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Formulation of nonlocal damage models based on spectral methods for application to complex microstructures

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ABSTRACT

The increasing interest in modelling local deformations and damage evolution within materials with complex microstructures leads to an increasing demand for efficient numerical methods. A method designed to study damage evolution within the microstructure should be able to deal with complex geometries and to capture system sizes that are large enough to rectify the assumptions made when naming them representative volume elements (RVEs). We introduce a nonlocal damage model into the framework of a spectral solver and study initiation and evolution of damage on the microstructural scale, where regions susceptible to damage are identified.

1. Introduction

In 1998 Moulinec and Suquet [1] introduced a numerical method, based on the Fast Fourier Transform (FFT) to calculate deformation within complex microstructures. They proposed a fixpoint iterative scheme that solves a boundary value problem, consisting of a rectangular geometry with arbitrary microstructure, iteratively starting from an initial guess of the strain field. In their model, elastic and non-linear material behaviours at small strains are introduced. During the following years, the concept got more and more accepted in solid mechanics and material science because it is numerically efficient and meshing, which is an inherent problem using the finite element method (FEM) for complex microstructures [2], is not necessary due to the regular sampling used in spectral methods. Further studies were dedicated to improve the convergence of spectral methods for high phase contrasts using augmented Lagrangians [3] or Conjugate gradients [4], which showed an improved convergence rate. Lebensohn [5] introduced rate dependent material models and more recently finite strain crystal plasticity models have been implemented [6]. The models introduced above all have in common that they consider only hardening type material models, while neglecting softening behaviour that occurs during damage evolution.

Among other models, continuum damage models are being widely applied in the literature to study nucleation and growth of cracks for complex geometries under various loading conditions. Within the framework of continuum damage mechanics, a field variable is introduced which describes the material degradation in a continuum mechanics sense [7]. The evolution of this field variable is governed by a constitutive law determining onset and development of damage, whereas the direction of damage propagation is determined by stress (re-)distributions near the damaged zone and is a result of the simulation. An essential property of any numerical method is the convergence upon mesh refinement, which is no problem using hardening material models. But in the 1980s several authors found that softening materials show spurious mesh sensitivity and do not converge to a meaningful solution upon mesh refinement [8]. The problem does not arise due to the numerical model used but due to the fact that the physical processes of damage are not described properly by local

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Nomenclature

$\bar{\kappa}$	nonlocal field variable
$\boldsymbol{\psi}$	Fourier frequencies
$\boldsymbol{\sigma}$	stress tensor
$\boldsymbol{\varepsilon}$	total strain tensor
$\boldsymbol{\varepsilon}^*$	fluctuating part of strain tensor
$\boldsymbol{\varepsilon}_{\mathrm{e}}$	elastic strain tensor
$\boldsymbol{\varepsilon}_{\mathrm{p}}$	plastic strain tensor
$\boldsymbol{C}$	elastic stiffness tensor
Δ	laplace operator
$\dot{a}$	derivation of variable a with respect to time
$\hat{\boldsymbol{\tau}}$	polarization tensor in Fourier space
$\hat{\boldsymbol{K}}$	reference stiffness in Fourier space
$\hat{\boldsymbol{N}}$	compliance tensor in Fourier space
$\hat{\Gamma}$	Green operator in Fourier space
$\hat{a}$	variable a in Fourier space
κ	local field variable
κ_0	onset value for damage
κ_c	finale failure value for damage
$\mathbf{E}$	average strain tensor
$\tilde{\boldsymbol{\sigma}}$	stress tensor in effective space
$\hat{\boldsymbol{\tau}}$	polarization tensor in Fourier space
D	damage parameter
p	equivalent plastic strain

continuum damage models [9]. Using a continuous damage variable in the domain, a certain smoothness of the damage field is assumed. In contrast to that, in the general context of local continuum damage mechanics, discontinuous solutions are admissible as for decreasing mesh size the damage band will localize progressively [10]. Thus using a local continuum damage model, damage will condense into a small region and the width of this region will depend on the discretization used. This is an unphysical solution as it is discovered experimentally that damage takes place in a zone of finite width.

A widely applied simple solution for this problem is the use of a constant discretization and calibration of the model parameters for this discretization. Following this solution, the discretization has to be the same in all further investigations, which already leads to problems for rather simple model geometries as systematic convergence studies are not directly possible. In the case of complex RVEs, this restriction is harsh and the approach cannot be followed as the complexity of the RVE morphology permits the use of a constant discretization.

Among other extensions, models in which gradients of constitutive variables governing the damage evolution are introduced, show a regularization effect [11–13] and are referred to as gradient dependent or nonlocal damage models. Within this models the local variable reaching high values under consideration of a local damage model is evaluated in a finite domain. In this finite domain the neighbouring damage states are also considered. The size of this finite domain introduces a length scale to the model and can be connected to the material length scale on which damage processes take place.

While most nonlocal damage models are implemented for application with finite element solvers, the general nonlocal continuum damage theory is also applicable to other numerical methods. In [14] it is already shown that a classical elastic damage model can be implemented into a FFT-solver, while neglecting the fact that damage models are mesh dependent. In [15] a damage model for brittle and quasi-brittle materials is formulated, in which the problem of local damage models is overcome by a Gaussian type of weighting function. In [16] a gradient enhanced energy functional is used to overcome mesh-dependency of an elastic damage model within the spectral method and the model is applied to RVEs representing concrete.

In this paper, we follow the numerical concept of Moos [16] and introduce a nonlocal continuum damage model, extend the concept to hardening plasticity and apply the model to a realistic RVE. The strengths of the proposed model are, on the one hand, the numerical efficiency and the mesh independency due to the use of the nonlocal damage model and, on the other hand, the easy discretization of complex RVEs due to the use of the FFT solver. The damage model is implemented in the open-source phase-field framework OpenPhase (Reference: www.openphase.de) [17].

2. Implementation

2.1. Governing equations

Considering a rectangular 3D body where strain and stress field are defined for each spatial point in $\boldsymbol{x} = (x, y, z)$ and following the pioneering work of Suquet [1], the local strain field $\boldsymbol{\varepsilon}$ can be split into an average strain $\boldsymbol{E}$ and a fluctuation term $\boldsymbol{\varepsilon}^*$ so that