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A multiscale approach for modeling progressive damage of composite materials using fast Fourier transforms

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ABSTRACT

Composite materials possess a highly complex material behavior, and thus advanced simulation techniques are necessary to compute their mechanical response. In this regard, especially modeling failure and progressive damage presents a challenging task. Conventional macro mechanical methods and even closed form estimates are in many cases not sufficient to predict the appropriate mechanical material response. Full-field simulations must be resorted to, but these are known to be very expensive from the computational point of view. In this contribution we propose a more efficient multiscale approach similar to FE^2. Nonlinear material effects caused by progressive damage behavior are captured directly on the discretized material level using simple isotropic continuum damage laws. In contrast to conventional FE^2 methods which use the Finite Element Method (FEM) to solve both scales numerically, the fine scale problem (material level) is rewritten in an integral form of Lippmann–Schwinger type and solved efficiently using the fast Fourier transformation (FFT). The calculation is carried out on a regular voxel grid that can be obtained from 3D images like tomographies. The fine scale problem is integrated in a standard Finite Element framework which is used to solve the macroscopic BVP (component level). In the work at hand, the scale coupling technique and the computation of the macroscopic tangent are described, and in some numerical examples the convergence behavior of the macroscopic Newton algorithm is investigated. Thereby the simulations were considered until localization and softening on the material scale occurred. It is shown that the proposed method presents an effective way to determine the exact physical macroscopic response considering arbitrary microstructures and loading conditions.

1. Introduction

Besides their outstanding mechanical properties in terms of strength and stiffness related to their weight, fiber-reinforced composite materials possess a highly complex material behavior. In order to use these composite materials efficiently, advanced simulation techniques are necessary. Especially modeling failure and progressive damage of composite materials, presents a major challenge in current research activities. Composite failure occurs as a result of a variety of complex microstructural damage mechanisms, such as matrix damage, fiber pull out and fiber breakage.

Recently, phenomenological macroscale models are state of the art, especially for failure investigations of laminated composite applications, see for instance the work of Maimí et al. [31] or Pinho et al. [44]. These models assume homogeneous

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material behavior and are usually based on macroscopic failure criteria, like those proposed by Puck [45] or Cuntze [10]. Disadvantages are the extensive identification of material parameters in dependence of the material structure and the loading conditions. Physical phenomena occurring on a finer length scale are not considered.

A more accurate approach is to capture nonlinear material effects directly on a finer length scale. Recent multiscale modeling and simulation techniques were developed to limit the increasing computational effort to an acceptable extent [25,53]. In this context, analytical methods based on closed form estimates to consider the micro mechanical material structure by means of analytical approximations, represent an efficient and practicable way. Mean field approaches are based on Eshelby's inclusion theory [14] and make use of analytical approximations like the Mori–Tanaka model [39], the double inclusion method [43], or self-consistent schemes [21] to obtain effective material properties. These closed form estimates are restricted to certain inclusion shapes (ellipsoidal, convex, unbent) and are therefore restricted to simple microstructures which are locally uniformly distributed in terms of their size, orientation and volume density. Further the volume fraction of the inclusions is restricted, the stress in the inclusions is assumed to be constant and the interactions between inclusions are only captured to a limited degree, what is an important limitation for the simulation of the evolution of micro cracks. Progressive damage is usually modeled using empirical failure criteria, like e.g. Tsai-Wu, Tsai-Hill, maximum stress or strain criterion, which are based on the work of Tsai and Wu [50] and Hill [22]. An overview of classical analytical methods can be found in [42,43]. Moreover, higher order theories have been proposed using nonlinear extensions of the Hashin–Shtrikman [18] variational principle [5] or the secant/tangent moduli of the phases [6,7]. Furthermore, semi-analytical methods like the Generalized Method of Cells [1] or the Transformation Field analysis (TFA) proposed by Dvorak [13] and extended by e.g. Chaboche et al. [8] or Fish et al. [17] were developed. Moreover in this context, Michel and Suquet [36] introduced the so called nonuniform TFA.

However, to overcome the essential shortcomings related to these kind of models one has to resort to direct or full-field simulations. Therein, the microstructural constituents are modeled explicitly on the interesting scale instead of forming effective constitutive equations. The resulting material response is based on genuine physical effects and consequently arbitrary complex non-proportional, multiaxial loading conditions can be captured. Moreover, simple (isotropic) constitutive laws can be used to define the material behavior of the microstructural constituents and the required parameters can be measured directly in physical experiments. In the last decade, several numerical multiscale modeling and simulation techniques were developed. According to [3,51], these numerical multiscale methods can be divided into concurrent and hierarchical ones. In concurrent methods the scales are strongly coupled and solved simultaneously. The domain is decomposed into a fine- and a coarse-scale model, whereby both scales are linked together "on the fly". Information is mutually exchanged between both scales. On the other hand hierarchical methods pre-compute effective properties from the microscale and pass this information to the uncoupled macroscale. Both scale problems are separated from each other and are solved sequentially. If the assumption of the separation of scales is valid, then the micro problem can be regarded as a representative sample of the microscopic material behavior. One well-known method, which has characteristics of both classes, is the FE^2 approach introduced by Feyel and Chaboche [16] and Smit et al. [48]. The scales are solved separately and every macroscopic point is equipped with a certain microstructure, which describes the material behavior and can be regarded as a representative volume element (RVE). The constitutive equation of the coarse scale is replaced by an associated microscopic boundary value problem (BVP). Information passes in both directions and a mutual exchange between both scales takes place. This class of models can be denoted as semi-concurrent or coupled hierarchical methods.

However, the detailed resolution of the microstructural constituents leads to a fine discretization of the computational model and thus to large algebraic systems with many degrees of freedom. Despite increasing computational power, simulations of macroscopic components using explicitly modeled realistic microstructures can today hardly be realized with reasonable CPU times. Due to the increased computational costs coming along with the application of a multiscale framework, an effective solution of the micro boundary value problem is necessary. In this work an alternative method is applied which uses the fast Fourier transformation (FFT) to solve an equivalent micro BVP (material level). A periodic BVP known from ordinary elasticity problems is reformulated in an integral equation of a so called Lippmann–Schwinger type, as proposed by Zeller and Dederichs [52] and Kröner [27]. The numerical method was introduced by Moulinec and Suquet [40,41,33]. Advantages of this method are its efficiency in terms of memory consumption and computational time. Further the calculation is carried out on a regular voxel grid and could therefore directly be applied to calculate homogenized quantities on 3D images like tomographies without using any complicated mesh generation. The fine scale problem can easily be integrated in a standard Finite Element framework which is used to solve the macroscopic BVP (component level).

In the first part of this paper, the constitutive equation and the numerical solution of the microscale model are introduced and demonstrated by an illustrative numerical example. The second part presents the coupling technique of the two geometrical scales by combining the two numerical methods. The numerical homogenization process including the computation of the macroscopic tangent by using the FFT method are explained. Finally, the paper closes with numerical examples of some scale coupling problems to illustrate the macroscopic convergence behavior of the numerical method. The examples shown in this work were considered until material softening appeared. This means the simulations were stopped when localization on the material scale occurred, so that the governing equation keep its ellipticity and the assumption of separation of scales remains valid.[1]

[1] In the opinion of the authors this should be satisfactory in this case, due to the brittle fracture characteristics of the considered fiber reinforced composite materials.