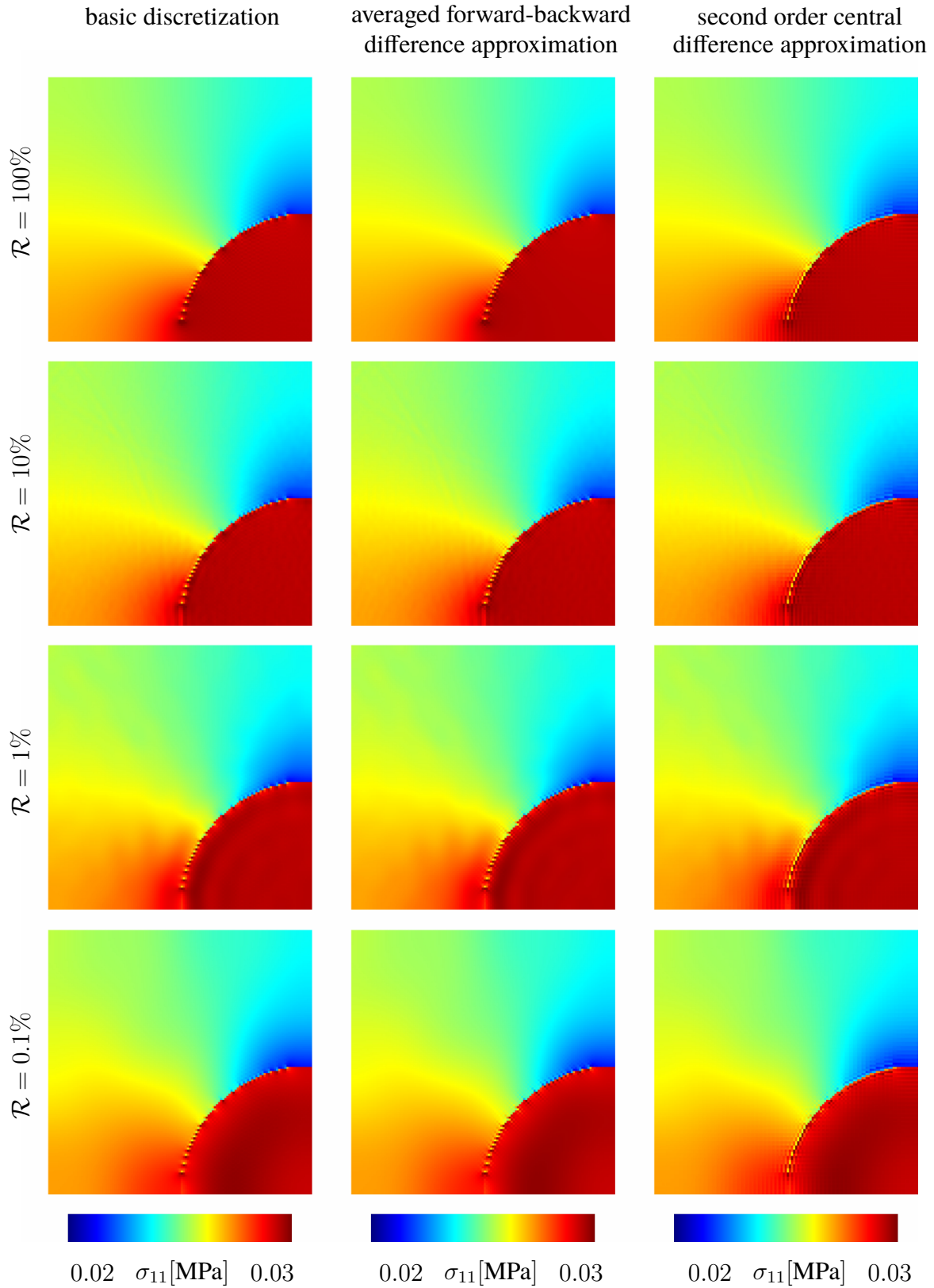


Figure 9.5: Comparison of σ_{11} for a circular inclusion considering the basic discretization, the averaged forward-backward and second order central difference approximation for varying $\mathcal{R}$.

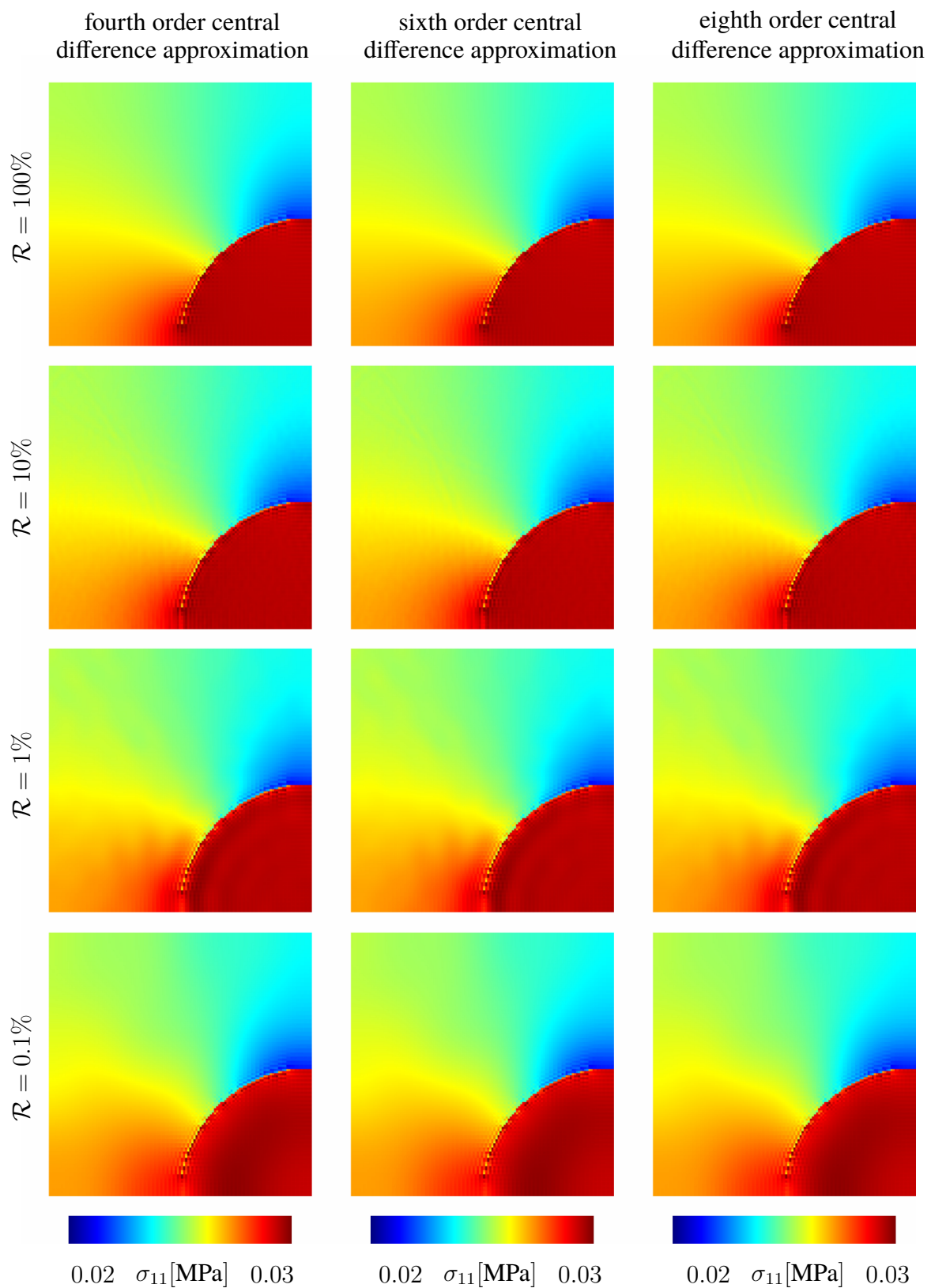


Figure 9.6: Comparison of σ_{11} for a circular inclusion considering the fourth, sixth and eighth order central difference approximation for varying $\mathcal{R}$.

component σ_{11} for the different discretizations considering a reduced amount of Fourier modes $\mathcal{R}$ [%] are shown in Figures 9.5 and 9.6 (only the upper left quarter is plotted), while the corresponding strain-based sampling patterns are depicted in Figures 9.7 and 9.8. In addition, Figure 9.9 displays the relative macroscopic and microscopic errors $\bar{\mathcal{E}}$ [%] and $\mathcal{E}$ [%] (with a logarithmic y-axis). Figure 9.10 shows the relative CPU times for solving the Lippmann-Schwinger equation in Fourier space $t_{\text{LippEq}}^{\text{rel}}$ [%] as well as the relative CPU times for computing

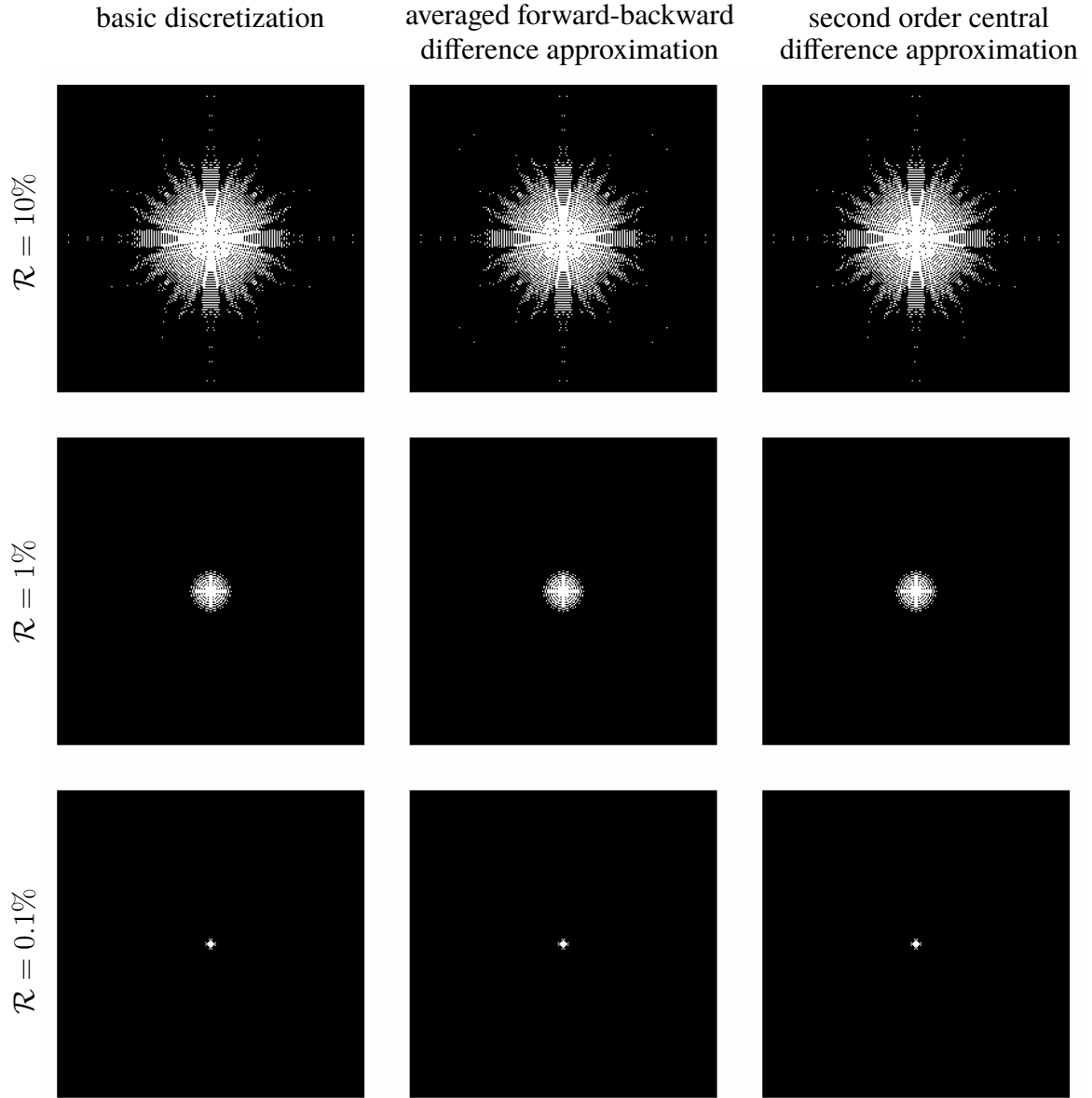


Figure 9.7: Comparison of the strain-based sampling patterns for a circular inclusion considering the basic discretization, the averaged forward-backward and second order central difference approximation for varying $\mathcal{R}$.

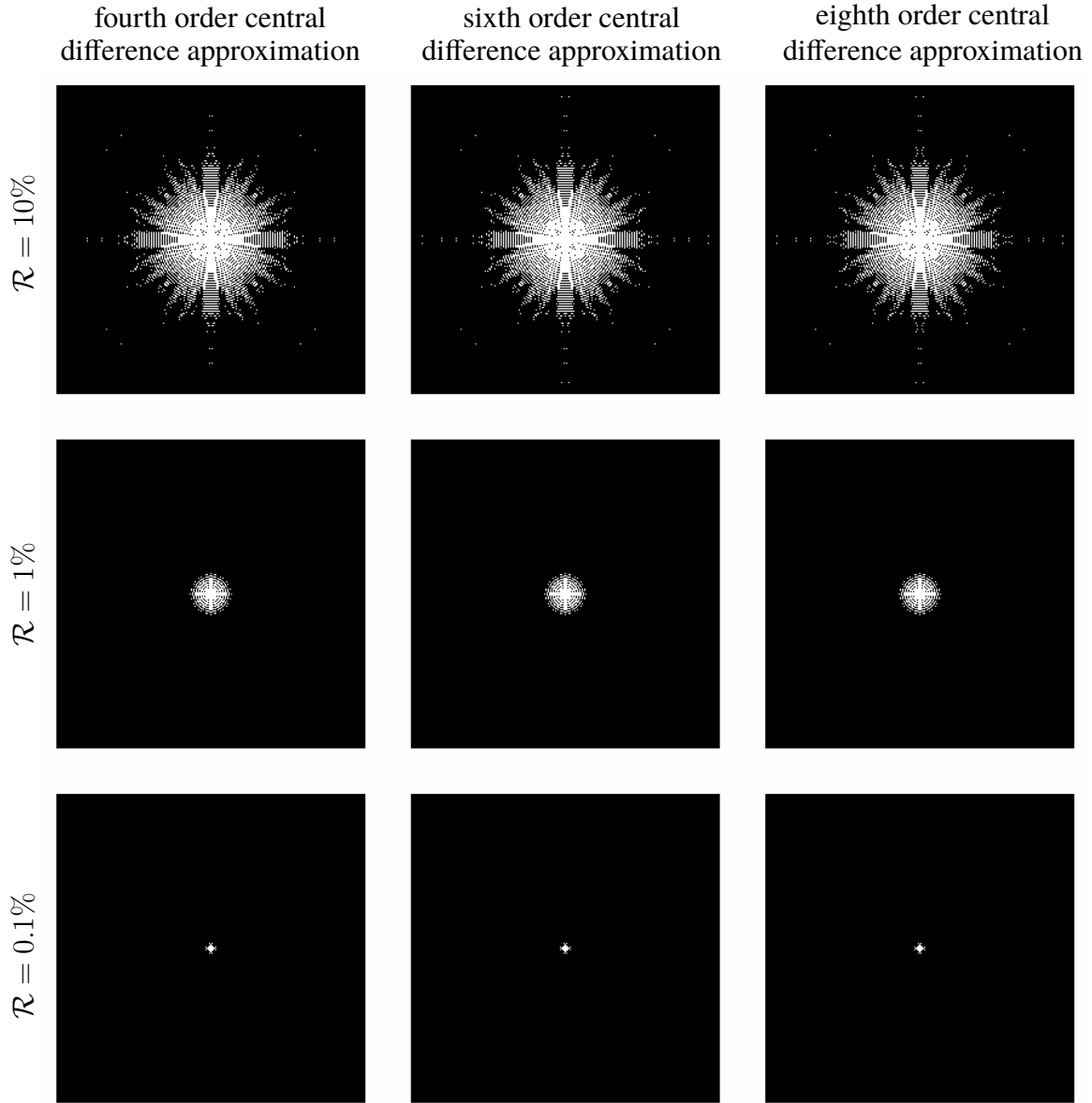


Figure 9.8: Comparison of the strain-based sampling patterns for a circular inclusion considering the fourth, sixth and eighth order central difference approximation for varying $\mathcal{R}$.

one iteration $t_{\text{Iter}}^{\text{rel}} [\%]$. Table 9.1 summarizes the number of iterations needed to reach equilibrium.

Comparing the stress distribution σ_{11} in Figures 9.5 and 9.6, it can be seen that the results computed based on a reduced set of Fourier modes ($\mathcal{R} < 100\%$) are always quite similar to the reference solution ($\mathcal{R} = 100\%$). Even considering only $\mathcal{R} = 0.1\%$ of Fourier modes, leads to relative macroscopic and microscopic errors (Figure 9.9) of only $\bar{\mathcal{E}} \approx 0.003\%$ and $\mathcal{E} \approx 0.4\%$. Although this is the case for all different types of discretizations, the typical characteristics of

the discretizations remain. While the basic discretization shows the typical ringing artifact, the averaged forward-backward difference approximation leads to checkerboarding and the different orders of the central difference approximations result in oscillatory behavior near the interface.

The strain-based sampling patterns in Figures 9.7 and 9.8 are also nearly independent of the discretizations. While small differences can be observed when considering a higher amount of Fourier modes (here $\mathcal{R} = 10\%$), no differences are visible when considering a very reduced amount of Fourier modes. Hence the dominant Fourier modes can be considered independent of the discretization. Since the different discretizations only reduce the effect of Gibbs oscillations that occur near the interface and are related to a truncation of high Fourier modes, these results are predictable, since these high Fourier modes are in general the first to be neglected in the context of the applied model order reduction technique.

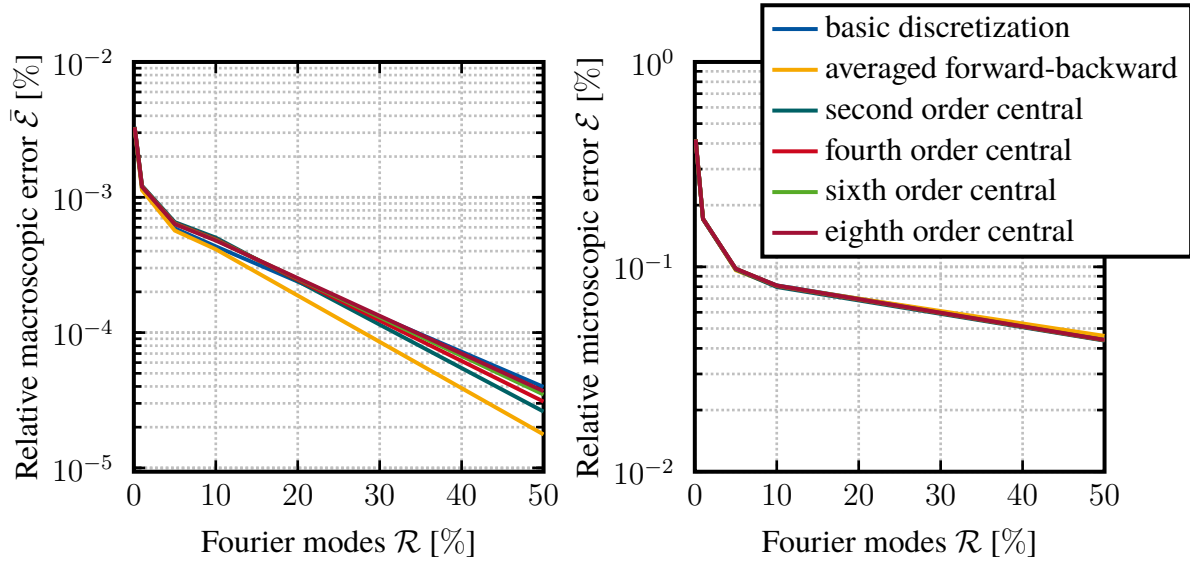


Figure 9.9: Error measurements for the microstructure with one circular inclusion. Left: Relative macroscopic error $\bar{\mathcal{E}}$ [%]. Right: Relative microscopic error $\mathcal{E}$ [%].

Figure 9.10 reveals that, independently of the discretization considered, using a reduced set of Fourier modes approximately linearly decreases the relative CPU time for solving the Lippmann-Schwinger equation in Fourier space to $t_{\text{LippEq}} \approx 0.1\%$. Consequently, also the relative CPU time for the computation of a complete iteration is approximately linearly reduced by a value of $t_{\text{Iter}} \approx 40\%$. Furthermore, as shown in Table 9.1, the number of iterations needed to reach equilibrium is more or less independent of the different discretizations and amounts of Fourier modes considered when examining a microstructure with a small phase contrast. Therefore, the total CPU time is reduced by approximately the same amount as the CPU time

per iteration.

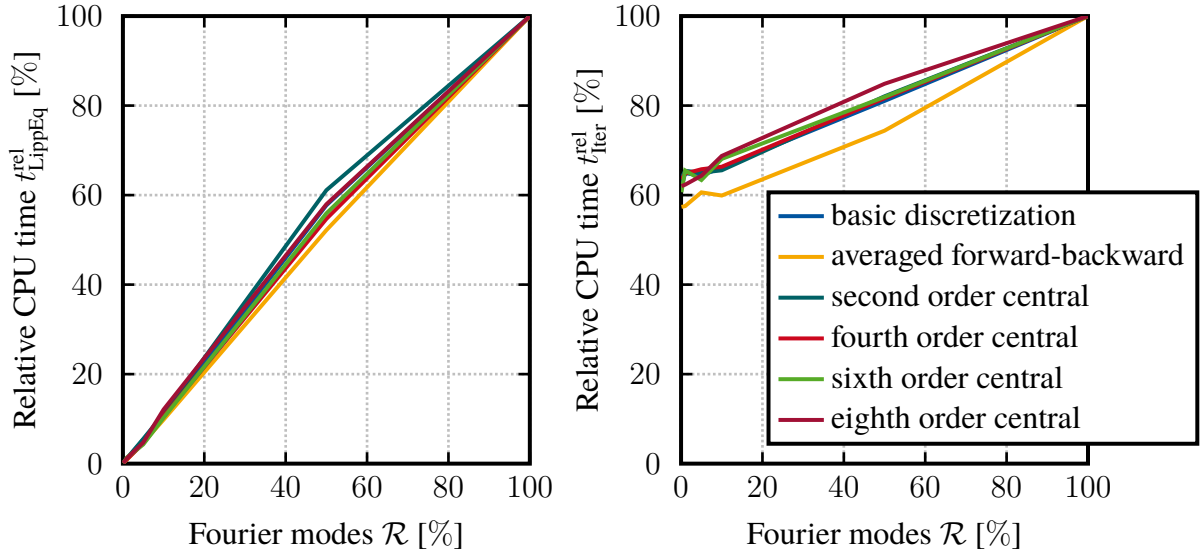


Figure 9.10: CPU time measurements for the microstructure with one circular inclusion. Left: Relative CPU time for solving the Lippmann-Schwinger equation in Fourier space $t_{\text{LippEq}}^{\text{rel}}$ [%]. Right: Relative CPU time for computing one iteration $t_{\text{iter}}^{\text{rel}}$ [%].

$\mathcal{R}$ [%]	100	50	10	5	1	0.1
basic discretization	8	7	8	8	8	9
averaged forward-backward	8	7	8	8	8	9
second order central	8	8	8	8	8	9
fourth order central	8	7	8	8	8	9
sixth order central	8	7	8	8	8	9
eighth order central	8	7	8	8	8	9

Table 9.1: Number of iterations needed to reach equilibrium for the different discretizations and different amounts of considered Fourier modes $\mathcal{R}$ [%] for the microstructure with one circular inclusion.

9.6.1.2 Squared inclusion with high phase contrast

The second example is similar to one found in [30] and deals with a microstructure with a centered squared inclusion of side length $L_I = 0.25L$, which is discretized by 511×511 grid points. The Lamé parameters of the matrix and inclusion phase are set to $\lambda^M = 1.0$ MPa and $\mu^M = 1.0$ MPa and $\lambda^I = 1000.0$ MPa and $\mu^I = 1000.0$ MPa, respectively, and the macroscopic shearing

$$\bar{\epsilon} = \begin{bmatrix} 0.0 & 0.01 \\ 0.01 & 0.0 \end{bmatrix}$$

is applied. This macroscopic strain is again artificially prescribed within two load steps, so that the strain of the first load step is used to define the strain-based sampling pattern. Since the differences between the different orders of the central difference approximation are rather small, in the following, only the second order central difference approximation is compared to the basic discretization and the averaged forward-backward difference approximation. The results are presented analogously to the first example: First, the distribution of the stress component σ_{12} for the second load step considering a reduced number of Fourier modes $\mathcal{R}$ [%] are shown for the different discretizations in Figure 9.11 (only the upper left quarter is plotted), while the corresponding strain-based sampling patterns are presented second in Figure 9.12. In Figure 9.13 the relative macroscopic and microscopic errors $\bar{\mathcal{E}}$ [%] and $\mathcal{E}$ [%] (with a logarithmic y-axis) are displayed. Finally, Figure 9.14 shows the relative CPU times for solving the Lippmann-Schwinger equation in Fourier space $t_{\text{LippEq}}^{\text{rel}}$ [%] as well as the relative CPU times for computing one iteration $t_{\text{Iter}}^{\text{rel}}$ [%]. The number of iterations needed to reach equilibrium are given in Table 9.2.

Comparing the results in Figure 9.11 as well as the relative macroscopic and microscopic errors in Figure 9.13, it becomes obvious, that the differences between the reference solution (computed with $\mathcal{R} = 100\%$) and the reduced simulations considering different $\mathcal{R} < 100\%$ are much higher for microstructures with high phase contrasts. Considering $\mathcal{R} = 0.1\%$ of the Fourier modes, the macroscopic and microscopic errors are given by $\bar{\mathcal{E}} \approx 1.3\%$ and $\mathcal{E} \approx 40\%$, respectively. Although, the characteristics of the different discretizations are hardly visible from the stress distributions resulting from the reduced simulations, the strain-based sampling patterns, shown in Figure 9.12, depend much more on the different discretizations (for the high phase contrast compared to the simulation of the low phase contrast microstructure discussed in the first example).

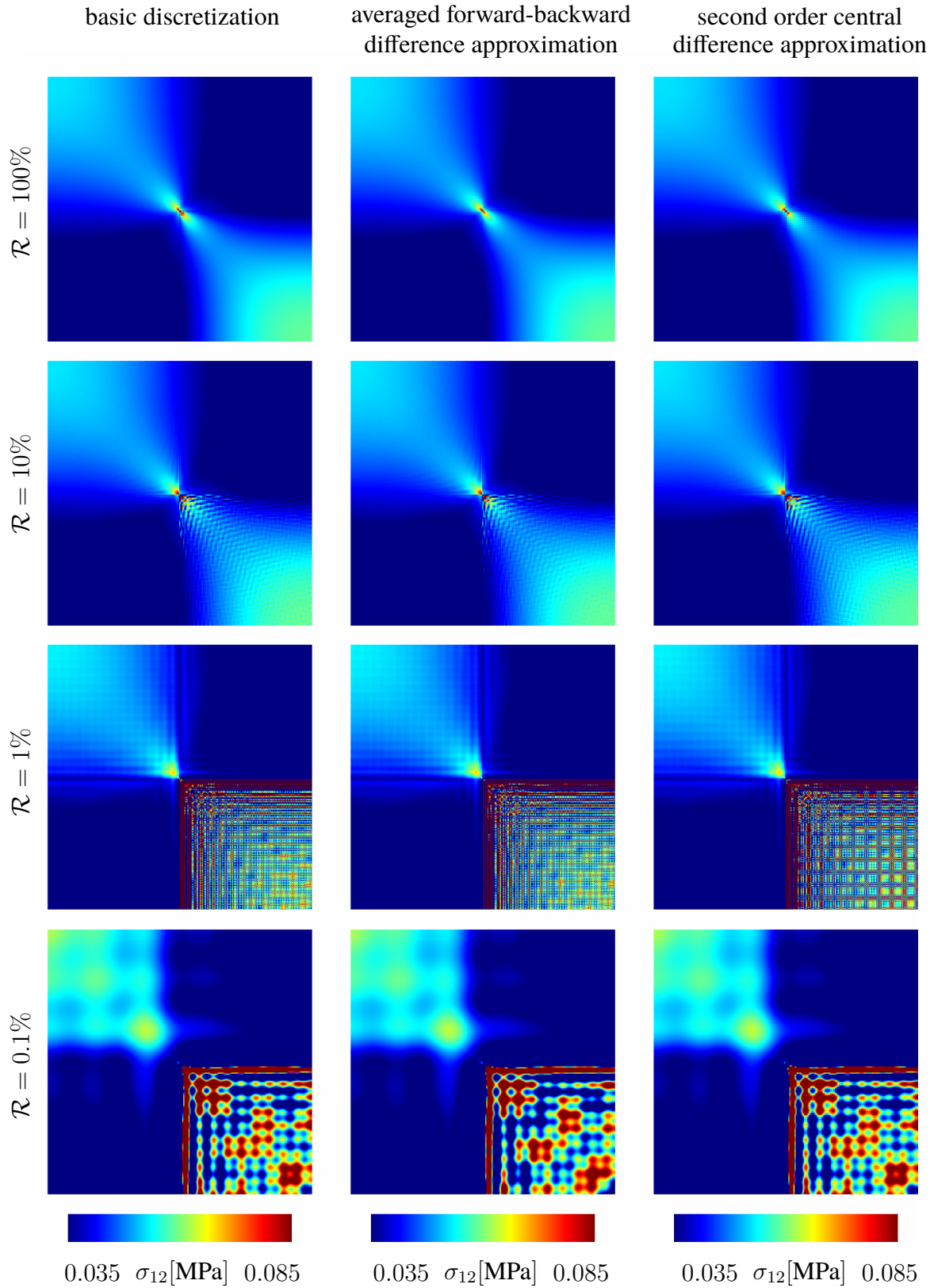


Figure 9.11: Comparison of σ_{12} for a squared inclusion considering the basic discretization, the averaged forward-backward and second order central difference approximation for varying $\mathcal{R}$.

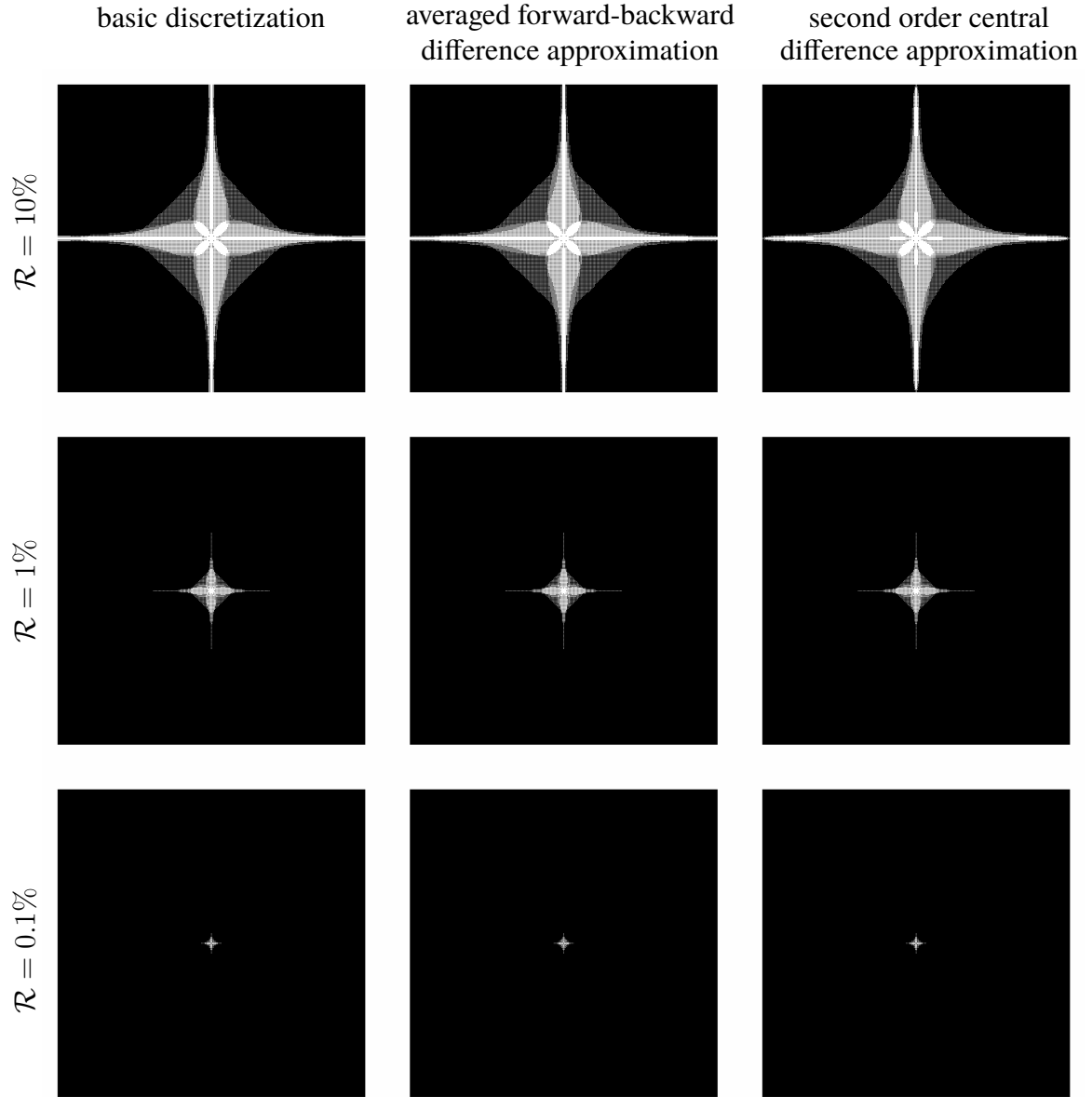


Figure 9.12: Comparison of the strain-based sampling patterns for a squared inclusion considering the basic discretization, the averaged forward-backward and second order central difference approximation for varying $\mathcal{R}$.

As shown in Figure 9.14, the relative CPU time for solving the Lippmann-Schwinger equation is again linearly decreased to $t_{\text{LippEq}}^{\text{rel}} \approx 0.1\%$, which reduces the CPU time for a full iteration by $t_{\text{Iter}}^{\text{rel}} \approx 25\%$. Besides, Table 9.2 shows that the number of iterations necessary to obtain equilibrium strongly depends on the number of Fourier modes considered as well as the chosen discretizations. While for the basic discretization a high number of iterations is needed to reach equilibrium (even when considering the full set of Fourier modes), much

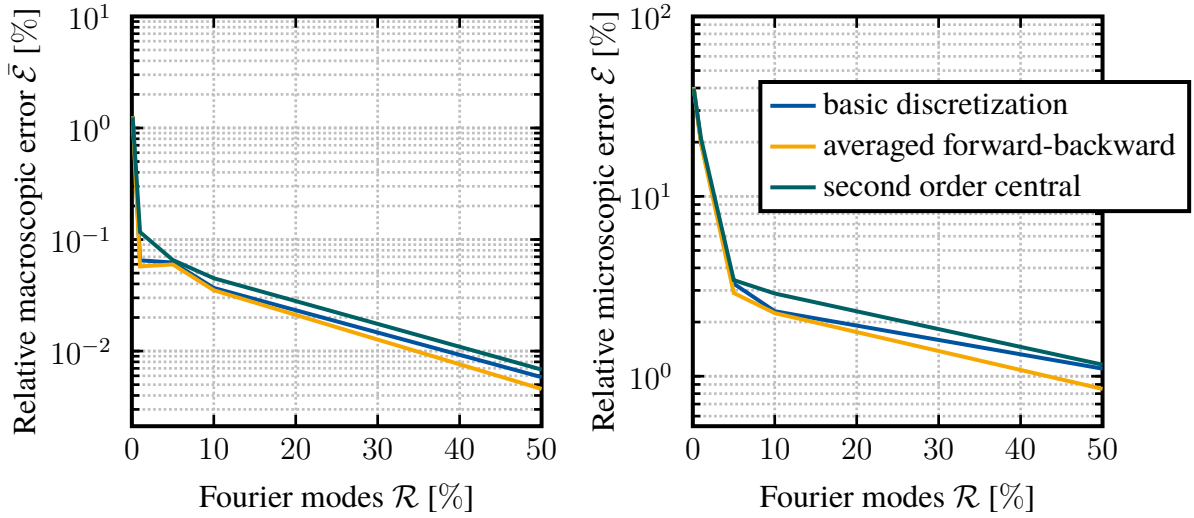


Figure 9.13: Error measurements for the microstructure with one squared inclusion. Left: Relative macroscopic error $\bar{\mathcal{E}}$ [%]. Right: Relative microscopic error $\mathcal{E}$ [%].

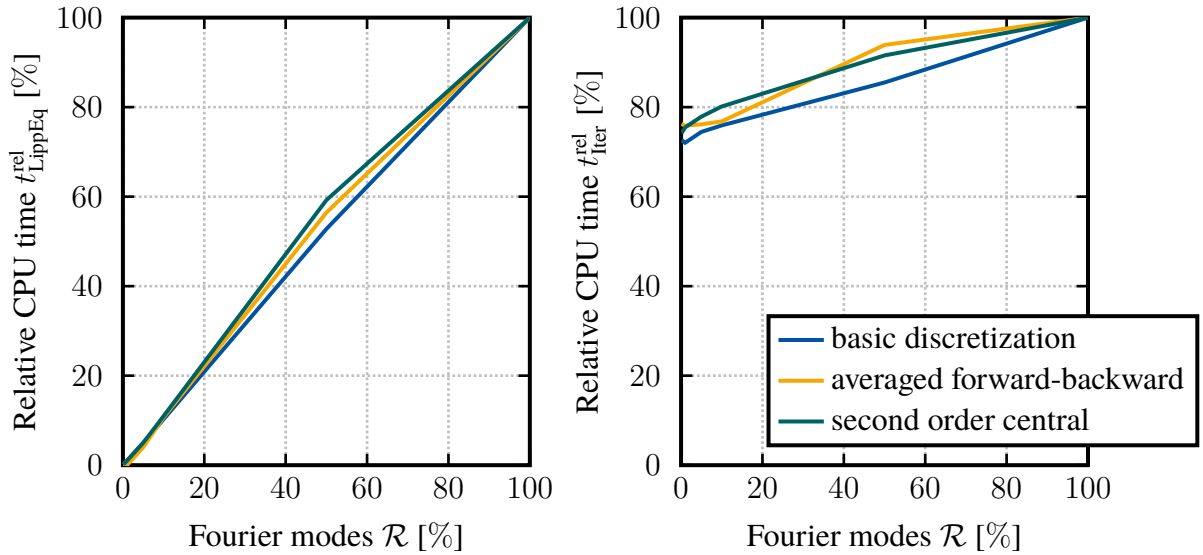


Figure 9.14: CPU time measurements for the microstructure with one squared inclusion. Left: Relative CPU time for solving the Lippmann-Schwinger equation in Fourier space $t_{\text{LippEq}}^{\text{rel}}$ [%]. Right: Relative CPU time for computing one iteration $t_{\text{Iter}}^{\text{rel}}$ [%].

fewer iterations are needed for the averaged forward-backward and the second order central difference approximation. This effect is eliminated by using a reduced set of Fourier modes, so that in this case, applying the model order reduction technique would paradoxically lead to higher overall CPU times when using the averaged forward-backward or central difference approximation.

$\mathcal{R}$ [%]	100	50	10	5	1	0.1
basic discretization	2418	2210	2318	2199	2622	1121
averaged forward-backward	32	2000	2329	2207	2622	1137
second order central	114	2251	2190	2228	2622	1120

Table 9.2: Number of iterations needed to reach equilibrium for the different discretizations and different amounts of considered Fourier modes $\mathcal{R}$ [%] for the microstructure with one squared inclusion.

9.6.1.3 Polycrystalline microstructure

As a last example to investigate the different discretizations, we consider a polycrystalline microstructure with $n^{\text{grain}} = 100$ grains per unit cell (given in Figure 9.1, right), which is discretized by 255×255 grid points. In this example an elastic material behavior is assumed, where the corresponding material parameters of the cubic anisotropic elasticity tensor $C_{11}^{\text{grain}} = 170.2$ GPa, $C_{12}^{\text{grain}} = 114.9$ GPa, and $C_{44}^{\text{grain}} = 61.0$ GPa (cf. [375]) are associated to copper. The macroscopic strain

$$\bar{\varepsilon} = \begin{bmatrix} 0.01 & 0.0 \\ 0.0 & -0.01 \end{bmatrix}$$

is applied. As in the previous examples, the macroscopic strain is artificially prescribed within two load steps so that a strain-based sampling pattern can be used in the second load step, and the following results are again compared for the basic discretization, the second order central, and the averaged forward-backward difference approximation: The results of the stress component σ_{11} considering a reduced number of Fourier modes $\mathcal{R}$ [%] are shown in Figure 9.15 for the different discretizations, while the corresponding strain-based sampling patterns are displayed in Figure 9.16. In Figure 9.17 the relative macroscopic and microscopic errors $\bar{\mathcal{E}}$ [%] and $\mathcal{E}$ [%] (with a logarithmic y-axis) are presented, while Figure 9.18 shows the relative CPU times for solving the Lippmann-Schwinger equation in Fourier space $t_{\text{LippEq}}^{\text{rel}}$ [%] as well as the relative CPU times for computing one iteration $t_{\text{Iter}}^{\text{rel}}$ [%]. The number of iterations needed to reach equilibrium are summarized in Table 9.3. Considering this polycrystalline microstructure, the sharp contrast within the local properties does not result from a phase contrast (as observed for the two-phase microstructures), but is related to a change in the crystal orientation of the individual grains.

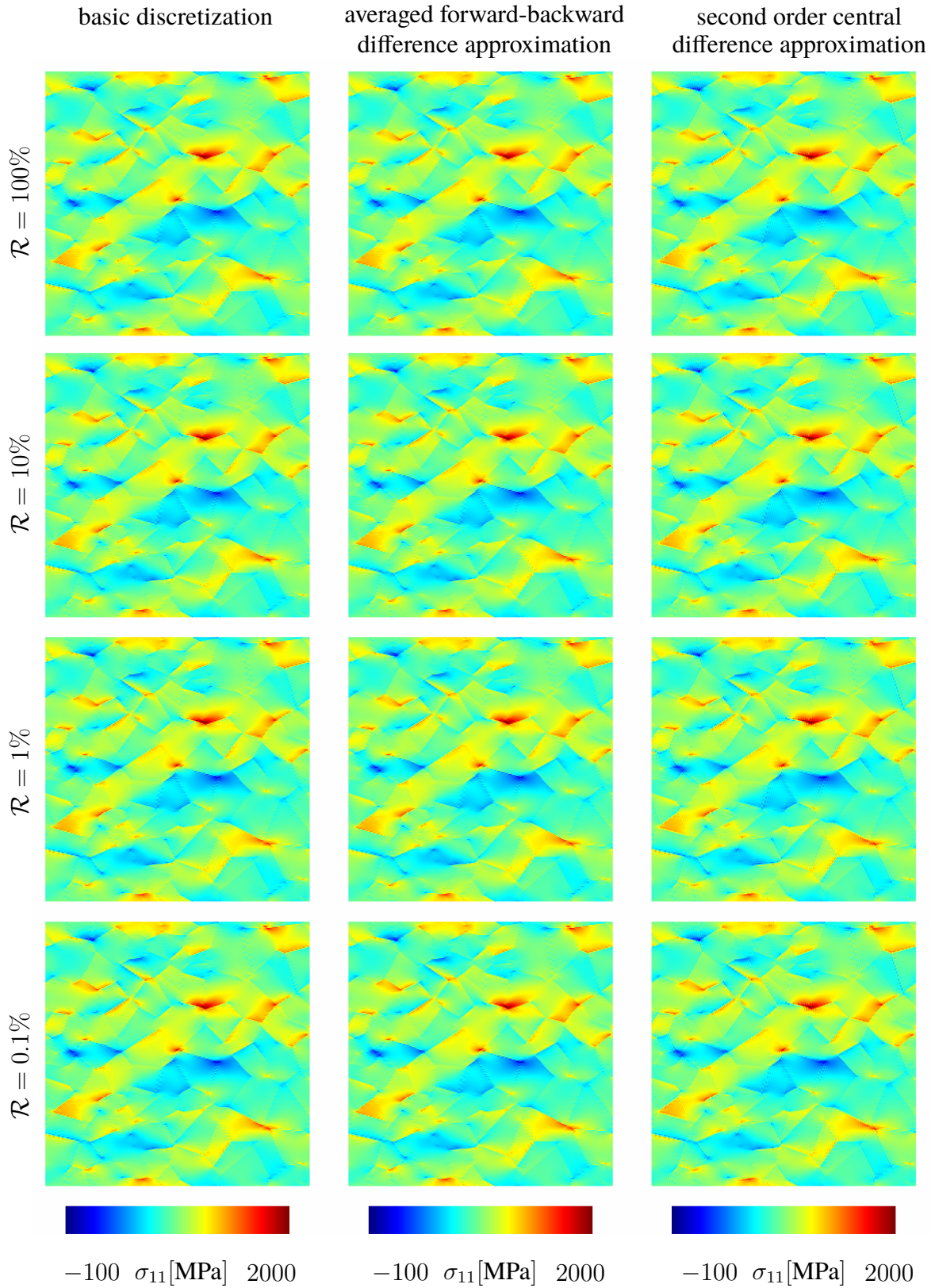


Figure 9.15: Comparison of σ_{11} for a polycrystal considering the basic discretization, the averaged forward-backward and second order central difference approximation for varying $\mathcal{R}$.

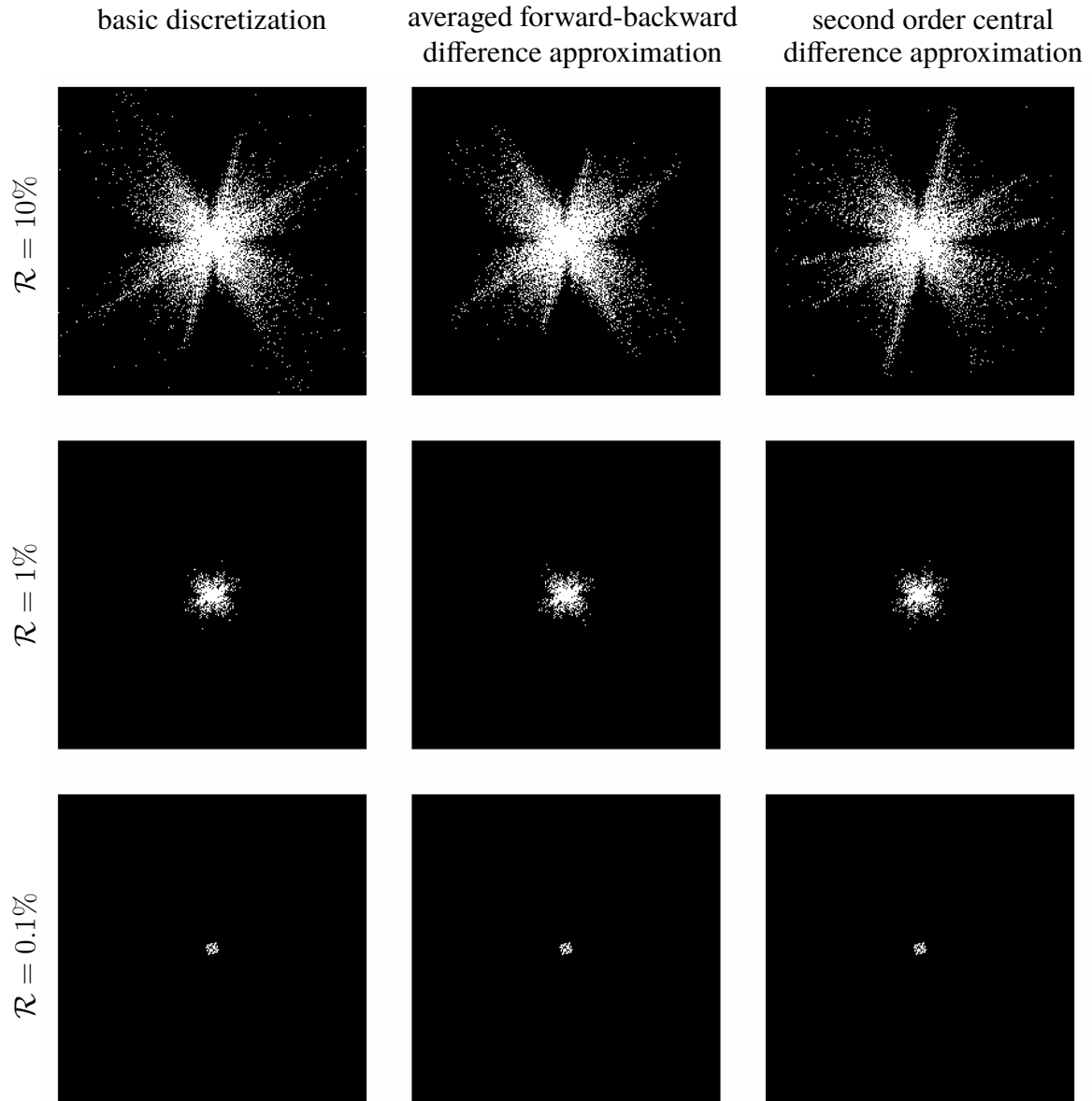


Figure 9.16: Comparison of the strain-based sampling patterns for a polycrystal considering the basic discretization, the averaged forward-backward and second order central difference approximation for varying $\mathcal{R}$.

As shown by the different stress distributions σ_{11} in Figure 9.15 and the error measurements, given in Figure 9.17, the approximated results computed using a reduced number of Fourier modes are nearly as good as the solutions for the microstructure with a small phase contrast discussed in Section 9.6.1.1. Using $\mathcal{R} = 0.1\%$ of Fourier modes, the macroscopic and microscopic errors are given by $\bar{\mathcal{E}} \approx 0.03\%$ and $\mathcal{E} \approx 1.3\%$, respectively. In addition, the characteristics of the different discretizations remain again visible even if only $\mathcal{R} = 0.1\%$ of

the Fourier modes are considered. Investigating the different sampling patterns in Figure 9.16, it is interesting to see, that even though the accuracy of the different discretizations is rather similar, the resulting sampling patterns differ comparatively widely.

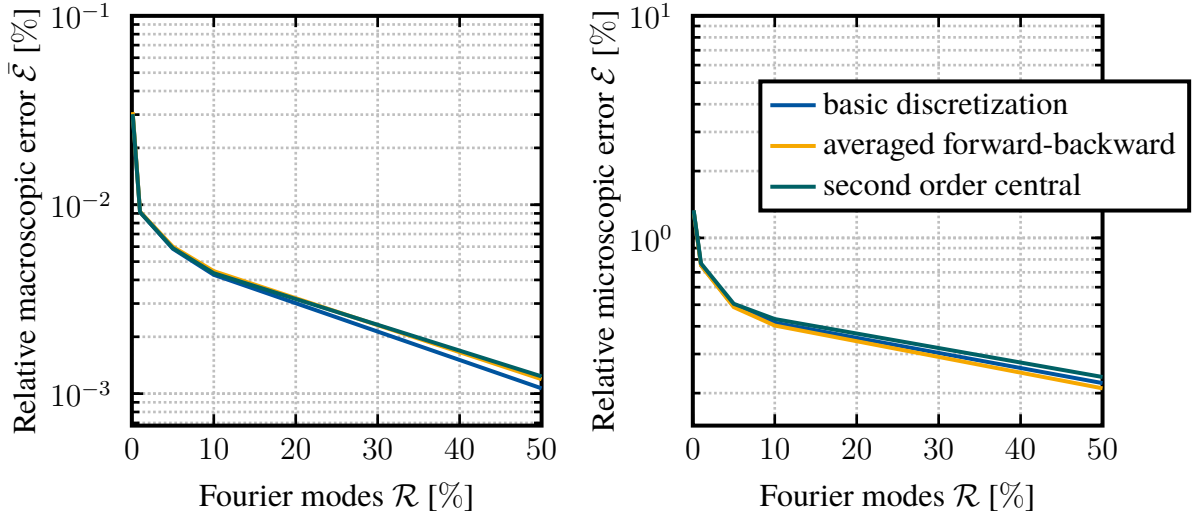


Figure 9.17: Error measurements for the polycrystalline microstructure. Left: Relative macroscopic error $\bar{\mathcal{E}}$ [%]. Right: Relative microscopic error $\mathcal{E}$ [%].

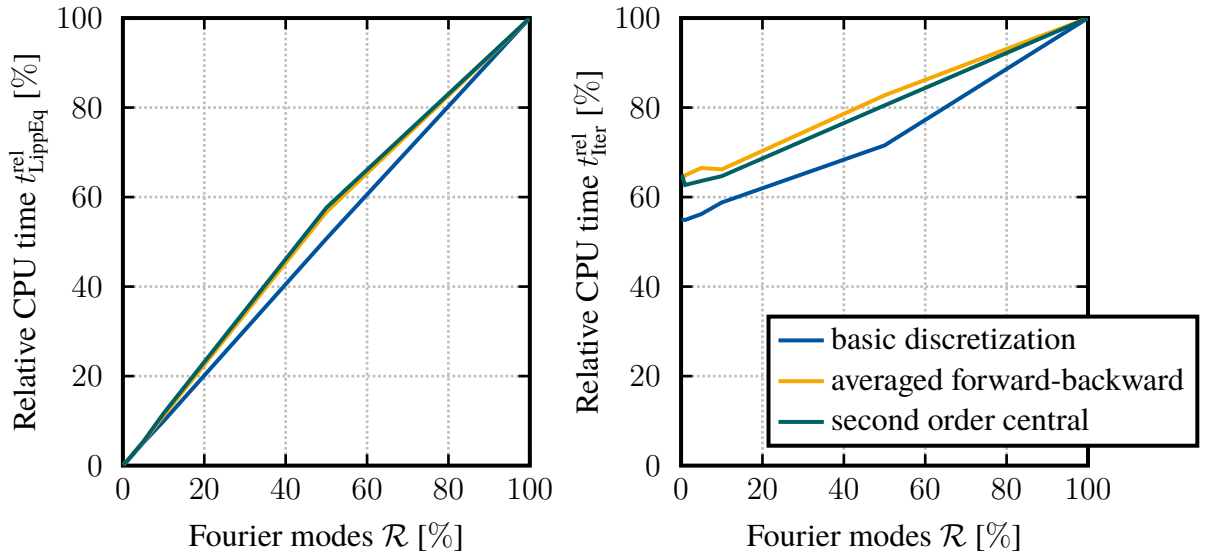


Figure 9.18: CPU time measurements for the polycrystalline microstructure. Left: Relative CPU time for solving the Lippmann-Schwinger equation in Fourier space $t_{\text{LippEq}}^{\text{rel}}$ [%]. Right: Relative CPU time for computing one iteration $t_{\text{iter}}^{\text{rel}}$ [%].

Figure 9.18 shows that the relative CPU time for solving the Lippmann-Schwinger equation in Fourier space is again approximately linearly reduced to $t_{\text{LippEq}}^{\text{rel}} \approx 0.1\%$, which decreases

the relative CPU time for computing one iteration by $t_{\text{iter}}^{\text{rel}} \approx 40\%$. In addition, Table 9.3 reveals that, in case of a polycrystalline microstructure, the number of iterations needed to reach equilibrium can even be reduced by using a reduced set of Fourier modes, leading to a further reduction in the overall CPU time.

$\mathcal{R}$ [%]	100	50	10	5	1	0.1
basic discretization	11	11	10	10	10	8
averaged forward-backward	11	11	10	10	10	8
second order central	11	11	10	10	10	8

Table 9.3: Number of iterations needed to reach equilibrium for the different discretizations and different amounts of considered Fourier modes $\mathcal{R}$ [%] for the polycrystalline microstructure.

9.6.2 Investigation on different solvers

To investigate the performance of the solvers, introduced in Section 9.4.2, we consider the same microstructure as in Section 9.6.1.3, i.e. a polycrystal with $n^{\text{grain}} = 100$ grains per unit cell discretized by 255×255 grid points. In this case, an elasto-viscoplastic material behavior of copper is assumed. The material parameters of the cubic anisotropic elasticity tensor are still set to $C_{11}^{\text{grain}} = 170.2$ GPa, $C_{12}^{\text{grain}} = 114.9$ GPa, and $C_{44}^{\text{grain}} = 61.0$ GPa (cf. [375]). In addition, the critical resolved shear stress, the drag stress, the rate sensitivity parameter and the reference shear rate are set to $\tau_0^c = 0.1$ MPa, $\tau_D = 10$ MPa, $p = 20$ and $\dot{\gamma}_0 = 10^{-3} \text{ s}^{-1}$, respectively, and the parameters for isotropic hardening are given by $\tau_\infty = 31$ MPa, $h_\infty = 50$ MPa and $h_0 = 1$ MPa (cf. [202, 319]). The macroscopic strain

$$\bar{\epsilon} = \begin{bmatrix} 0.01 & 0.0 \\ 0.0 & -0.01 \end{bmatrix}$$

is imposed within 200 load steps, while the strain rate is set to $\dot{\epsilon}_{11} = 1 \text{ s}^{-1}$. Since the difference between the investigated discretizations is rather small and the highest CPU time reduction could be achieved for the basic discretization in the elastic case (see Figure 9.18), the basic discretization is also used here to compare the performance of the different solvers considering an elasto-viscoplastic material behavior. Note that, in general, any other discretization could have been considered.

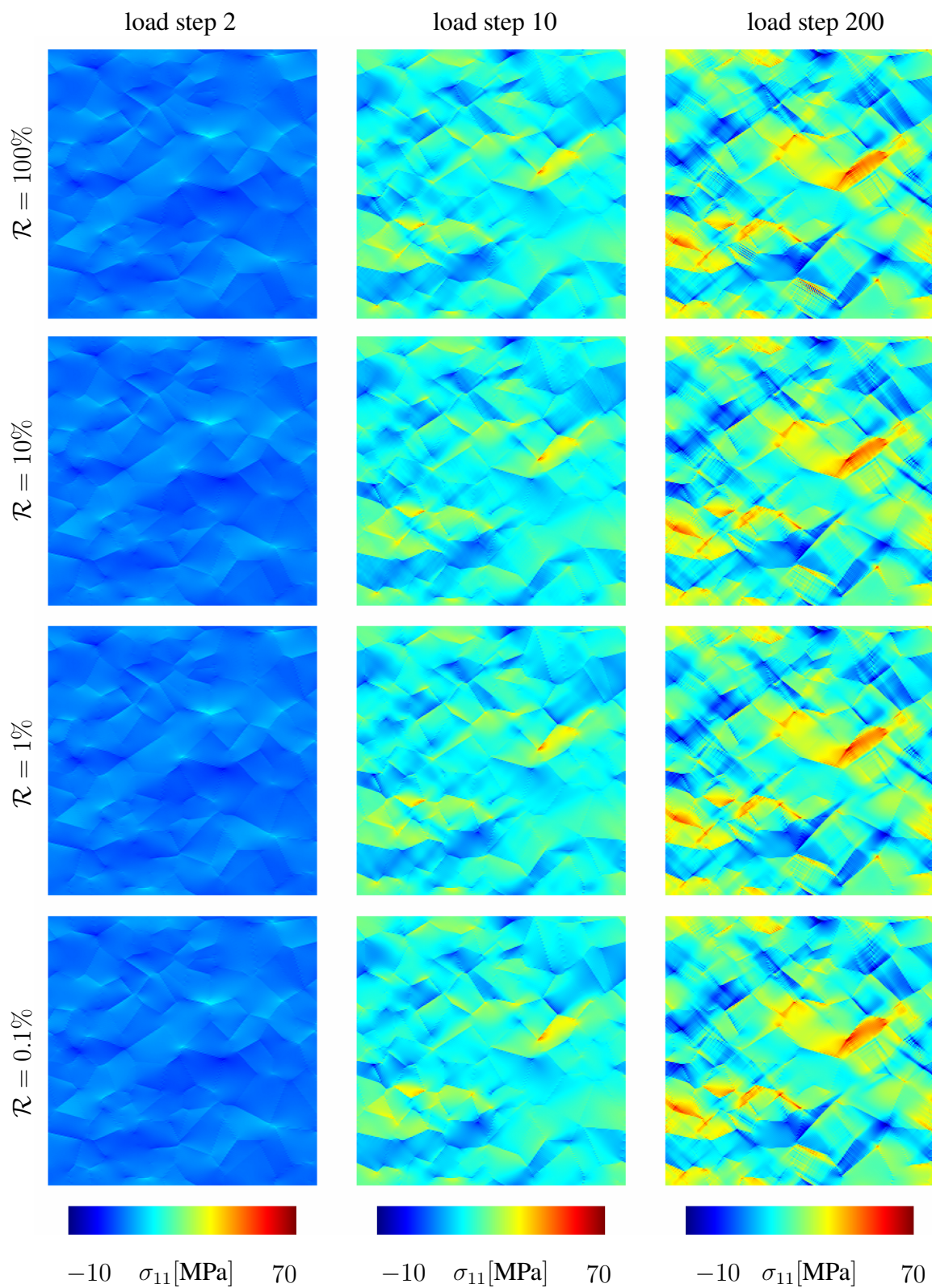


Figure 9.19: Comparison of σ_{11} for the elasto-viscoplastic polycrystal considering varying time steps (2, 10 and 200) for different $\mathcal{R}$.

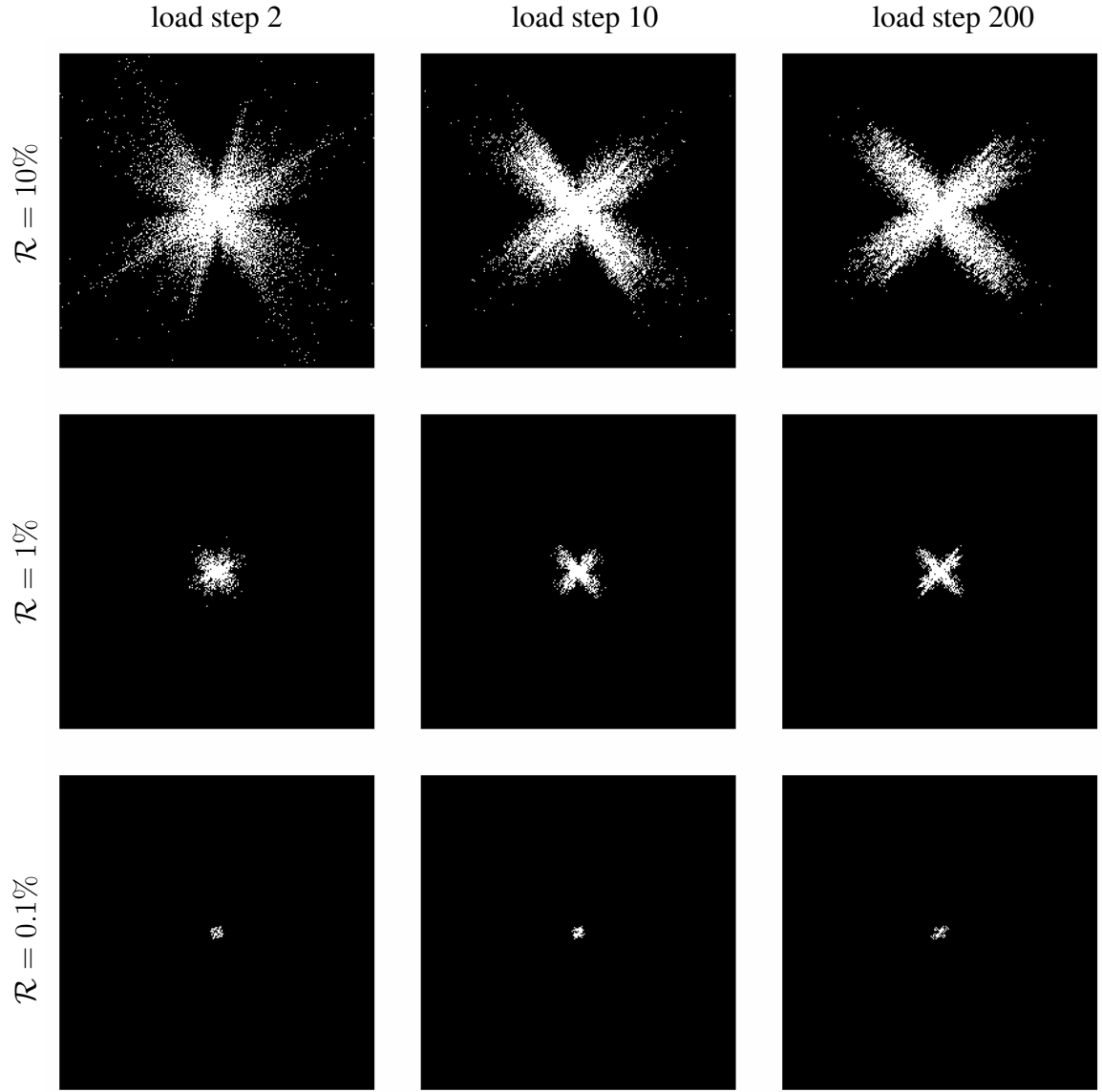


Figure 9.20: Comparison of the strain-based sampling patterns for the elasto-viscoplastic polycrystal considering different time steps (2, 10 and 200) and varying $\mathcal{R}$.

The distribution of the stress component σ_{11} considering a reduced number of Fourier modes $\mathcal{R}$ [%] are depicted for three different load steps (2, 10 and 200) in Figure 9.19, while the corresponding strain-based sampling patterns are depicted in Figure 9.20. In addition, Figure 9.21 shows the macroscopic stress-strain curve for the $\bar{\sigma}_{11}$ and $\bar{\varepsilon}_{11}$ components, while Figure 9.22 presents the relative macroscopic and microscopic errors $\bar{\mathcal{E}}$ [%] and $\mathcal{E}$ [%] (with a logarithmic y-axis) for the last load step. Examining the different solvers, Figure 9.23 shows the relative total CPU times $t_{\text{Tot}}^{\text{rel}} = t_{\text{Tot}}/t_{\text{Tot}}^{\text{ref}}$ [%], each normalized to the CPU time for computing one iteration for the corresponding solver using all of Fourier modes ($\mathcal{R} = 100\%$).

In Figure 9.24 the number of necessary iterations to obtain equilibrium for the individual load steps are given. In each case, six different amounts of Fourier modes are considered $\mathcal{R} = \{100\%, 50\%, 10\%, 5\%, 1\%, 0.1\%\}$.

Although a complex nonlinear material behavior was investigated, the differences between the reference solution computed with $\mathcal{R} = 100\%$ and the reduced simulations are still very small. The good agreement of the reduced simulation and the reference solution

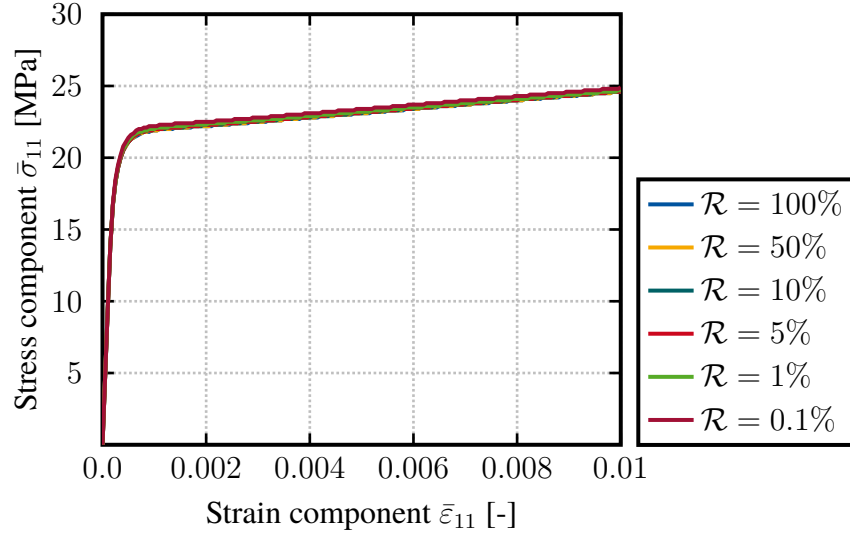


Figure 9.21: Macroscopic stress-strain curve for the $\bar{\sigma}_{11}$ and $\bar{\epsilon}_{11}$ components for different numbers of Fourier modes $\mathcal{R}$ [%].

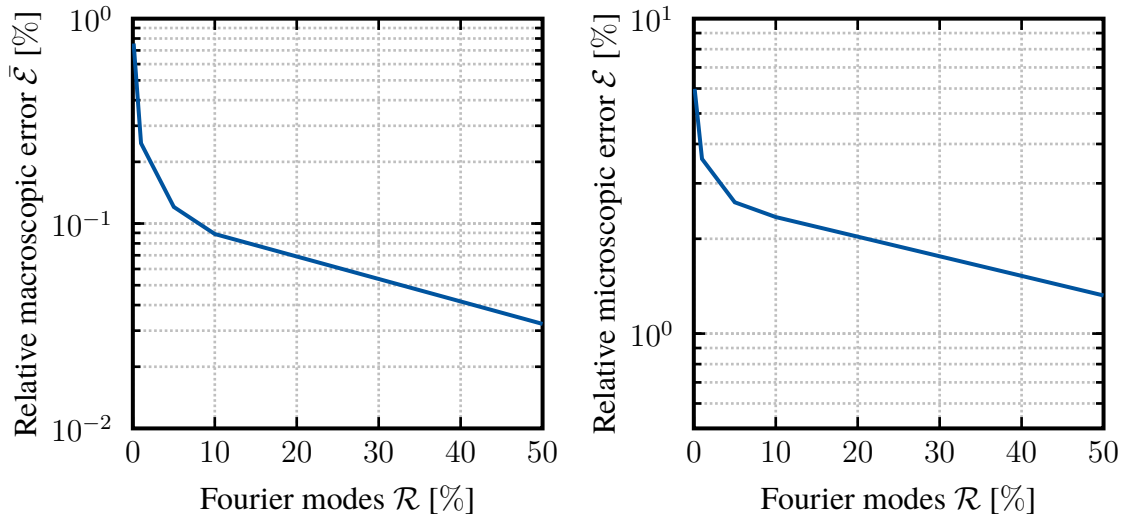


Figure 9.22: Error measurements for the elasto-viscoplastic polycrystalline microstructure. Left: Relative macroscopic error $\bar{\mathcal{E}}$ [%]. Right: Relative microscopic error $\mathcal{E}$ [%].

is also revealed by the numerical results given in Figure 9.19. Considering only $\mathcal{R} = 0.1\%$ of the Fourier modes, the macroscopic and microscopic errors are given by $\bar{\mathcal{E}} \approx 0.75\%$ and $\mathcal{E} \approx 6\%$ (cf. Figure 9.22). The presented results and the sampling patterns shown in Figure 9.20 are also independent of the solver. However, since we are considering a strain-based sampling pattern, which is dependent on the current strain field, the distribution of the considered Fourier modes changes once local phenomena due to the nonlinear material behavior set in.

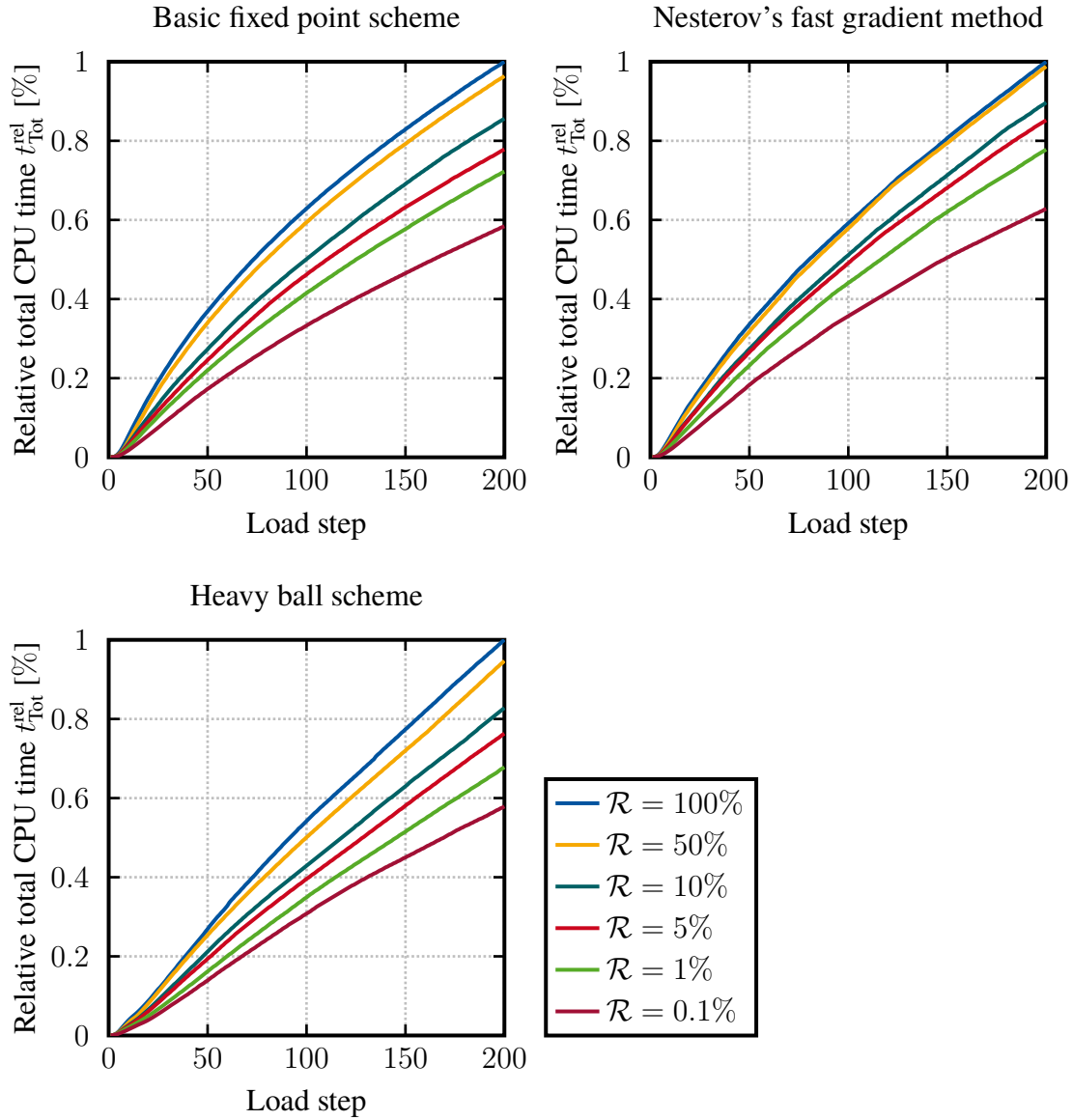


Figure 9.23: Sum of the relative CPU times for the elasto-viscoplastic polycrystalline microstructure for computing one iteration $\sum t_{\text{Iter}}^{\text{rel}}$ [%] considering the different solvers and varying amounts of Fourier modes $\mathcal{R} = \{100\%, 50\%, 10\%, 5\%, 1\%, 0.1\%\}$.

Finally, the CPU times for using the different solvers are compared in Figures 9.23 and 9.24. Using the full number of Fourier modes, the total CPU time for the basic fixed point scheme is $t_{\text{Tot}} = 2.2\text{h}$, for Nesterov's fast gradient method it is $t_{\text{Tot}} = 1.8\text{h}$ and for the heavy ball scheme it is $t_{\text{Tot}} = 1.2\text{h}$.

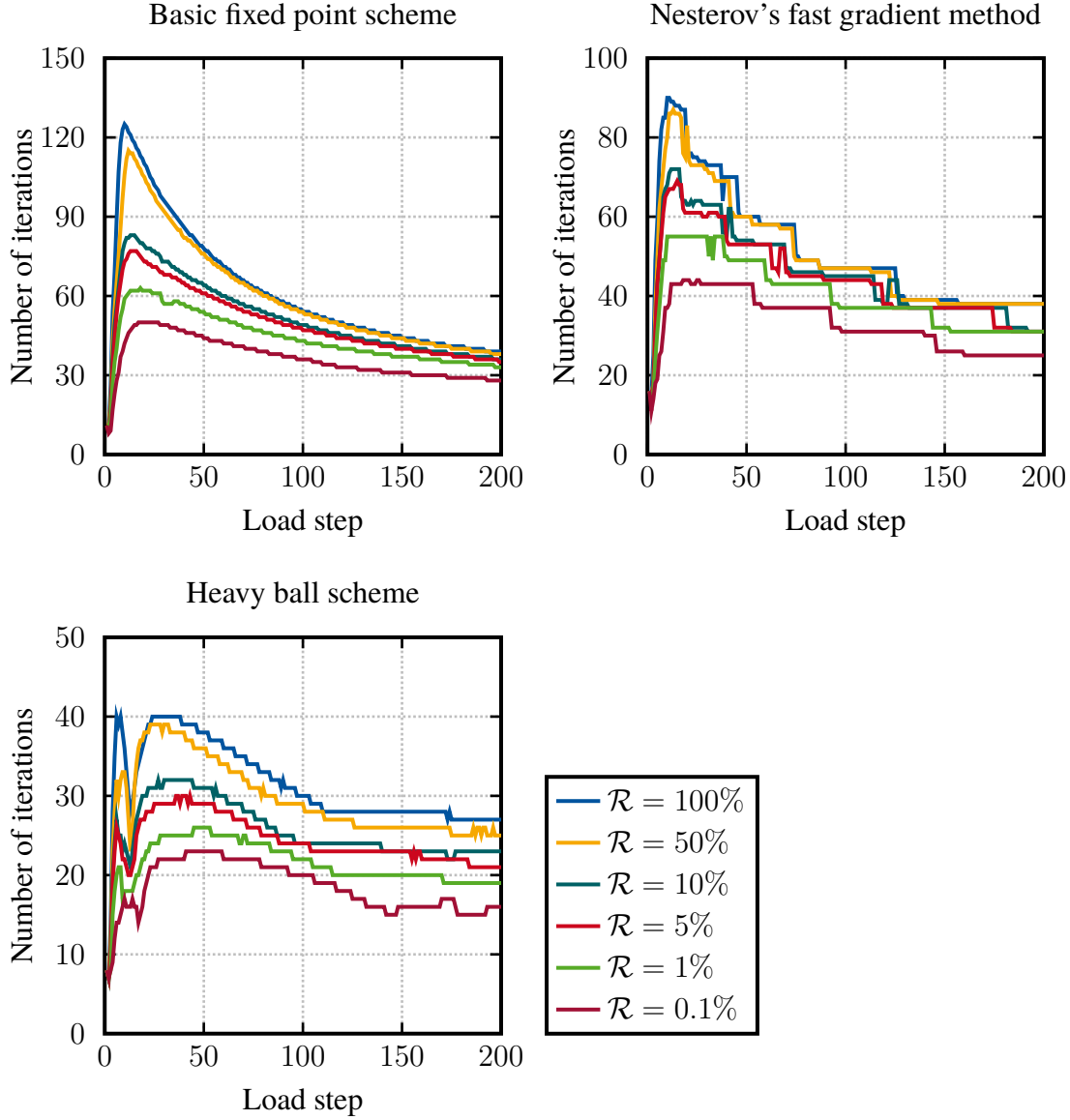


Figure 9.24: Number of iterations needed to reach equilibrium per load step for the elasto-viscoplastic polycrystalline microstructure considering the different solvers and varying amounts of Fourier modes $\mathcal{R} = \{100\%, 50\%, 10\%, 5\%, 1\%, 0.1\%\}$.

As expected, the total CPU time decreases when using the fast gradient solvers instead of the basic fixed point scheme. As shown in Figure 9.23, the use of a reduced number of Fourier

modes leads to a further reduction of CPU times, which is similar for the different solvers. In any case, the CPU times can be reduced by $t_{\text{Tot}}^{\text{rel}} \approx 40\%$. Although the CPU time for solving the Lippmann-Schwinger equation in Fourier space is again decreased to $t_{\text{LippEq}}^{\text{rel}} \approx 0.1\%$ the reduction in total CPU time is not primarily due to this reduction. This is related to the more complex nonlinear material behavior, which basically defines the entire computational effort during the iteration and which can not be reduced by considering a reduced number of Fourier modes. However, Figure 9.24 shows that the number of iterations decreases again when considering a reduced number of Fourier modes, as already shown in Section 9.6.1.3 for the polycrystalline microstructure with linear elastic material behavior. This reduction in the number of iterations occurs for all different solvers and leads to a decrease in the overall CPU time.

9.7 Conclusion and outlook

We presented the possibility to combine a reduced number of Fourier modes with modified Green's operators, which are based on finite differences, and fast gradient solvers. Since the model order reduction technique of using a reduced set of Fourier modes only decreases the computational effort of solving the Lippmann-Schwinger equation in Fourier space, the application of these modifications is straightforward and easily possible. As shown for several numerical examples, the CPU time for solving the Lippmann-Schwinger equation in Fourier space is reduced to almost zero. For two-phase microstructures with a small phase contrast or polycrystalline microstructures, this leads to a total CPU time reduction of about 40% when a linear elastic material behavior is considered. In this case, the characteristics of the various modified Green's operators are also retained and the number of iterations slightly decreases as the number of Fourier modes is reduced. When investigating two-phase microstructures with high phase contrast, the effect of the modified Green's operators is lost when considering a reduced number of Fourier modes, which leads to a significant increase in the number of iterations required and therefore, to an increase of the overall CPU time. Considering the different solvers and investigating a polycrystalline microstructure with an elasto-viscoplastic material behavior, the CPU time for solving the Lippmann-Schwinger equation is still reduced to almost zero, but since solving the complex nonlinear material behavior is computationally demanding, the effect of reducing the CPU time for solving the Lippmann-Schwinger equation in Fourier space on the total computational time for one iteration is significantly smaller. However, the number of iterations needed to obtain convergence is decreased by reducing the number of Fourier modes considered. Therefore, a CPU time reduction of about 40% is still

possible, almost independent of the solver used.

The current work shows that the combination of the model order reduction using a reduced number of Fourier modes with various improvements known from general FFT-based microstructure simulation is straightforward and easily possible. The great advantage of the model order reduction technique lies in the fact that no pre-processing or similar is required, while still achieving a reasonable CPU time reduction with accurate microscopic and macroscopic results. Nevertheless, when considering a complex material behavior, the CPU time during an iteration is mainly determined by the evaluation of the constitutive law and less dependent on the solution of the Lippmann-Schwinger equation in Fourier space. Therefore, future work will focus on reducing the CPU time for computing the microstructural stresses, e.g. by using a clustered microstructure (cf. [115, 128, 351]). This will lead to a further reduction in CPU time, but requires pre-processing steps, which were, up to now, not necessary.

10 | Conclusions and Outlook

The present cumulative dissertation dealt with model order reduction techniques for the FE-FFT-based two-scale and the related FFT-based microscale method. In particular, the novelties developed in this thesis include the generalization of an efficient FE-FFT-based two-scale simulation strategy to the finite strain regime as well as to thermomechanically coupled crystal plasticity models. Furthermore, by introducing a geometrically adapted and strain-based sampling pattern, fundamental improvements for the FFT-based microscale simulation with a reduced set of Fourier modes have been proposed. These sampling strategies significantly increase the accuracy of this model order reduction technique and enable an accurate investigation of polycrystalline microstructures characterized by complex microstructural effects, e.g. crystal plasticity or solid-solid phase transformations. Finally, it was demonstrated that the universality of this technique allows a straightforward application of several improvements to the FFT-based microscale method as well as an extension to investigate 3D problems.

While the current trends in computational multiscale material modeling, including the latest developments for the FE-FFT-based two-scale and related FFT-based microscale methods were presented in Chapter 1, a general and comprehensive literature review summarizing earlier works (published before 2022) on the FE-FFT-based two-scale and FFT-based microscale methods was provided in the first journal article (Chapter 2). In this article, several FFT-based algorithms and solvers as well as their applications, methods to reduce the effect of Gibbs oscillations, and model order reduction techniques for the spectral solver were discussed.

Subsequently, Chapters 3 and 4 dealt with the generalization of an efficient two-scale FE-FFT-based simulation strategy, where the two-scale simulation was performed using a coarsely discretized microstructure. The solution strategy was generalized to the finite strain regime to predict the local and global mechanical behavior of polycrystalline materials with elasto-viscoplastic constitutive behavior, which allowed the two-scale simulation of a deep rolling process of an iron-based specimen (see Chapter 3). Additionally, the method has been extended to simulate two-scale thermomechanically coupled processes (see Chapter 4). In this case, the balance of linear momentum and the balance of internal energy must be solved on both scales, with the temperature or its gradient introduced as additional unknowns (compared to

the purely mechanical boundary value problem, where the displacement or the deformation gradient are the only unknowns).

Chapters 5 to 9 were concerned with the reduced FFT-based microscale simulation, where the computations in Fourier space were performed using a decreased number of Fourier modes. First in Chapter 5, a geometrically adapted sampling pattern was introduced, based on which the Fourier modes suitable for the reduced computations are selected. The idea relies on the definition of a characteristic function for the microscale, which represents the distribution of phases in a two-phase microstructure. The sampling pattern is defined by first transforming the characteristic function into Fourier space, and then choosing the Fourier modes characterized by the highest amplitudes. Compared to the initially proposed fixed sampling pattern (cf. [17]), significantly more accurate results can be obtained for both linear and nonlinear material behavior. In addition, the extension of the model order reduction technique to the 3D case was presented. In Chapter 6, the identification process of the reduced set of Fourier modes used for the reduced FFT-based simulation was further optimized by introducing a strain-based sampling pattern, where the characteristic function was replaced by a microstructural strain field. Again, significantly more accurate results were achieved using this sampling strategy. Furthermore, the need to define the characteristic function was eliminated, which can be a challenging task for complex microstructures such as polycrystalline microstructures or microstructures with changing phase distributions. In Chapters 7 and 8, this new sampling strategy was applied to predict the microscopic and overall fields in a polycrystalline microstructure considering a crystal plasticity constitutive model or solid-solid phase transformations between austenite and martensite, respectively. Finally, in Chapter 9, the preliminary version of an article by the author (and his co-authors) was presented, in which the advantages and the universality of the model order reduction technique based on the use of a reduced set of Fourier modes were highlighted. The method reduces the computations in Fourier space that are independent of modifications made to the Green's operator or the spectral solver itself. Therefore, the model order reduction technique can be used in combination with finite-difference-based operator approximations in order to reduce the effect of Gibbs oscillations as well as in combination with fast gradient solvers in order to improve the convergence behavior of the method.

In this cumulative dissertation, various developments for model order reduction techniques for the FE-FFT-based two-scale and the FFT-based microscale methods have been introduced and investigated in order to reduce the computational effort of both two-scale and microscale simulations. However, to enable 3D two-scale simulations of complex macroscopic boundary value problems with highly resolved microstructures and highly nonlinear constitutive behavior within reasonable CPU times, further research is still required.

Up to now, the efficient two-scale FE-FFT-based simulation strategy has only been used to simulate 2D plane strain problems, limiting the investigation to a simplified problem setting. However, a straightforward extension of this model order reduction technique to the simulation of 3D problems to allow the investigation of more realistic mechanical and thermomechanically coupled processes is possible. In addition, the thermomechanical coupling enables the investigation of various microstructural phenomena. In [70] mechanically induced solid-solid phase transformations have already been modeled within the efficient two-scale simulation framework. Future works should also address the simulation of the heat generated from these transformations as well as the simulation of their thermally motivated initiation. This would, for example, enable concurrent two-scale simulations of shape memory alloys. Finally, the two-scale simulation results should be compared to and validated against experimental data, which is also a challenging task.

Due to the universality of the reduced FFT-based microscale simulation with a decreased number of Fourier modes, further improvements for the FFT-based method itself, such as other spectral solvers or other strategies to reduce the effect of Gibbs oscillations (see e.g. [15] for an overview of the different methods), could be applied. However, while this model order reduction technique reduces the computational effort of the calculations in Fourier space, for complex constitutive behaviors, the evaluation of the stress computed in real space consumes most of the required CPU time. Therefore, further developments should also focus on reducing this computational effort in real space (see e.g. [41, 42, 351]) and on combining both strategies to reduce the CPU times in Fourier and in real space.

Finally, the FFT-based microscale simulation with the presented model order reduction techniques, i.e. a microscale simulation performed either using a coarsely discretized microstructure or using a reduced number of Fourier modes, can also be used for an efficient data generation in the sense of data-driven multiscale methods. Hence, for example, the development of a coupled model-free data-driven macroscopic and reduced FFT-based microscale method (DD-FFT-based two-scale method), similar to the works presented in [104, 108, 109], is of high interest. This method could lead to an extremely efficient concurrent two-scale simulation strategy through an on-the-fly data generation based on reduced FFT-based microscale simulations. In this context the model-free data-driven method has several advantages. For example, only data that is not yet included in the data set needs to be generated by highly resolved microscale simulations, continuously reducing the number of microscale simulations required. Furthermore, there is no need to compute a macroscopic tangent operator, which is a highly demanding computation in classical concurrent two-scale methods such as the FE-FFT-based approach. Additionally, a DD-FFT-based method also allows an easy investi-

gation of microstructural uncertainties by considering variations of the microstructure within the simulations performed to enrich the data set.

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