Chapter 5
Parallel inelastic heterogeneous multiscale simulations

Ramin Shirazi Nejad and Christian Wieners

Abstract We recall the heterogeneous multiscale method for elasticity and its extension to inelasticity within a two-scale energetic approach, where the fine-scale material properties are evaluated in Representative Volume Elements. These RVEs are located at Gauss points of a coarse finite element mesh. Within this FE² method the displacement is approximated on a coarse-scale, and depending on the strain at the Gauss points in every RVE a periodic micro-fluctuation and the internal variables describing the material history in this RVE are computed. Together, this defines the global energy and the dissipation functional, both depending on coarse-scale displacements as well as on fluctuations and internal variables on the micro-scale.

Here we introduce a parallel realization of this method which allows the computation of 3D micro-structures with fine resolution. It is based on the parallel representation of the RVE with distributed internal variables associated to each Gauss points, and a parallel multigrid solution method in the nonlinear computation of the micro-fluctuations and for the up-scaling of the algorithmic tangent within the incremental loading steps of the macro-problem. The efficiency of the method is demonstrated for a simple damage model combined with elasto-plasticity describing a PBT matrix material with glass fiber inclusions.

For this investigation we use the material models in J. Spahn (PhD thesis Kaiserslautern 2015) and the software developed by R. Shirazi Nejad (PhD thesis Karlsruhe 2017).
5.1 Introduction

Materials with micro-structures can be described effectively by homogenization. Formally, the effective description can be obtained by a two-scale limit, where in every material point a periodic representative volume element (RVE) describing the material on the micro-scale is appended. Classical homogenization computes an effective material response in one RVE and inserts the result into the macroscopic problem. This procedure is analytically well investigated, see, e.g., [1, 2, 3] for homogenization and [4] for the two-scale limit. This is extended to heterogeneous materials, and for a corresponding numerical method the finite element convergence can be estimated with separate terms for the modeling error and the approximation on micro- and macro-scale [5].

For inelastic materials the heterogeneous multiscale method introduced in [6, 7, 8, 9] is called the FE² method, see [10] for an overview. It is now well established for two-scale model in plasticity, damage and fracture. In case of rate-independent energetic material models [11] a full two-scale analysis for generalized standard materials with periodic coefficients is established in [12].

Here we apply this method to a short fiber-reinforced material with a polymer matrix and glass fiber inclusions. Experimentally this material is investigated in [13], and appropriate models combining damage and plasticity effects and derived in [14, 15]. Here, the micro-structure requires a very fine resolution, so that for a full 3D simulation, e.g., cyclic loading in a tensile test, massive parallel computing is required.

Our contribution is the formulation of these models as rate-independent energetic material systems and the development of a fully scalable parallel algorithm for the incremental problem. This is realized in the parallel finite element software M++ [16] using multigrid methods for the solution of the linearizations on both scales. It includes a highly scalable periodic parallel direct coarse grid solver [17] for the linear system on the coarse level.

This work is organized as follows. We start in Sect. 5.2 with the heterogeneous two-scale finite element method for linear elasticity by defining the corresponding two-scale energy minimization for the displacements on the macro-level and the micro-fluctuations in all RVEs. It is shown that this is equivalent to the classical homogenization procedure where the macro-solution can be computed in two stages. In the first step, in the RVEs a basis of periodic micro-fluctuations corresponding to the symmetric tensor basis is computed, which then defines the homogenized Hookian tensor describing the effective material behavior. This is inserted into the macro-problem which directly determines the homogenization limit by the solution of the coarse mesh problem. For this standard procedure we propose an efficient parallel scheme, which is then in Sect. 5.3 evaluated numerically for a tensile test with different micro-structures. For the extension to inelastic models we introduce in Sect. 5.4 the analytic framework for rate-independent systems based on an energy functional depending on displacement and internal mem-
ory variables, and on a dissipation functional depending on the rate of the internal variables. Energy and dissipation are defined for small strain damage and plasticity models, the incremental stress response for these models are defined and the consistent tangent operator is derived explicitly. This is extended to nonlinear two-scale algorithms in Sect. 5.5 and finally in Sect. 5.6 the nonlinear numerical methods are evaluated by various test scenarios.

All results in this chapter are part of the PhD thesis of the first author [18], where the numerical realization and the parallelization strategy is explained in detail.
5.2 Parallel heterogeneous two-scale FEM for linear elasticity

We introduce the two-scale method for elastic solids in $\Omega \subset \mathbb{R}^D$ in the case of small deformations. The method aims to approximate the deformation with a coarse mesh size $H$ in a heterogeneous medium with much smaller characteristic length scale $\delta$.

**Small strain elasticity** In the continuous problem the displacement vector $u$ is characterized by minimizing the total energy

$$\mathcal{E}(u) = \int_{\Omega} W(x, \varepsilon(u)) \, dx - \langle \ell, u \rangle$$

subject to boundary conditions $u = u_D$ on $\Gamma_D \subset \partial \Omega$. Here, a load functional

$$\langle \ell, v \rangle = \int_{\Omega} b(x) \cdot v(x) \, dx + \int_{\Gamma_N} t_N(x) \cdot v(x) \, da,$$

with body forces $b$ and surface tractions $t_N$ is applied, and the small strain isotropic elastic energy is of the form

$$W(x, \varepsilon) = \frac{1}{2} C(x) [\varepsilon(x)] : \varepsilon(x) \quad (5.1)$$

only depending on the linearized strain $\varepsilon = \varepsilon(u)$ with $\varepsilon(u) = \text{sym} \, Du$.

We consider the case that $C(\cdot)$ is strongly inhomogeneous and cannot be resolved on coarse meshes of mesh size $H$, i.e., we consider the case that $C(\cdot)$ can be resolved only on a mesh size $h < \delta$ with $\delta \ll H$, so that it is not feasible to compute the full fine mesh solution in $\Omega$.

**The multiscale idea** A multiscale method aims to approximate the exact solution $u$ on the coarse level in a finite element space with mesh size parameter $H > 0$, where the coarse approximation $u_H$ (referred as macro-solution) is obtained by solving a suitable averaged problem. Therefore, we define a suitable averaged energy $\mathcal{E}_H(\cdot)$ so that the coarse approximation can be determined as minimizer of this energy.

The construction of the averaged energy relies on the solution of local problems in **representative volume elements** (RVE)

$$Y_\xi = \xi + \delta(-0.5, 0.5)^D \subset \Omega$$

at sample points $\xi \in Z_H \subset \Omega$. On the RVEs we define locally micro-solutions $u_{\xi,h} = u_{\xi,H} + v_{\xi,h}$, where $u_{\xi,H}$ is the linearization of the macro-solution and $v_{\xi,h}$ is the so-called micro-fluctuation. This is approximated in a finite element space with mesh size parameter $h > 0$. The two-scale setting is illustrated in Fig. 5.1.
Fig. 5.1: Illustrations of the two-scale model with isotropic and unidirectional fiber directions: In the domain $\Omega$, the macroscopic solution $u_H$ is approximated on a coarse scale with mesh size $H$. The micro-structure of size $\delta \ll H$ is approximated at sample points $\xi$. The micro-fluctuation $v_{\xi,h}$ and the effective material response is computed in the representative volume element $Y_{\xi} = \xi + \delta(-0.5,0.5)^D \subset \Omega$. The symmetries of the tensile test can be exploited to reduce the computational domain for the approximation of the macro-solution.

The heterogeneous multiscale method extends the two-scale homogenization of periodic micro-structures to applications, where the micro-structure in every RVE is representative at least for a small neighborhood extending the RVE. It is a modeling assumption that a periodic continuation of the micro-fluctuation is appropriate. These assumptions are quite restrictive but they allow for a full mathematical analysis of the homogenization error which is enhanced by the modeling error due to the approximation of the heterogeneous micro-structure [5].

**The discrete multiscale setting** Let $\Omega \subset \mathbb{R}^D$ be a Lipschitz domain, and define the space $V = H^1(\Omega; \mathbb{R}^D)$. For given Dirichlet data $u_D$, we define the affine space $V(u_D) = \{v \in V : v = u_D \text{ on } \Gamma_D \subset \partial \Omega\}$. The macro-solution is approximated in a finite element space $V_H \subset V$, and we set

$$V_H(u_D) = \{v_H \in V_H : v_H(x) = u_D(x) \text{ for all nodal points } x \in \Gamma_D \}.$$

On the mesh corresponding to $V_H$ we select quadrature points $\Xi_H \subset \Omega$ with weights $\omega_\xi$ for $\xi \in \Xi_H$, and we introduce the notation

$$\int_{\Xi_H} f(\xi) = \sum_{\xi \in \Xi_H} \omega_\xi f(\xi) \approx \int_{\Omega} f(x) \, dx.$$

We assume that the quadrature is exact for $\varepsilon(u_H)$. 
Locally in every RVE, the micro-fluctuation is approximated in a finite element space $V_{\xi,h} \subset V_{\xi}$ with

$$V_{\xi} = \{ v_{\xi} \in H^1_{\text{per}}(Y_{\xi}, \mathbb{R}^D) : \int_{Y_{\xi}} v_{\xi} \, dx = 0 \},$$

where $H^1_{\text{per}}(Y_{\xi}, \mathbb{R}^D)$ denotes the restriction of $Y_{\xi}$-periodic $H^1_{\text{loc}}(\mathbb{R}^D, \mathbb{R}^D)$ functions to $Y_{\xi}$. On the micro-scale we set the global finite element approximation space as the product space $V_h = \prod_{\xi \in \Xi} V_{\xi,h}$. Furthermore, we assume that the elasticity tensor $C(x)$ for $x \in Y_{\xi}$ is representative for the material properties in a neighborhood of any sample point $\xi \in \Xi_H$.

**The multiscale problem** The multiscale approximation represented by the macro-solution and the micro-fluctuations in every RVE is defined as the minimizer $(u_H, v_h) \in V_H(u_D) \times V_h$ of the two-scale energy

$$\mathcal{E}_H(u_H, v_h) = \int_{\Xi_H} W_{\xi}(\varepsilon(u_H) + \varepsilon(v_{\xi,h}), \varepsilon_h) - \langle \ell, u_H \rangle,$$

where the micro-energy is evaluated on the RVEs by

$$W_{\xi}(\varepsilon_H, v_{\xi,h}) = \frac{1}{|Y_{\xi}|} \int_{Y_{\xi}} W(x, \varepsilon_H(x) + \varepsilon(v_{\xi,h})) \, dx$$

depending on the strain $\varepsilon_H = \varepsilon(u_H)$ of the macro-solution and micro-fluctuations $v_{\xi,h}$. In the RVE we define the linear approximation of the macro-solution by $u_{\xi,h}(x) = u_H(\xi) + Du_H(\xi)(x - \xi)$. This defines together with the micro-fluctuation the micro-solution $u_{\xi,h} = u_{\xi,H} + v_{\xi,h}$, so that by construction $u_{\xi,h} - u_{\xi,H}$ is periodic, and the strain of the macro-solution $\varepsilon_{\xi,H} = \varepsilon(u_{\xi,H}) \equiv \varepsilon(u_H)(\xi)$ is constant in the RVE $Y_{\xi}$.

**The two-scale problem and the multiscale tensor** The minimizer of the two-scale energy is characterized as the critical point of the two-scale energy: find $(u_H, v_h) \in V_H(u_D) \times V_h$ satisfying

**Macro-Equilibrium**

$$0 = \partial_u \mathcal{E}_H(u_H, v_h), \quad (5.2a)$$

**Micro-Equilibrium**

$$0 = \partial_{v_{\xi,h}} \mathcal{E}_H(u_H, v_h), \quad (5.2b)$$

i.e., solving the coupled linear problems

$$\sum_{\xi} \frac{\omega_{\xi}}{|Y_{\xi}|} \int_{Y_{\xi}} C(x)[\varepsilon(u_H)(\xi) + \varepsilon(v_{\xi,h})(x)] : \varepsilon(\delta u_H)(\xi) \, dx = \langle \ell, \delta u_H \rangle, \quad (5.3a)$$

$$\frac{1}{|Y_{\xi}|} \int_{Y_{\xi}} C(x)[\varepsilon(u_H)(\xi) + \varepsilon(v_{\xi,h})(x)] : \varepsilon(\delta v_{\xi,h}) \, dx = 0 \quad (5.3b)$$

for test functions $(\delta u_H, \delta v_{\xi,h}) \in V_H(0) \times V_{\xi,h}$. 
Now we reduce this system to an averaged macro-problem. Therefore, we introduce an orthonormal basis $\eta_1, \ldots, \eta_6$ of $\text{Sym}(3) = \mathbb{R}^{3 \times 3}_{\text{sym}}$. Corresponding to this basis we compute micro-fluctuations $w_{\xi,h,1}, \ldots, w_{\xi,h,6} \in V_{\xi,h}$ solving

$$
\frac{1}{|Y_{\xi}|} \int_{Y_{\xi}} C(x)[\eta_j + \varepsilon(w_{\xi,h,j})(x)] : \varepsilon(\delta v_{\xi,h})(x) \, dx = 0, \quad \delta v_{\xi,h} \in V_{\xi,h}. \quad (5.4)
$$

Inserting the representation of the macro-strain $\varepsilon_{\xi,H} = \varepsilon(u_H)(\xi)$ with respect to this basis

$$
\varepsilon_{\xi,H} = \sum_{j=1}^{6} (\varepsilon_{\xi,H} : \eta_j) \eta_j,
$$

we obtain for the micro-fluctuation solving (5.3b)

$$
v_{\xi,h} = \sum_{j=1}^{6} (\varepsilon_{\xi,H} : \eta_j) w_{\xi,h,j}.
$$

This is now inserted into the macro-equation (5.3a), which yields

$$
\int_{\Sigma_H} C_{\xi,H}[\varepsilon(u_H)] : \varepsilon(\delta u_H) = \langle \ell, \delta u_H \rangle, \quad \delta u_H \in V_H(0)
$$

with the two-scale elasticity tensor

$$
C_{\xi,H} = \sum_{j,k=1}^{6} \left( \frac{1}{|Y_{\xi}|} \int_{Y_{\xi}} C(x)[\eta_j + \varepsilon(w_{\xi,h,j})(x)] : \eta_k \, dx \right) \eta_j \otimes \eta_k. \quad (5.5)
$$

Together, we obtain the following result.

**Lemma 5.1.** The macro-solution $u_H \in V_H(u_D)$ of the heterogeneous multiscale method minimizes the averaged energy

$$
E_{\text{avg}}^H(u_H) = \frac{1}{2} \int_{\Sigma_H} C_{\xi,H}[\varepsilon(u_H)] : \varepsilon(u_H) - \langle \ell, u_H \rangle. \quad (5.6)
$$

The definition of the micro-fluctuations $w_{\xi,h,1}, \ldots, w_{\xi,h,6}$ by equation (5.4) ensures that the two-scale elasticity tensor $C_{\xi,H}$ is symmetric. Due to Korn’s inequality the averaged energy is uniformly convex, which assures the existence and uniqueness of the minimizer in (5.6).

**The parallel two-scale model** In our parallel model we assume that the meshes to resolve the geometry in the RVEs are so large that they can be distributed to all processes. On the other hand, we do expect that we do not need to compute a micro-fluctuation in all RVEs $Y_{\xi}$, e.g., if the microstructure is identical. In the most simple case of two-scale homogenization, we compute the micro-problem only once, as it is now described for our first parallel two-scale FEM of the heterogeneous small strain elasticity problem.
For the implementation, the RVEs $\mathcal{Y}_\xi = \xi + \delta(-0.5, 0.5)D \subset \Omega$ are mapped to the unit cube $\mathcal{Y} = (0, 1)^3$. In the simple case the micro-structure described by the elasticity tensor $C$ is mapped to the same tensor for all $\xi \in \Xi_H$. Nevertheless, since this cannot be expected for general applications, we describe the parallel algorithm in a more general case which allows for different micro-structures and which also is flexible for cases where only some of the RVE computations are required.

Here we consider the case, that the approximation of the micro-structure requires a very fine mesh size, so that also the micro-problem has to be computed in parallel. Therefore, we determine by a load balancing procedure a domain decomposition $\Omega = \bar{\Omega}_1 \cup \cdots \cup \bar{\Omega}_P$ and a further decomposition for the reference RVE $\bar{\mathcal{Y}} = \bar{\mathcal{Y}}_1 \cup \cdots \cup \bar{\mathcal{Y}}_P$. The finite element spaces $V_H$ and $V_{\xi,h}$ are distributed to the processes $p \in \mathcal{P} = \{1, \ldots, P\}$ which results into a consistent representation of the macro-deformation $u_H$ and the micro-fluctuations $w_{\xi,h}^1, \ldots, w_{\xi,h}^6$ by local functions $u_H^p = u_H|_{\bar{\Omega}_p}$ and $w_{\xi,h}^p = w_{\xi,h}^p|_{\bar{\mathcal{Y}}_p}$ on process $p$. For the elastic two-scale solution the multiscale tensor $C_{\xi,H}$ is evaluated only for a subset $\Xi_H^\text{active}$ with different micro-structure, i.e., we assume that for all other points $\xi \in \Xi_H \setminus \Xi_H^\text{active}$ some active point $\xi' \in \Xi_H^\text{active}$ exists so that we can choose $C_{\xi,H} = C_{\xi',H}$. The full parallel two-scale method is summarized in Alg. 1.

**Algorithm 1** Parallel heterogeneous two-scale method for linear elasticity.

E1) Sequentially for all points $\xi \in \Xi_H^\text{active}$ with different micro-structure perform the following steps:

M1) Compute the micro-fluctuations $w_{\xi,h,1}, \ldots, w_{\xi,h,6} \in V_{\xi,h}$ solving in parallel

$$\frac{1}{|Y_\xi|} \int_{Y_\xi} C(x)[\eta_l + \varepsilon(w_{\xi,h,l})] : \varepsilon(\delta v_{\xi,h}) \, dx = 0, \quad \delta v_{\xi,h} \in V_{\xi,h}. $$

M2) Evaluate the local contributions of the multiscale tensor

$$C_{\xi,H}^p = \frac{1}{|Y_\xi|} \sum_{l,j=1}^6 \left( \int_{Y_\xi} C(x)[\eta_l + \varepsilon(w_{\xi,h,l}^p)] : \eta_j \, dx \right) \eta_l \otimes \eta_j, \quad p \in \mathcal{P}. $$

M3) On the process $q$ with $\xi \in \Xi_H \cap \Omega^q$ collect the full multiscale tensor

$$C_{\xi,H} = \sum_{p=1}^P C_{\xi,H}^p. $$

E2) Sequentially for all points $\xi \in \Xi_H \setminus \Xi_H^\text{active} \cap \Omega^p$ find $\xi' \in \Xi_H^\text{active}$ with $C_{\xi,H} = C_{\xi',H}$ and send the multiscale tensor to process $p$.

E3) Compute $u_H \in V_H(u_D)$ solving in parallel

$$\int_{\Xi_H} C_{\xi,H}[\varepsilon(u_H)] : \varepsilon(\delta u_H) = \langle \ell, \delta u_H \rangle, \quad \delta u_H \in V_H(0). $$
5.3 Numerical experiments for linear elastic two-scale models

We evaluate the two-scale method for two component composites with the thermoplastic polymer polybutylene terephthalate as carrier matrix and embedded glass fibers. We use isotropic linear elasticity with Lamé parameters $\lambda_M = 3571.43$ and $\mu_M = 892.857$ for the polymer and $\lambda_F = 30000$ and $\mu_F = 20000$ for the glass fiber.

For the test scenario we use a standardized uniaxial tensile test configuration ISO 527-2:1996 type 1A, where experimental data are available. The computational domain $\Omega \subset (-0.2, 0.2) \times (-2, 2) \times (-6.5, 6.5)$ is approximated by a hexahedral mesh, cf. Fig. 5.2.

Corresponding to the experimental setting we prescribe the displacement at the Dirichlet boundary $\Gamma_D = \{ x \in \partial \Omega : x_3 = -6.5 \text{ or } x_3 = 6.5 \}$ with

$$u_D(t, x) = \begin{cases} 0 & \text{for } x_3 = 6.5, \\ 0 & \text{for } x_3 = -6.5, \\ u_0 t & \end{cases}$$

$$\sigma(\varepsilon(u)) n = 0 \text{ on } \Gamma_N = \partial \Omega \setminus \Gamma_D.$$  \hspace{1cm} (5.7)

The scaling factor is set to $u_0 = 0.01$, and the linear model is tested for $t = 1$. For the investigation of the convergence properties, we reduce the computation to one fourth of the geometry $\Omega_{sym} \subset \Omega$ with symmetry boundary conditions on $\Gamma_{sym} = \{ x \in \partial \Omega_{sym} : x_3 = 0 \text{ or } x_2 = 0 \}$ which corresponds to two-sided loading with $u_0$ replaced by $0.5u_0$.

In $V_H$ and in $V_{\xi,h}$ we use conforming hexahedral $Q_1$ finite elements.

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1 BASF data sheet on http://www.plasticsportal.net
2 Data sheet on http://www.matweb.com
Numerical tests for different resolutions of the micro-structure

In our first experiment, the convergence of the classical two-scale homogenization is tested, where only one representative micro-structure is computed, and where the same effective material response is used at all integration points. Therefore, we select from the collection [20] one micro-structure $\mathcal{Y}_\delta$ of characteristic length scale $\delta$ with isotropic glass fiber distribution and 10% fiber volume fraction. Corresponding to a basis of the symmetric tensors, 6 periodic micro-fluctuations are computed by (5.4), see Fig. 5.3.

Fig. 5.3: Deformation of the 6 periodic micro-fluctuations $\mathbf{w}_{\xi,h,k}^\delta$ and the Frobenius norm distribution of the stress $|\mathbf{\sigma}_{\xi,h,k}^\delta|$ in $\mathcal{Y}_\delta$ corresponding to the symmetric tensor basis $\eta_1,...,\eta_6$.

This defines by (5.5) the effective elasticity tensor

$$
\mathbf{C}_{\xi,H}^{\delta_0} = 
\begin{pmatrix}
6813.81 & 4103.21 & 4091.94 & -31.99 & -1.79 & -30.05 \\
4103.21 & 6746.61 & 4090.63 & -1.79 & 26.43 & -3.04 \\
4091.94 & 4090.63 & 6750.23 & 9.40 & 2.73 & -22.82 \\
-31.99 & -1.79 & 9.40 & 2630.59 & -7.91 & -1.96 \\
-1.79 & 26.43 & 2.73 & -7.91 & 2598.53 & 10.05 \\
-30.05 & -3.04 & 22.82 & -1.96 & 10.05 & 2597.09
\end{pmatrix}.
$$

The accuracy of the two-scale approximation depends on the mesh size of the macro- and the micro-problem, and on the resolution $\delta$ of the geometry in the RVE. Since the complex micro-structure in the RVE requires a very fine resolution of the micro-problem, we test if smaller RVEs $\mathcal{Y}_{\delta/2}^\xi$ and $\mathcal{Y}_{\delta/4}^\xi$ with a coarser resolution of the micro-problem are sufficient.
For the quantitative evaluation we compute the macroscopic stress integral
\[
\sigma^\delta_H = \int_{\Xi_H} \sigma^\delta_{\xi,H} \quad \text{with} \quad \sigma^\delta_{\xi,H} = \frac{1}{|Y_\xi|} \int_{Y_\delta} C(y) \left[ \varepsilon_{\xi,H} + \varepsilon(v_{\xi,h}) \right] \, dy
\]
depending on \( \varepsilon_{\xi,H} = \varepsilon(u_H)(\xi) \), see Tab. 5.1.

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<td>3.93153</td>
</tr>
</tbody>
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Table 5.1: Numerical results for \(|\sigma^\delta_H|\) computed on the macro-scale in \(V_H\) (row) and on the micro-scale in \(V_{\xi,h}\) (column) for the micro-structures \(Y_\delta\), \(Y_{\delta/2}\), and \(Y_{\delta/4}\) with isotropic fiber distribution and 10% fiber volume fraction.

We observe, that the coarse resolution with \(\dim V_H = 765\) for the macro-problem is sufficient to approximate \(|\sigma^\delta_H|\) with a relative error of less than 2%. On the micro-scale, a relative error of less than 10% requires at least \(\dim V_{\xi,h} = 6 440 067\) on \(Y_\delta\), and \(\dim V_{\xi,h} = 823 875\) on \(Y_{\delta/2}\). The asymptotic results for \(Y_{\delta/4}\) show that in this case the resolution of the micro-structure is not sufficient to obtain approximations with a relative error smaller than 10%. For a detailed convergence analysis we refer to [18, Chap. 4].
Numerical tests for different fiber orientations and filler contents

Now we investigate the elastic material properties for 10%, 20% and 30% fiber volume content and 0°, 45°, 60° and 90° fiber orientation with respect to the applied load in the tensile test. We use a fine resolution in the RVE with $\dim V_{\xi,h} = 6440067$, and $\dim V_H = 6551523$ for the macro-solution. Each computation is performed on a single node\(^3\) with 64 cores in approx. one hour.

<table>
<thead>
<tr>
<th></th>
<th>PBT 0°</th>
<th>45°</th>
<th>60°</th>
<th>90°</th>
</tr>
</thead>
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<tr>
<td>$E_x$</td>
<td>2500</td>
<td>6116</td>
<td>3333</td>
<td>3167</td>
</tr>
<tr>
<td>$\nu_{xy}$</td>
<td>0.40</td>
<td>0.38</td>
<td>0.44</td>
<td>0.36</td>
</tr>
<tr>
<td>$\nu_{xx}$</td>
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<td>0.38</td>
<td>0.36</td>
<td>0.41</td>
</tr>
<tr>
<td>$\sigma_z$</td>
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<td>5.30179</td>
<td>2.94166</td>
<td>2.78511</td>
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<tr>
<td>$\varepsilon_x$</td>
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<td>-3.32e-4</td>
<td>-3.15e-4</td>
<td>-3.56e-4</td>
</tr>
<tr>
<td>$\varepsilon_y$</td>
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<td>-3.33e-4</td>
<td>-3.86e-4</td>
<td>-3.20e-4</td>
</tr>
<tr>
<td>$\varepsilon_z$</td>
<td>8.77e-4</td>
<td>8.66e-4</td>
<td>8.82e-4</td>
<td>8.79e-4</td>
</tr>
</tbody>
</table>

Table 5.2: Characteristic material values for a uniaxial tensile test with uni-directional short fibers with 10%, 20% and 30% fiber volume fraction and orientations between 0° and 90°.

\(^3\) AMD Opteron 6376 processor with 2.3 GHz and 512 GB RAM.
The characteristic material values are evaluated by averaging in the cross section \( \Omega_{\text{ctr}} = (0,0.5) \times (-0.2,0.2) \times (0,2) \subset \Omega \). Stress and strain in tensile direction are numerically computed by

\[
\sigma_z = \frac{1}{|\Omega_{\text{ctr}}|} \int_{\Omega_{\text{ctr}}} \mathbb{C}_{\xi,H}[\varepsilon(u_H)]_{zz}, \quad \varepsilon_z = \frac{1}{|\Omega_{\text{ctr}}|} \int_{\Omega_{\text{ctr}}} \varepsilon(u_H)_{zz}
\]

to approximate Young’s modulus \( E_z = \frac{\sigma_z}{\varepsilon_z} \) in \( z \)-direction. Analogously, the strain averages \( \varepsilon_x \) and \( \varepsilon_y \) are defined to determine Poisson’s ratios \( \nu_{zx} = -\frac{\varepsilon_y}{\varepsilon_x} \) and \( \nu_{zy} = -\frac{\varepsilon_x}{\varepsilon_y} \), cf. Tab. 5.2. All other orientations have a nearly equal stiffness character. Very accurate transverse isotropy, i.e. \( \nu_{zx} = \nu_{zy} \), can be observed in the case of parallel fiber and tensile alignment. This corresponds to the symmetry of the rotational axis along the fiber direction. For each different fiber alignment to the acting force the material behaves strongly anisotropic. The full elastic properties of the multiscale material are contained in the effective elasticity tensors

\[
\mathbb{C}_{\xi,H}^{0^\circ} = \begin{pmatrix}
6136.42 & 3976.58 & 3892.41 \\
3976.58 & 6196.72 & 3906.77 \\
3892.41 & 3906.77 & 9111.39
\end{pmatrix}
\]

\[
\mathbb{C}_{\xi,H}^{45^\circ} = \begin{pmatrix}
6189.56 & 3937.77 & 3936.05 \\
3937.77 & 6886.21 & 4576.09 \\
3936.05 & 4576.09 & 6897.25
\end{pmatrix}
\]

\[
\mathbb{C}_{\xi,H}^{90^\circ} = \begin{pmatrix}
6228.66 & 3938.61 & 3960.34 \\
3938.61 & 7439.97 & 4308.68 \\
3960.34 & 4308.68 & 6343.01
\end{pmatrix}
\]

The results fit well to experimental data provided by C. Rörig [13,21]. For a directly extruded specimen of type 1A with parallel aligned load fiber orientation and fiber volume content of 11.3% a Young’s modulus of \( E_z^{0^\circ} = 5960 \) and for 17.9% a modulus of \( E_z^{0^\circ} = 8240 \) is measured. For fiber orientations with angle 0°, 45°, 60° and 90° measurements of Young’s modulus of a specimen type 5A gives \( E_z^{0^\circ} = 6050 \), \( E_z^{45^\circ} = 4300 \), \( E_z^{60^\circ} = 3485 \) and \( E_z^{90^\circ} = 3840 \) for a volume filler content of 11.3%, and \( E_z^{0^\circ} = 7910 \), \( E_z^{45^\circ} = 4500 \), \( E_z^{60^\circ} = 4550 \) and \( E_z^{90^\circ} = 4430 \) for 17.3% fiber volume content.
5.4 Rate-independent material models with memory

Inelastic effects can be described by material models with history variables. In this section we introduce small-strain damage and plasticity model and the framework of energetic models as it is analyzed in [22]. We specify the constitutive settings of these models, and we derive the return mapping and the corresponding consistent tangent operators.

**Materials with memory** We aim to find displacements \( u : [0, T] \times \Omega \to \mathbb{R}^3 \) in the time interval \([0, T]\) of a material which is described by internal variables \( z : [0, T] \times \Omega \to \mathbb{R}^N \) and where the evolution is determined by the total energy and dissipation functionals

\[
\mathcal{E}(t, u, z) = \int_\Omega W(x, \varepsilon(u), z) \, dx - \langle \ell(t), u \rangle,
\]
\[
\mathcal{R}(\dot{z}) = \int_\Omega R(x, \dot{z}) \, dx.
\]

The load functional is given by

\[
\langle \ell(t), u \rangle = \int_\Omega b(t) \cdot v \, dx + \int_{\Gamma_N} t_N(t) \cdot v \, da
\]

with body forces \( b : [0, T] \times \Omega \to \mathbb{R}^3 \) and traction forces \( t_N : [0, T] \times \Gamma_N \to \mathbb{R}^3 \). We assume that the material is rate-independent, i.e., the inelastic deformation is independent from scaling in time. This is achieved if the dissipation function \( R \) is 1-homogeneous.

We only consider small strains with the ansatz space \( V = H^1(\Omega, \mathbb{R}^N) \) for the displacements, and the test space \( V(0) = \{ v \in V : v = 0 \text{ on } \Gamma_D \} \) including homogeneous boundary conditions on the Dirichlet boundary \( \Gamma_D \subset \partial\Omega \). For the internal variables we use the space \( Z = L_2(\Omega, \mathbb{R}^N) \). If the total energy functional \( \mathcal{E} : [0, T] \times V \times Z \to \mathbb{R} \) is bounded and uniformly convex in \( V(0) \times Z \) for all \( t \in [0, T] \), and if the dissipation functional \( \mathcal{R} : Z \to \mathbb{R} \cup \{\infty\} \) is convex, proper and lower semi-continuous (l.s.c.), an energetic solution

\[
(u, z) : [0, T] \to V \times Z
\]

exists which is characterized by

**Equilibrium** \( 0 = \partial_u \mathcal{E}(t, u(t), z(t)) \),

**Flow Rule** \( 0 \in \partial_z \mathcal{E}(t, u(t), z(t)) + \partial \mathcal{R}(\dot{z}(t)) \)

and boundary conditions for the displacement \( u(t) = u_D(t) \) on the Dirichlet boundary \( \Gamma_D \).
The incremental problem The evolution in time is approximated by a series of incremental problems. Let $0 = t_0 < t_1 < \cdots < t_{N_{\text{max}}} = T$ be a time series with $\Delta t_n = t_n - t_{n-1}$. Starting with $(u^0, z^0)$ we define for $n = 1, \ldots, N_{\text{max}}$ the following incremental problems depending on the given history variable $z^{n-1}$, the load functional $\ell^n = \ell(t_n)$ and the Dirichlet data $u^n_D = u_D(t_n)$: find a minimizer $(u^n, z^n) \in V(u^n_D) \times Z$ of the incremental functional

$$
J_n(u^n, z^n) = E(t_n, u^n, z^n) + R(z^n - z^{n-1}).
$$

In our applications $J_n(\cdot)$ is uniformly convex, so that a unique minimizer exists. It is determined by computing a critical point of $J_n(\cdot)$ characterized by the nonlinear system

\begin{align}
\text{Equilibrium} & \quad 0 = \partial_u E(t_n, u^n, z^n), \quad (5.9a) \\
\text{Flow Rule} & \quad 0 \in \partial_z E(t_n, u^n, z^n) + \partial R(\Delta z^n). \quad (5.9b)
\end{align}

Since we consider rate-independent materials, the flow rule is 1-homogeneous satisfying $\Delta t_n R((\Delta t_n)^{-1}(z^n - z^{n-1})) = R(z^n - z^{n-1})$ and thus depending only on the increment $\Delta z^n = z^n - z^{n-1}$.

A simple damage model Continuum damage mechanics phenomenologically describes the expansion of micro-cracks and cavities with a single additional state variable

$$
d = \frac{A_d}{A_0} \in [0, 1]
$$

defined by the proportion of damaged area $A_d$ of a representative cross sectional area $A_0$ (see, e.g., [23, 24, 25, 26]). This results into the effective stress response $\sigma = (1 - d)C[\varepsilon]$.

Within the energetic framework we set $N = 1$ and $z = d$. The free energy is defined by

$$
W(\varepsilon, d) = (1 - d)W_{\text{elastic}}(\varepsilon) + W_{\text{damage}}(d)
$$

with $W_{\text{elastic}}(\varepsilon) = \frac{1}{2} \varepsilon : C[\varepsilon]$, so that $\sigma = \partial_\varepsilon W(\varepsilon, d) = (1 - d)C[\varepsilon]$. The dissipation functional

$$
R_{\text{damage}}(d) = \begin{cases} 
0 & d \geq 0, \\
+\infty & \text{otherwise} 
\end{cases} \quad (5.10)
$$

just ensures the irreversibility of the damage process.

The additional term $W_{\text{damage}}$ determines the evolution of the damage variable and guarantees $d < 1$. It is constructed in analogy to isotropic plasticity. We assume that the damage evolution is locally controlled by a strictly monotone function $\Phi$ depending on the local elastic energy $Y = W_{\text{elastic}}(\varepsilon(u))$ and...
the complementarity conditions
\[ \dot{d} \geq 0, \quad \Phi(Y) - d \leq 0, \quad (\Phi(Y) - d)\dot{d} = 0, \] (5.11)
i.e., \( d \) can only increase and not decrease and the material remains elastic, if the local elastic energy is small satisfying \( \Phi(Y) < d \). Here, the choice
\[ \Phi(Y) = 1 - \exp \left( -H(\sqrt{2Y} - Y_0) \right) \]
with damping and yielding point material parameters \( H, Y_0 \geq 0 \) is designed such that the material responds elastic for \( \Phi(Y) < 0 \), i.e., \( \sqrt{2Y} < Y_0 \), and \( \Phi(Y) \to 1 \) for large \( Y \). Nevertheless, since \( \Phi(Y) < 1 \) for all \( Y \), the damage variable will not reach \( d = 1 \) which prevents fracture in this model.

Since \( \Phi(\cdot) \) is assumed to be strictly monotone, the inverse is uniquely defined and the complementarity conditions (5.11) take the form
\[ \dot{d} \geq 0, \quad Y - \Phi^{-1}(d) \leq 0, \quad (Y - \Phi^{-1}(d))\dot{d} = 0. \]
Due to our choice of the dissipation this is equivalent to
\[ Y - \Phi^{-1}(d) \in \partial R_{\text{damage}}(\dot{d}). \]
This motivates the definition of the defect energy
\[ W_{\text{damage}}(d) = \int_0^d \Phi^{-1}(\delta) \, d\delta, \] (5.12)
i.e., \( \Phi^{-1}(d) = \partial_d W_{\text{damage}}(d) \) and \( Y - \Phi^{-1}(d) = -\partial_d W(\varepsilon, d) \).

For fixed \( \varepsilon \) the flow rule \( 0 \in \partial_d W(\varepsilon, d) + \partial R_{\text{damage}}(\dot{d}) \) characterizes the minimum of \( f(d; \varepsilon) = W(\varepsilon, d) + R_{\text{damage}}(\dot{d}) \). Together, we observe that the minimizer is characterized by (5.11).

For our choice of \( \Phi \) we observe \( \Phi^{-1}(d) = \frac{1}{2} \left( Y_0 - \frac{1}{H} \log(1 - d) \right)^2 \), so that \( W_{\text{damage}}(d) \to \infty \) for \( d \to 1 \) prevents to reach a fully damaged material in this model. Nevertheless, we will see below that the inelastic energy is not uniformly convex, so that a well-defined evolution is only determined for sufficiently small loads or displacements.

Remark 5.1. This simple model does not allow to compute the transition to fracture. Due to the choice of \( \Phi(\cdot) \), the energy in this model is only convex for sufficiently small damage, and the consistent tangent gets indefinite for \( d \) close to 1, so that one cannot expect convergence for the Newton method for large loads, and simulations for larger loads need an extension of the model.
The incremental flow rule for the damage model In the first step, we consider the semi-discrete problem in time. For given history variable \( d^{n-1} \), the incremental problem \(*5.9*\) determines \((u^n, d^n) \in V(u^n_D) \times L^2(\Omega)\) with

\[
0 = \int_{\Omega} \partial_\varepsilon W(\varepsilon(u^n), d^n) : \varepsilon(\delta u) \, dx - \langle t^n, \delta u \rangle, \quad \delta u \in V(0), \tag{5.13a}
\]

\[
0 \in \partial_d W(\varepsilon(u^n), d^n) + \partial R_{\text{damage}}(d^n - d^{n-1}). \tag{5.13b}
\]

The solution \((u^n, d^n)\) of \(5.13\) is a critical point of the functional

\[
J_n(u_d) = \int_{\Omega} W(\varepsilon(u), d) \, dx - \langle t, u \rangle + \int_{\Omega} R_{\text{damage}}(d - d^{n-1}) \, dx \tag{5.14}
\]

subject to the essential boundary conditions \(u = u_D\) on \(\Gamma_D\).

The incremental damage problem can be reduced to a nonlinear problem for the displacement by inserting the local solution of the incremental flow rule depending on the strain. This is based on the following result.

**Lemma 5.2.** For given history variable \( d^{n-1} \) and fixed strain \( \varepsilon \) the unique solution \( \Delta d \) of the local incremental flow rule in every material point

\[
0 \in \partial_d W(\varepsilon, d^{n-1} + \Delta d) + \partial R_{\text{damage}}(\Delta d)
\]

is given by

\[
\Delta d = \max \{0, \Phi(Y(\varepsilon)) - d^{n-1}\}, \quad Y(\varepsilon) = W_{\text{elastic}}(\varepsilon).
\]

**Proof.** Evaluating \( \partial_d W(\varepsilon, d^{n-1} + \Delta d) = -Y(\varepsilon) + \Phi^{-1}(d^{n-1} + \Delta d) \) in the incremental flow rule yields

\[
Y(\varepsilon) - \Phi^{-1}(d^{n-1} + \Delta d) \in \partial R_{\text{damage}}(\Delta d) = \begin{cases} 
\{0\} & \Delta d > 0, \\
(-\infty, 0] & \Delta d = 0, \\
\emptyset & \Delta d < 0.
\end{cases}
\]

This is equivalent to the complementarity condition

\[
\Delta d \geq 0, \quad \Phi(Y(\varepsilon)) - d^{n-1} - \Delta d \leq 0, \quad \left(\Phi(Y(\varepsilon)) - d^{n-1} - \Delta d\right) \Delta d = 0
\]

which directly implies \( \Delta d = \max \{0, \Phi(Y(\varepsilon)) - d^{n-1}\} \). \(\square\)

The evaluation of the flow rule defines the update of the damage variable

\[
d_n(\varepsilon) = d^{n-1} + \Delta d = d^{n-1} + \max \{0, \Phi(Y(\varepsilon)) - d^{n-1}\}
\]

and the incremental stress response

\[
\sigma_n(\varepsilon) = (1 - d_n(\varepsilon)) C[\varepsilon].
\]
Choosing $\text{sgn}(s) \in \partial \max\{0, s\}$ with

$$\text{sgn}(s) = \begin{cases} 1 & s > 0, \\ 0 & \text{otherwise} \end{cases}$$

defines the consistent tangent $C_n(\varepsilon) \in \partial \sigma_n(\varepsilon)$ by

$$C_n(\varepsilon)\|\delta\varepsilon\| = (1 - d_n(\varepsilon))C(\varepsilon)\|\delta\varepsilon\| - \text{sgn} \left( \max \{0, \Phi(Y(\varepsilon)) - d_n^{-1}\} \right) \Phi'(Y(\varepsilon)) (C[\varepsilon] \cdot \delta\varepsilon) C[\varepsilon]$$

with $\Phi'(Y) = \frac{H}{2\sqrt{Y}} \exp(-H(\sqrt{2}Y - Y_0))$.

The incremental problem can be solved by minimizing the reduced functional for the displacement

$$J_n^{\text{red}}(u) = \int_{\Omega} \left( \int_0^{Y(\varepsilon(u))} \left( 1 - d_n^{-1} - \max \{0, \Phi(y) - d_n^{-1}\} \right) dy \right) dx - \langle \ell^n, u \rangle$$

with first variation

$$\partial J_n^{\text{red}}(u)[\delta u] = \int_{\Omega} \left( 1 - d_n^{-1} - \max \{0, \Phi(Y(\varepsilon(u))) - d_n^{-1}\} \right) C(\varepsilon(u)) [\varepsilon(\delta u)] dx - \langle \ell^n, \delta u \rangle$$

corresponding to (5.13a). Within a generalized Newton method, the consistent tangent defines

$$\partial^2 J_n^{\text{red}}(u)[\Delta u, \delta u] = \int_{\Omega} C_n(\varepsilon(u)) [\varepsilon(\Delta u)] : \varepsilon(\delta u) dx.$$

We observe $C_n(\varepsilon)[\varepsilon] : \varepsilon < 0$ for large $\varepsilon$, so that for our choice of $\Phi$ the second variation of $J_n^{\text{red}}$ is not positive and thus $J_n^{\text{red}}$ is only convex for sufficiently small strains. This restricts the application of this damage model to moderate loads. An extended damage model with convex energy can be obtained by including gradient terms, see, e.g., [27].
Small strain elasto-plasticity

For the elasto-plastic model with hardening, the internal variables \( \mathbf{z} = (\varepsilon_p, r) \) are the plastic strain \( \varepsilon_p \) with trace \( \varepsilon_p = 0 \) and the isotropic hardening parameter \( r \), i.e., \( N = 6 \). The strain is decomposed into elastic and plastic part \( \varepsilon(u) = \varepsilon_e + \varepsilon_p \), and the free energy is given by

\[
W(\mathbf{x}, \varepsilon, \varepsilon_p, r) = W_{\text{elastic}}(\mathbf{x}, \varepsilon(u) - \varepsilon_p) + W_{\text{plastic}}(\varepsilon_p, r)
\]

with the elastic energy (5.1) and defect energy

\[
W_{\text{plastic}}(\varepsilon_p, r) = W_{\text{kin}}(\varepsilon_p) + W_{\text{iso}}(r) \tag{5.15}
\]

combining kinematic and isotropic hardening. The translation of the yield surface is described by kinematic hardening with

\[
W_{\text{kin}}(\varepsilon_p) = \frac{1}{2} K \varepsilon_p : \varepsilon_p
\]

depending on the hardening parameter \( K \geq 0 \). The expansion of the yield surface is described by isotropic hardening determined by the yield function

\[
\Psi(r) = \sigma_y + H_0 r + (K_{\infty} - K_0)(1 - \exp(\delta r))
\]

for given material parameters \( \sigma_y, H_0, \delta \geq 0 \) and \( K_{\infty} \geq K_0 \geq 0 \). Now we construct the remaining energy contribution and the dissipation such that the plastic evolution satisfies the yield condition \( |\text{dev} \sigma - \beta| + \Psi(r) \leq 0 \).

The energy definition corresponds to the constitutive stress-stain relation

\[
\sigma = \partial_\varepsilon W(\varepsilon, \varepsilon_p, r) = \partial_\varepsilon W_{\text{elastic}}(\varepsilon(u) - \varepsilon_p) = \mathcal{C} [\varepsilon(u) - \varepsilon_p].
\]

It defines the back stress \( \beta = \partial_\varepsilon W_{\text{kin}}(\varepsilon_e) = K \varepsilon_p \), and the conjugated variables \( \mathbf{y} = (\alpha, \zeta) = -\partial_\varepsilon W(\varepsilon, \mathbf{z}) \) with

\[
\begin{align*}
\alpha &= \partial_{\varepsilon_p} W_{\text{elastic}}(\varepsilon(u) - \varepsilon_p) - \partial_{\varepsilon_p} W_{\text{kin}}(\varepsilon_p) = \text{dev} \sigma - \beta, \\
\zeta &= -\partial_r W_{\text{iso}}(r).
\end{align*}
\]

This yields the constitutive relation \( \zeta = -\partial_r W_{\text{iso}}(r) = -\Psi(r) \) by defining

\[
W_{\text{iso}}(r) = \int_0^r \Psi(\rho) \, d\rho.
\]

The plastic evolution is determined by the plastic potential

\[
R^{\star}_{\text{plastic}}(\alpha, \zeta) = \begin{cases} 
0 & |\alpha| + \zeta \leq 0 \text{ and } \zeta \leq 0, \\
+\infty & \text{otherwise},
\end{cases}
\]

which is by duality equivalent to the dissipation functional

\[
R_{\text{plastic}}(\dot{\varepsilon}_p, \dot{r}) = \begin{cases} 
0 & \dot{r} \geq |\dot{\varepsilon}_p|, \\
+\infty & \text{otherwise}. 
\end{cases}
\tag{5.16}
\]
The flow rule \((\alpha, \zeta) \in \partial R_{\text{plastic}}(\dot{\varepsilon}_p, \dot{r})\) in every material point is evaluated by duality, i.e., \((\dot{\varepsilon}_p, \dot{r}) \in \partial R^*_{\text{plastic}}(\alpha, \zeta)\). Introducing a consistency parameter \(\lambda_p\) this is equivalent to the normality rule
\[
\dot{\varepsilon}_p = \lambda_p \frac{\alpha}{|\alpha|}, \quad \dot{r} = \lambda_p,
\]
and the complementarity conditions
\[
\lambda_p \geq 0, \quad |\alpha| + \zeta \leq 0, \quad \lambda_p (|\alpha| + \zeta) = 0.
\]
In particular, this implies \(|\dot{\varepsilon}_p| = \dot{r}\), and assuming \(\varepsilon_p(0) = 0\) and \(r(0) = 0\) at initial time \(t = 0\), we obtain
\[
r(t) = \int_0^t \dot{r} \, dt = \int_0^t |\dot{\varepsilon}_p| \, dt,
\]
i.e., \(r\) is the equivalent plastic strain.

**The incremental flow rule for elasto-plasticity** For the incremental problem the local computation of the stress response and the consistent tangent in every material point in the RVEs is reduced to a scalar nonlinear problem for the equivalent plastic strain increment.

**Lemma 5.3.** For given history variables \((\varepsilon_p^{n-1}, r^{n-1})\) and strain \(\varepsilon\) a unique solution \((\Delta \varepsilon_p, \Delta r)\) of the local flow rule in every material point
\[
0 \in \partial (\varepsilon_p, r) W(\varepsilon, \varepsilon_p^{n-1} + \Delta \varepsilon_p, r^{n-1} + \Delta r) + \partial R_{\text{plastic}}(\Delta \varepsilon_p, \Delta r)
\]
exists.

**Proof.** For fixed history and given strain \(\varepsilon\), the increment is a minimizer of
\[
\Phi(\Delta \varepsilon_p, \Delta r; \varepsilon) = W(\varepsilon, \varepsilon_p^{n-1} + \Delta \varepsilon_p, r^{n-1} + \Delta r) + R_{\text{plastic}}(\Delta \varepsilon_p, \Delta r).
\]
Since the functional is uniformly convex in \(\mathbb{R}^6\), the minimizer exists and it is unique. For the evaluation we define the conjugated variables
\[
(\alpha, \zeta) = -\partial (\varepsilon_p, r) W(\varepsilon, \varepsilon_p^{n-1} + \Delta \varepsilon_p, r^{n-1} + \Delta r)
\]
we obtain \(\alpha = \text{dev } \sigma - K(\varepsilon_p^{n-1} + \Delta \varepsilon_p)\) from the stress \(\sigma = \mathbb{C}[\varepsilon - \varepsilon_p^{n-1} - \Delta \varepsilon_p]\), and \(\zeta = -\Psi(r^{n-1} + \Delta r)\). Evaluating
\[
(\Delta \varepsilon_p, \Delta r) \in \partial R^*_{\text{plastic}}(\alpha, \zeta) = \begin{cases} 
\{0\} & |\alpha| + \zeta < 0, \\
[0, \infty) \left( \frac{\alpha}{|\alpha|} \right) & |\alpha| + \zeta = 0, \\
0 & |\alpha| + \zeta > 0
\end{cases}
\]
yields the normality rule.
\[
\begin{bmatrix}
(\Delta \varepsilon_p) \\
(\Delta r)
\end{bmatrix} = \lambda_p \begin{bmatrix}
\frac{\alpha}{|\alpha|} \\
1
\end{bmatrix}
\]

and the complementarity conditions for the consistency parameter \(\lambda_p\)

\[
\lambda_p \geq 0, \quad |\alpha| + \zeta \leq 0, \quad \lambda_p(|\alpha| + \zeta) = 0.
\]

The normality rule yields \(\Delta \varepsilon = \lambda_p |\Delta \varepsilon_p|\) and for the flow direction

\[
\frac{\Delta \varepsilon}{|\Delta \varepsilon|} = \frac{\alpha}{|\alpha|} = \frac{2 \mu \text{dev} \varepsilon - (2 \mu + K)(\varepsilon^n_{p} - 1 + \Delta \varepsilon_p)}{[2 \mu \text{dev} \varepsilon - (2 \mu + K)(\varepsilon^n_{p} - 1 + \Delta \varepsilon_p)]} = \frac{\alpha^{tr}_n(\varepsilon)}{|\alpha^{tr}_n(\varepsilon)|}
\]

with the relative trial stress \(\alpha^{tr}_n(\varepsilon) = 2 \mu \text{dev} \varepsilon - (2 \mu + K)\varepsilon^n_{p} - 1\). Thus, defining the flow function

\[
F_n(\Delta r; \varepsilon) = |\alpha^{tr}_n(\varepsilon)| - (2 \mu + K)\Delta r - \Psi'(r^n_{\varepsilon} + \Delta r)
\]

we observe \(|\alpha| + \zeta = F_n(\Delta r; \varepsilon)\). Now, for the given strain \(\varepsilon\) we have to distinguish two cases. If \(F_n(0; \varepsilon) \leq 0\), we set \(\Delta r = 0\). Otherwise, since \(F_n(\cdot; \varepsilon)\) is strictly monotone and negative for large \(\Delta r\), the equation \(F_n(\Delta r; \varepsilon) = 0\) uniquely determines \(\Delta r > 0\). Then, we obtain

\[
\Delta \varepsilon_p = \Delta r \frac{\alpha^{tr}_n(\varepsilon)}{|\alpha^{tr}_n(\varepsilon)|}.
\]

Evaluating the increment \(\Delta r_n(\varepsilon)\) defines the update of the history variables

\[
r_n(\varepsilon) = r^n_{\varepsilon} + \Delta r_n(\varepsilon),
\]

\[
\varepsilon_{p,n}(\varepsilon) = \varepsilon^n_{p} + \Delta r_n(\varepsilon) \frac{\alpha^{tr}_n(\varepsilon)}{|\alpha^{tr}_n(\varepsilon)|},
\]

the incremental stress response

\[
\sigma_n(\varepsilon) = \mathbb{C}[\varepsilon - \varepsilon_{p,n}(\varepsilon)],
\]

and the consistent tangent \(\mathbb{C}_n(\varepsilon) \in \partial \sigma_n(\varepsilon)\) by

\[
\mathbb{C}_n(\varepsilon)[\delta \varepsilon] = \mathbb{C}[\delta \varepsilon] - \frac{4 \mu^2 \Delta r_n(\varepsilon)}{|\alpha^{tr}_n(\varepsilon)|} \text{dev}(\delta \varepsilon)
\]

\[
+ \left( \frac{4 \mu^2 \Delta r_n(\varepsilon)}{|\alpha^{tr}_n(\varepsilon)|} - \frac{4 \mu^2}{2 \mu + K + \Psi'(r_n(\varepsilon))} \right) \frac{\alpha^{tr}_n(\varepsilon) \cdot \delta \varepsilon}{|\alpha^{tr}_n(\varepsilon)|} \frac{\alpha^{tr}_n(\varepsilon)}{|\alpha^{tr}_n(\varepsilon)|},
\]

cf. [28, Sect. 3.3.2].
Damage and elasto-plasticity For the model combining damage and elasto-plasticity we use the internal variables \( z = (d, \varepsilon_p, r) \) with \( N = 7 \) components and the free energy

\[
W(x, \varepsilon, z) = (1 - d)W_{\text{elastic}}(x, \varepsilon(u) - \varepsilon_p) + W_{\text{defect}}(z)
\]

\[
= (1 - d)(W_{\text{elastic}}(x, \varepsilon(u) - \varepsilon_p) + W_{\text{plastic}}(\varepsilon_p, r)) + W_{\text{damage}}(d)
\]

with the elastic energy \([5.1] \) and defect energy components \([5.12] \) and \([5.15] \). The dissipation combines \([5.10] \) and \([5.16] \) to

\[
R(\ddot{d}, \dot{\varepsilon}_p, \dot{r}) = \int_{\Omega} R(\ddot{d}, \dot{\varepsilon}_p, \dot{r}) \, dx, \quad R(\ddot{d}, \dot{\varepsilon}_p, \dot{r}) = R_{\text{damage}}(\ddot{d}) + R_{\text{plastic}}(\dot{\varepsilon}_p, \dot{r}).
\]

The incremental two-scale elasto-plastic damage model For the incremental problem the local computation of the stress response and the consistent tangent in every material point in the RVEs is evaluated first for the plasticity variables and then for the damage variable.

**Lemma 5.4.** For given history variables \((d^{n-1}, \varepsilon_p^{n-1}, r^{n-1})\) and strain \( \varepsilon \) a unique solution \((\Delta d, \Delta \varepsilon_p, \Delta r)\) of the local flow rule in every material point

\[
0 \in \partial_{(d,\varepsilon_p,r)} W(\varepsilon, d^{n-1} + \Delta d, \varepsilon_p^{n-1} + \Delta \varepsilon_p, r^{n-1} + \Delta r) + \partial R(\Delta d, \Delta \varepsilon_p, \Delta r)
\]

exists.

**Proof.** Inserting the conjugated variables

\[
-\partial_{(d,\varepsilon_p,r)} W(\varepsilon, d^{n-1} + \Delta d, \varepsilon_p^{n-1} + \Delta \varepsilon_p, r^{n-1} + \Delta r)
\]

\[
= \left( Y - \Phi^{-1}(d^{n-1} + \Delta d) \right) \left( \partial_{\Phi^{-1}(d^{n-1} + \Delta d)} \right)
\]

\[
= \left( 1 - d^{n-1} + \Delta d \right) \left( \text{dev}(\sigma) - K(\varepsilon_p^{n-1} + \Delta \varepsilon_p) \right) - \left( 1 - d^{n-1} + \Delta d \right) \Psi(r^{n-1} + \Delta r)
\]

with \( Y = W_{\text{elastic}}(\varepsilon - \varepsilon_p^{n-1} - \Delta \varepsilon_p) \), the back stress \( \alpha = \text{dev} \sigma - K(\varepsilon_p^{n-1} + \Delta \varepsilon_p) \), \( \zeta = -\Psi(r^{n-1} + \Delta r) \), and \( \sigma = C[\varepsilon - \varepsilon_p^{n-1} - \Delta \varepsilon_p] \) into the flow rule yields

\[
Y - \Phi^{-1}(d^{n-1} + \Delta d) \in \partial R_{\text{damage}}(\Delta d),
\]

and, since \( R_{\text{plastic}}^{\ast}(\cdot) \) is 1-homogeneous,

\[
(\Delta \varepsilon_p, \Delta r) \in \partial R_{\text{plastic}}^{\ast}(\alpha, \zeta) = \partial R_{\text{plastic}}^{\ast} \left( (1 - d^{n-1} + \Delta d)(\alpha, \zeta) \right).
\]

This shows that in the first step, the plastic increment can be evaluated from the plastic flow rule independent from the damage variable. We proceed as in Lem. 5.3 The plastic flow rule is equivalent to the normality rule

\[
\left( \frac{\Delta \varepsilon_p}{\Delta r} \right) = \lambda_p \left( \frac{\alpha}{|\alpha|} \right)
\]
and the complementarity conditions for the consistency parameter $\lambda_p$

$$\lambda_p \geq 0, \quad |\alpha| + \zeta \leq 0, \quad \lambda_p(|\alpha| + \zeta) = 0.$$ 

The normality rule yields $\Delta r = \lambda_p = |\Delta \varepsilon_p|$ and for the flow direction

$$\frac{\Delta \varepsilon}{|\Delta \varepsilon|} = \frac{\alpha}{|\alpha|} = \frac{2\mu \text{dev } \varepsilon - (2\mu + K)(\varepsilon_p^{n-1} + \Delta \varepsilon_p)}{2\mu \text{dev } \varepsilon - (2\mu + K)(\varepsilon_p^{n-1} + \Delta \varepsilon_p)} = \frac{\alpha_{n}^{tr}(\varepsilon)}{|\alpha_{n}^{tr}(\varepsilon)|}$$

with the relative trial stress $\alpha_{n}^{tr}(\varepsilon) = 2\mu \text{dev } \varepsilon - (2\mu + K)\varepsilon_p^{n-1}$. Thus, defining

$$F_n(\Delta r; \varepsilon) = |\alpha_{n}^{tr}(\varepsilon)| - (2\mu + K)\Delta r - \Psi(r_{n-1} + \Delta r)$$

we observe $|\alpha| + \zeta = F_n(\Delta r; \varepsilon)$. Now, for the given $\varepsilon$ we have to distinguish two cases. If $F_n(0; \varepsilon) \leq 0$, we set $\Delta r = 0$. Otherwise, $\Delta r > 0$ is uniquely determined by the equation $F_n(\Delta r; \varepsilon) = 0$. Then, we obtain

$$\Delta \varepsilon_p = \Delta r \frac{\alpha_{n}^{tr}(\varepsilon)}{|\alpha_{n}^{tr}(\varepsilon)|}$$

which also defines $Y_n(\varepsilon) = W_{\text{elastic}}(\varepsilon - \varepsilon_p^{n-1} - \Delta \varepsilon_p)$. Now, the increment of the damage variable is computed as in Lem. 5.2 depending on $Y_n(\varepsilon)$, i.e., $\Delta d = \max \{0, \Phi(Y_n(\varepsilon)) - d_{n-1}\}$.

The evaluation of the flow rule defines the update of the history variables

$$d_n(\varepsilon) = d^{n-1} + \Delta d,$$
$$\varepsilon_{p,n}(\varepsilon) = \varepsilon_p^{n-1} + \Delta \varepsilon_p,$$
$$r_n(\varepsilon) = r^{n-1} + \Delta r,$$

the incremental stress response $\sigma_n(\varepsilon) = (1 - d_n(\varepsilon))C[\varepsilon - \varepsilon_{p,n}(\varepsilon)]$, and the consistent tangent $C_n(\varepsilon) \in \partial \sigma_n(\varepsilon)$

$$C_n(\varepsilon)[\delta \varepsilon] = (1 - d_n(\varepsilon))C_{n}^{\text{plastic}}(\varepsilon)[\delta \varepsilon]$$
$$- \text{sgn}\left(\max \{0, \Phi(Y_n(\varepsilon)) - d^{n-1}\}\right)(C[\varepsilon - \varepsilon_{p,n}(\varepsilon)] \cdot \delta \varepsilon)C[\varepsilon]$$

with

$$C_{n}^{\text{plastic}}(\varepsilon)[\delta \varepsilon] = C[\delta \varepsilon] - \frac{4\mu^2 \Delta r}{|\alpha_{n}^{tr}(\varepsilon)|} \text{dev}(\delta \varepsilon)$$
$$+ \left(\frac{4\mu^2 \Delta r}{|\alpha_{n}^{tr}(\varepsilon)|} - \frac{4\mu^2}{2\mu + K + \Psi'(r_n(\varepsilon))}\right) \frac{\alpha_{n}^{tr}(\varepsilon) \cdot \delta \varepsilon}{|\alpha_{n}^{tr}(\varepsilon)|} \frac{\alpha_{n}^{tr}(\varepsilon)}{|\alpha_{n}^{tr}(\varepsilon)|}.$$
5.5 Heterogeneous two-scale FEM for inelasticity

The inelastic material behavior for short fiber-reinforced polymers is modeled by a two-scale infinitesimal elasto-plastic damage material \[14, 15\]. Here, this model is reformulated in the framework of generalized standard materials which directly defines the corresponding algorithmic realization within the FE\(^2\) framework.

Two-scale models with memory The energetic framework extends to the two-scale setting as follows. We consider \(u_H : [0, T] \to V_H\) on the macro-scale satisfying the Dirichlet boundary conditions, i.e., \(u_H(t) \in V_H(u_D(t))\), and locally in every RVE \(Y_\xi\) the micro-fluctuations \(v_{\xi,h} : [0, T] \to V_{\xi,h}\) and the internal variables describing the material history \(z_{\xi,h} : [0, T] \to Z_{\xi,h}\) has to be determined. Here, we use for the internal variables piecewise constant vectors in \(Z_{\xi,h} \subset L^2(Y_\xi, \mathbb{R}^N)\) represented by \(z_{\xi,h}(\zeta) \in \mathbb{R}^N\) at the integration points \(\zeta \in \Xi_{\xi,h} \subset Y_\xi\) in the RVE. Together, we define \(Z_h = \prod_{\xi \in \Xi_H} Z_{\xi,h}\).

The model is determined by the corresponding two-scale energy and dissipation functionals

\[
\mathcal{E}_H(t, u_H, v_h, z_h) = \int_{\Xi_H} W_\xi(\varepsilon(u_H), v_{\xi,h}, z_{\xi,h}) - \langle \ell(t), u_H \rangle,
\]

\[
\mathcal{R}_H(\dot{z}_h) = \int_{\Xi_H} R_\xi(\dot{z}_{\xi,h})
\]

where the contributions at every sample point \(\xi \in \Xi_H\) is evaluated in the RVEs \(Y_\xi\) by the locally averaged two-scale micro-energy and micro-dissipation

\[
W_\xi(\varepsilon_H, v_{\xi,h}, z_{\xi,h}) = \frac{1}{|Y_\xi|} \int_{Y_\xi} W(x, \varepsilon_{\xi,H} + \varepsilon(v_{\xi,h}), z_{\xi,h}) \, dx
\]

\[
R_\xi(\dot{z}_h) = \frac{1}{|Y_\xi|} \int_{Y_\xi} R(x, \dot{z}_{\xi,h}) \, dx,
\]

depending on the macro-strain \(\varepsilon_{\xi,H} = \varepsilon(u_H)(\xi)\). Again, this defines the micro-solution by \(u_{\xi,h} = u_{\xi,H} + v_{\xi,h}\) depending on the linearized macro-solution by \(u_{\xi,H}(x) = u_H(\xi) + Du_H(\xi)(x - \xi)\), i.e., by construction the micro-fluctuation is periodic and the strain of the macro-solution \(\varepsilon(u_{\xi,H}) = \varepsilon_{\xi,H}\) is constant in \(Y_\xi\).
The incremental two-scale problem  Starting with \((u_h^0, v_h^0, z_h^0)\) we solve for \(n = 1, \ldots, N_{\max}\) the following incremental problems depending on the given history variable \(z_h^{n-1}\), find a minimizer \((u_h^n, v_h^n, z_h^n) \in V_H(u_D^0) \times V_h \times Z_h\) of the two-scale incremental functional

\[
J_{h,n}(u_h^n, v_h^n, z_h^n) = \mathcal{E}_H(t_n, u_h^n, v_h^n, z_h^n) + \mathcal{R}_H(z_h^n - z_h^{n-1}).
\]

The minimizer is determined by computing a critical point of \(J_{h,n}(\cdot)\). This is characterized by the nonlinear system

<table>
<thead>
<tr>
<th>Macro-Equilibrium</th>
<th>(0 = \partial_n \mathcal{E}_H(t_n, u_h^n, v_h^n, z_h^n)), (5.17a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Micro-Equilibrium</td>
<td>(0 = \partial_v \mathcal{E}_H(t_n, u_h^n, v_h^n, z_h^n)), (5.17b)</td>
</tr>
<tr>
<td>Flow Rule</td>
<td>(0 \in \partial_{\delta} \mathcal{E}_H(t_n, u_h^n, v_h^n, z_h^n) + \partial \mathcal{R}_H(\delta z_h^n)). (5.17c)</td>
</tr>
</tbody>
</table>

The Macro-Equilibrium \(0 = \partial_n \mathcal{E}_H(t_n, u_h^n, v_h^n, z_h^n)\) reads in variational form

\[
\int_{\Xi} \frac{1}{|Y_\xi|} \int_{Y_\xi} \partial_\varepsilon W(\varepsilon_{\xi,h}^n + \varepsilon(v_{\xi,h}^n), z_{\xi,h}^n) : \varepsilon(\delta u_h) \, dx = \langle \ell^n, \delta u_H \rangle
\]

for \(\delta u_H \in V_H(0)\), where \(\varepsilon_{\xi,h}^n = \varepsilon(u_h^n)(\xi)\) denotes the macro-strain. We define the micro-stress

\[
\sigma_{\xi,h}^n = \partial_\varepsilon W(\varepsilon_{\xi,h}^n + \varepsilon(v_{\xi,h}^n), z_{\xi,h}^n)
\]

depending on the macro-strain and the micro-fluctuation \(v_{\xi,h}^n \in V_{\xi,h}\) and then by averaging in the RVE the macro-stress

\[
\sigma_{\xi,H}^n = \frac{1}{|Y_\xi|} \int_{Y_\xi} \sigma_{\xi,h}^n \, dx,
\]

which together yields the macro-equilibrium in the form

\[
\int_{\Xi} \sigma_{\xi,H}^n : \varepsilon(\delta u_h) = \langle \ell^n, \delta u_H \rangle, \quad \delta u_H \in V_H(0).
\]

The Micro-Equilibrium \(0 = \partial_v \mathcal{E}_H(t_n, u_h^n, v_h^n, z_h^n)\) reads in variational form

\[
\frac{1}{|Y_\xi|} \int_{Y_\xi} \sigma_{\xi,h}^n : \varepsilon(\delta v_{\xi,h}) \, dx = 0, \quad \delta v_{\xi,h} \in V_{\xi,h}.
\]

The Flow Rule \(0 \in \partial_{\delta} \mathcal{E}_H(t_n, u_h^n, v_h^n, z_h^n) + \partial \mathcal{R}_H(\delta z_h^n)\) determines the history variable \(z_h^n\) from the macro-solution \(u_h^n\) and the micro-fluctuation \(v_{\xi,h}^n\). Depending on the conjugated variable \(y_{\xi,h}^n = -\partial_\varepsilon W(\varepsilon_{\xi,h}^n + \varepsilon(v_{\xi,h}^n), z_{\xi,h}^n)\) it is evaluated in every integration point of the RVE \(Y_\xi\) and can be expressed by duality

\[
y_{\xi,h}^n \in \partial R(\Delta z_{\xi,h}^n) \iff \Delta z_{\xi,h}^n \in \partial R^*(y_{\xi,h}^n).
\]
The two-scale damage problem

We specify the incremental two-scale problem (5.17) for the damage model and we derive a generalized Newton method by inserting the results in Lem. 5.2. Here, for given damage history $d_{h,n}^{n-1}$ and time $t_n$, the incremental two-scale problem aims to compute the unique minimizer $(\mathbf{u}_{H}^{n}, \mathbf{v}_{h}^{n}, d_{h}^{n}) \in V_{H}(\mathbf{u}_{H}^{n}) \times V_{h} \times Z_{h}$ of the functional

$$J_{h,n}(\mathbf{u}_{H}^{n}, \mathbf{v}_{h}^{n}, d_{h}^{n}) = \mathcal{E}_{H}(t_n, \mathbf{u}_{H}^{n}, \mathbf{v}_{h}^{n}, d_{h}^{n}) + \mathcal{R}_{H}(d_{h}^{n} - d_{h,n}^{n-1})$$

by solving the nonlinear system

\begin{align}
0 &= \partial_{u}\mathcal{E}_{H}(t_n, \mathbf{u}_{H}^{n}, \mathbf{v}_{h}^{n}, d_{h}^{n}), \quad (5.18a) \\
0 &= \partial_{u}\mathcal{E}_{H}(t_n, \mathbf{u}_{H}^{n}, \mathbf{v}_{h}^{n}, d_{h}^{n}), \quad (5.18b) \\
0 &= \partial_{d}\mathcal{E}_{H}(t_n, \mathbf{u}_{H}^{n}, \mathbf{v}_{h}^{n}, d_{h}^{n}) + \partial\mathcal{R}_{H}(\Delta d_{h}^{n}). \quad (5.18c)
\end{align}

For this purpose, we define a return mapping procedure which evaluates the variational inequality (5.18c) which allows to determine a suitable Newton linearization.

The flow rule (5.18c) is evaluated at every integration point in the RVE $\mathcal{Y}_{\xi}$. Inserting $Y(\varepsilon_{\xi,h}) = \frac{1}{2}\varepsilon_{\xi,h} : \mathbb{C}[\varepsilon_{\xi,h}]$, we obtain from Lem. 5.2 for the damage variable

$$d_{\xi,h,n}(\varepsilon_{\xi,h}) = d_{\xi,h}^{n-1} + \max \left\{ 0, \Phi(Y(\varepsilon_{\xi,h}))-d_{\xi,h}^{n-1} \right\}$$

and the stress response $\sigma_{\xi,h}^{n} = \sigma_{\xi,h,n}(\varepsilon_{\xi,h})$ with

$$\sigma_{\xi,h,n}(\varepsilon_{\xi,h}) = (1-d_{\xi,h,n}(\varepsilon_{\xi,h}))\mathbb{C}[\varepsilon_{\xi,h}].$$

Inserting this result in (5.18) yields the reduced nonlinear problem to compute a critical point $(\mathbf{u}_{H}^{n}, \mathbf{v}_{h}^{n}) \in V_{H}(\mathbf{u}_{H}^{n}) \times V_{h}$ of

$$\langle \mathcal{F}_{h,n}(\mathbf{u}_{H}, \mathbf{v}_{h}), (\delta \mathbf{u}_{H}, \delta \mathbf{v}_{h}) \rangle = \int_{\mathcal{E}_{H}} \frac{1}{|\mathcal{Y}_{\xi}|} \int_{\mathcal{Y}_{\xi}} \sigma_{\xi,h,n}(\varepsilon_{\xi,h}) : (\varepsilon(\delta \mathbf{u}_{H}) + \varepsilon(\delta \mathbf{v}_{\xi,h})) \, dx - \langle \ell^{n}, \delta \mathbf{u}_{H} \rangle$$

for all $(\delta \mathbf{u}_{H}, \delta \mathbf{v}_{h}) \in V_{H}(0) \times V_{h}$. The consistent tangent operator

$$\mathbb{C}_{\xi,h,n}(\varepsilon_{\xi,h}) = \left(1-d_{\xi,h,n}(\varepsilon_{\xi,h})\right)\mathbb{C} - \operatorname{sgn} \left( \max \left\{ 0, \Phi(Y(\varepsilon_{\xi,h}))-d_{\xi,h}^{n-1} \right\} \right) \Phi'(Y(\varepsilon_{\xi,h})) \mathbb{C}[\varepsilon_{\xi,h}] \otimes \mathbb{C}[\varepsilon_{\xi,h}]$$

yields a Newton linearization

$$\langle \mathcal{F}'_{h,n}(\mathbf{u}_{H}, \mathbf{v}_{h}), (\Delta \mathbf{u}_{H}, \Delta \mathbf{v}_{h}), (\delta \mathbf{u}_{H}, \delta \mathbf{v}_{h}) \rangle = \int_{\mathcal{E}_{H}} \frac{1}{|\mathcal{Y}_{\xi}|} \int_{\mathcal{Y}_{\xi}} \mathbb{C}_{\xi,h,n}(\varepsilon_{\xi,h})[\varepsilon(\Delta \mathbf{u}_{H}) + \varepsilon(\Delta \mathbf{v}_{\xi,h})] : (\varepsilon(\delta \mathbf{u}_{H}) + \varepsilon(\delta \mathbf{v}_{\xi,h})) \, dx$$

for $(\Delta \mathbf{u}_{H}, \Delta \mathbf{v}_{h}), (\delta \mathbf{u}_{H}, \delta \mathbf{v}_{h}) \in V_{H}(0) \times V_{h}$. 


The two-scale residual $F_{h,n}$ and its linearization $F'_{h,n}$ allows for the construction of a generalized Newton method of the incremental problem. This can be formulated as follows: starting with $(u_H^{0}, v_h^{0}) \in V_H(u_H^0) \times V_h$, for $k = 1, 2, ...$ the Newton increment $(\Delta u_H^{n,k}, \Delta v_h^{n,k}) \in V_H(0) \times V_h$ is determined solving

\[
\langle F'_{h,n}(u_H^{n,k-1}, v_h^{n,k-1})(\Delta u_H^{n,k}, \Delta v_h^{n,k}), (\delta u_H, \delta v_h) \rangle = -\langle F_{h,n}(u_H^{n,k-1}, v_h^{n,k-1}), (\delta u_H, \delta v_h) \rangle
\]

for all $(\delta u_H, \delta v_h) \in V_H(0) \times V_h$. The next iterate is given by

\[
(u_H^{n,k}, v_h^{n,k}) = (u_H^{n,k-1}, v_h^{n,k-1}) + s_{n,k}(\Delta u_H^{n,k}, \Delta v_h^{n,k})
\]

with a suitable damping parameter $s_{n,k} \in (0, 1]$. The iteration stops, if the residual $F_{h,n}(u_H^{n,k}, v_h^{n,k})$ is small enough.

It turns out that this monolithic Newton method for the combined two-scale problem is not efficient, since for every Newton step a full micro-macro problem has to be solved. So we use an alternative approach to compute the Newton increment first on the micro-scale and then on the macro-scale.

In the first time step $n = 0$, we compute for every $\xi \in \Xi_H$ the micro-fluctuations $w_{\xi,h,1}^{0}, \ldots, w_{\xi,h,6}^{0} \in V_{\xi,h}$ with respect to the basis $\eta_1, \ldots, \eta_6$ solving (5.4).

In every time step $n \geq 1$ we set $w_{\xi,h,l}^{n,0} = w_{\xi,h,l}^{n-1}$ and we start with selecting $u_H^{n,0} \in V_H(u_H^0)$. For every macro-Newton step $k \geq 1$ and for every $\xi \in \Xi_H$, the micro-residual at $\varepsilon_{\xi,H}^{n,k-1} = \varepsilon(u_H^{n,k-1})(\xi)$ is given by

\[
\langle F_{\xi,h,n,k}(v_{\xi,h}), \delta v_{\xi,h} \rangle = \int_{\Omega_{\xi}} \sigma_{\xi,h,n}(\varepsilon_{\xi,H}^{n,k-1} + \varepsilon(v_{\xi,h})) : \varepsilon(\delta v_{\xi,h}) \, dx.
\]

The micro-fluctuation $v_{\xi,h}^{n,k}$ is computed by a micro-Newton method solving approximately the nonlinear problem $F_{\xi,h,n,k}(v_{\xi,h}) = 0$. Starting with

\[
v_{\xi,h}^{n,k,0} = \sum_{j=1}^{6} \left( \varepsilon_{\xi,H}^{n,k-1} : \eta_j \right) w_{\xi,h,j}^{n,k-1},
\]

we compute for $m = 1, 2, \ldots$ the strain $\varepsilon_{\xi,h}^{n,k,m-1} = \varepsilon_{\xi,H}^{n,k-1} + \varepsilon(v_{\xi,h}^{n,k,m-1})$, the stress response $\sigma_{\xi,h}^{n,k,m-1} = \sigma_{\xi,h,n}(\varepsilon_{\xi,h}^{n,k,m-1})$ and the consistent tangent operator $C_{\xi,h,n}^{n,k,m-1} = C_{\xi,h,n}(\varepsilon_{\xi,h}^{n,k,m-1})$. 
Then, the increment \( \Delta v^{n,k,m}_{\xi,h} \in V_{\xi,h} \) is computed by solving
\[
\int_{Y_{\xi}} C_{n,k,m-1}^{n,k,m}[\varepsilon(\Delta v^{n,k,m}_{\xi,h})] : \varepsilon(\delta v_{\xi,h}) \, dx = - \int_{Y_{\xi}} \sigma^{n,k,m-1}_{\xi,h} : \varepsilon(\delta v_{\xi,h}) \, dx
\]
for all \( \delta v_{\xi,h} \in V_{\xi,h} \) defining \( v^{n,k,m}_{\xi,h} = v^{n,k,m-1}_{\xi,h} + s^{n,k,m}_{\xi,n,k,m} \Delta v^{n,k,m}_{\xi,h} \) with \( s^{n,k,m}_{\xi,n,k,m} \in (0, 1] \). If the micro-residual is small enough, we set \( v^{n,k}_{\xi,h} = v^{n,k,m}_{\xi,h} \), \( \sigma^{n,k}_{\xi,h} = \sigma^{n,k,m}_{\xi,h} \),
\[
\sigma^{n,k}_{\xi,H} = \frac{1}{|Y_{\xi}|} \int_{Y_{\xi}} \sigma^{n,k}_{\xi,h} \, dx,
\]
and \( C^{n,k}_{\xi,h} = C^{n,k,m}_{\xi,h} \). If \( v^{n,k}_{\xi,h} \) is sufficiently close to the previous iterate, we use \( w^{n,k}_{\xi,h,l} = w^{n,k-1}_{\xi,h,l} \) and \( C^{n,k}_{\xi,H} = C^{n,k-1}_{\xi,H} \) from the previous iteration, otherwise we compute \( w^{n,k}_{\xi,h,l} \in V_{\xi,h} \) solving
\[
\frac{1}{|Y_{\xi}|} \int_{Y_{\xi}} C(x)[\eta_l + \varepsilon(w^{n,k}_{\xi,h,l})] : \varepsilon(\delta v_{\xi,h}) \, dx = 0, \quad \delta v_{\xi,h} \in V_{\xi,h}
\]
for \( l = 1, \ldots, 6 \) and the multiscale tensor
\[
C^{n,k}_{\xi,H} = \frac{1}{|Y_{\xi}|} \sum_{l,j=1}^{6} \left( \int_{Y_{\xi}} C^{n,k}_{\xi,h}[\eta_l + \varepsilon(w^{n,k}_{\xi,h,l})] : \eta_j \, dx \right) \eta_l \otimes \eta_j.
\]
The macro-update \( \Delta u^{n,k}_{H} \in V_{H}(0) \) is computed solving
\[
\int_{\Xi_{H}} C^{n,k}_{\xi,H}[\varepsilon(\Delta u^{n,k}_{H})] : \varepsilon(\delta u_{H}) = - \int_{\Xi_{H}} \sigma^{n,k}_{\xi,H} : \varepsilon(\delta u_{H}) + \langle \ell^n, \delta u_{H} \rangle
\]
for all \( \delta u_{H} \in V_{H}(0) \) defining \( u^{n,k}_{H} = u^{n,k-1}_{H} + s^{n,k}_{n,k} \Delta u^{n,k}_{H} \) with \( s^{n,k}_{n,k} \in (0, 1] \). If the macro-residual is small enough, we set \( u^n_H = u^{n,k}_{H} \), \( v^n_{\xi,h} = v^{n,k}_{\xi,h} \), we update the damage variable \( d_{m}\xi,h} = d_{m-1}\xi,h} + \max \{0, \Phi(\Psi(\varepsilon^{n}_{\xi,h})) - d_{m-1}\xi,h} \} \), and then we proceed to the next time step.
The two-scale elasto-plasticity model Specifying the incremental two-scale problem \(5.17\) for elasto-plasticity yields

\[
\begin{align*}
0 &= \partial_u \mathcal{E}(t_n, u^n_H, v^n_h, \varepsilon^n_{p,h}, r^n_h) , \\
0 &= \partial_\varepsilon \mathcal{E}(t_n, u^n_H, v^n_h, \varepsilon^n_{p,h}, r^n_h) , \\
0 &\in \partial_{(\varepsilon, r)} \mathcal{E}(t_n, u^n_H, v^n_h, \varepsilon^n_{p,h}, r^n_h) + \partial R(\Delta \varepsilon^n_{p,h}, \Delta r^n_h) .
\end{align*}
\]

(5.19)

For given material history \((\varepsilon^{n-1}_{p,h}, r^{n-1}_h)\) and strain \(\varepsilon^n_{\xi,h} = \varepsilon(u^n_H)(\xi) + \varepsilon(v^n_h)\), the stress \(\sigma^n_{\xi,h} = \sigma_{\xi,h,n}(\varepsilon^n_{\xi,h})\) is determined from the flow rule, cf. Lem. \(5.3\). Therefore, we define the relative trial stress

\[
\alpha^r_{\xi,h,n}(\varepsilon_{\xi,h}) = 2\mu \mathrm{dev} \varepsilon_{\xi,h} - (2\mu + K)\varepsilon^{n-1}_{p,h} ,
\]

and the flow function

\[
F_{\xi,h,n}(\Delta r_{\xi,h}; \varepsilon_{\xi,h}) = |\alpha^r_{\xi,h,n}(\varepsilon_{\xi,h})| - (2\mu + K)\Delta r_{\xi,h} - \Psi(r^{n-1}_h + \Delta r_{\xi,h}) .
\]

If \(F_{\xi,h,n}(0; \varepsilon_{\xi,h}) \leq 0\), we set \(\Delta r_{\xi,h,n}(\varepsilon_{\xi,h}) = 0\), otherwise the increment is defined by solving the nonlinear problem \(F_{\xi,h,n}(\Delta r_{\xi,h,n}(\varepsilon_{\xi,h}); \varepsilon_{\xi,h}) = 0\). This defines the update \(r_{\xi,h,n}(\varepsilon_{\xi,h}) = r^{n-1}_h + \Delta r_{\xi,h,n}(\varepsilon_{\xi,h})\) and the response for the plastic strain and the stress, and the consistent tangent operator

\[
\begin{align*}
\varepsilon_{p,\xi,h}(\varepsilon_{\xi,h}) &= \varepsilon^{n-1}_{p,\xi,h} + \Delta r_{\xi,h,n}(\varepsilon_{\xi,h}) \frac{\alpha^r_{\xi,h,n}(\varepsilon_{\xi,h})}{|\alpha^r_{\xi,h,n}(\varepsilon_{\xi,h})|} , \\
\sigma_{\xi,h,n}(\varepsilon_{\xi,h}) &= C[\varepsilon_{\xi,h} - \varepsilon_{p,\xi,h}(\varepsilon_{\xi,h})] , \\
C_{\xi,h,n}(\varepsilon_{\xi,h}) &= C - 4\mu^2 \Delta r_{\xi,h,n}(\varepsilon_{\xi,h}) |\alpha^r_{\xi,h,n}(\varepsilon_{\xi,h})| \left( \mathrm{dev} - \frac{\alpha_{\xi,h,n}(\varepsilon_{\xi,h})}{|\alpha_{\xi,h,n}(\varepsilon_{\xi,h})|} \otimes \frac{\alpha_{\xi,h,n}(\varepsilon_{\xi,h})}{|\alpha_{\xi,h,n}(\varepsilon_{\xi,h})|} \right) \\
&\quad - \frac{4\mu^2}{2\mu + K + \Psi'(r_{\xi,h,n}(\varepsilon_{\xi,h}))} \frac{\alpha_{\xi,h,n}(\varepsilon_{\xi,h})}{|\alpha_{\xi,h,n}(\varepsilon_{\xi,h})|} \otimes \frac{\alpha_{\xi,h,n}(\varepsilon_{\xi,h})}{|\alpha_{\xi,h,n}(\varepsilon_{\xi,h})|} .
\end{align*}
\]

Now, the residual, \(F_{n,h}\), the linearization \(F'_{n,h}\), and the generalized Newton method for the macro-problem can be defined as for the damage model, and inserting the elasto-plastic stress response yields the corresponding two-scale system for the combined model.

The two-scale model combining damage and elasto-plasticity Here, the internal variable has \(N = 7\) components \(\varepsilon^n_{\xi,h} = (d^n_{\xi,h}, \varepsilon^n_{p,\xi,h}, r^n_h)\), and in \(5.19\) we use the combined energy and dissipation functional, cf. Sect. \(5.4\). Inserting the stress response from Lem. \(5.3\) and the corresponding consistent tangent yields the residual and its linearization as in the previous cases.
Parallel nonlinear two-scale algorithms  The full algorithm is realized in three loops (see Fig. 5.4 for an overview): the outer loop for the time stepping, the Newton iteration for the macro-problem for every incremental problem, and in the inner loop the Newton iterations for the micro-problem for every RVE evaluating the local stress response.

given $z_h^{n-1} = (z_{\xi,h}^{n-1})_{\xi \in \Xi_H}$

select $u_{H}^{n,0} \in V_H(u_{H}^{n-1})$

$k := 0$

sequentially for all $\xi \in \Xi_H$:

communicate $\varepsilon_{n,k}^{\xi,H} = \varepsilon(u_{H}^{n,k})_{\xi}^H$

select $v_{\xi,h}^{n,k,0} \in V_{\xi,h}$

set $z_{\xi,h}^{n,k,0} = z_{\xi,h}^{n-1}$

$m := 0$

evaluate $\sigma_{n,k,m}^{\xi,h} \xi,h$ and residual $F_{\xi,h}^{n,k,m}$

$m := m + 1$

$F_{n,k}^{\xi,h}$ large

compute $\Delta v_{n,k}^{\xi,h}$

update $v_{n,k,m+1}^{\xi,h}$

evaluate residual $F_{H}^{n,k}$

$F_{H}^{n,k}$ small

$F_{H}^{n,k}$ large

$n := n + 1$

go to next time step

$k := k + 1$

Fig. 5.4: The parallel incremental two-scale algorithm.
We extend the parallel algorithm in Sect. [5.2] to inelastic applications. Every Newton iteration in the incremental problem has the structure of the linear two-scale model, provided that the residual and the consistent tangent is evaluated in every RVE. To obtain an efficient method, we use heuristic criteria in the RVE whether a new multiscale basis is required.

The Newton method in every RVE is described in detail in Alg. 2. This is used in the full parallel two-scale method in Alg. 3 for the evaluation of the residual and for the computation of the linearization on macro-scale. The damping factors in S5) and N7) are chosen by a line search strategy such that the next residual is decreasing.

**Algorithm 2** Nonlinear computation of the micro-fluctuation \( v^{n,k}_{\xi,h} \) at time \( t_n \) and Newton iteration \( k \) in step N1) of Alg. 3 depending on the strain approximation \( \varepsilon^{n,k}_{\xi,h} \) of the incremental macro-problem.

S0) On \( p \) with \( \xi \in \Omega^p \) evaluate \( \varepsilon^{n,k}_{\xi,H} = \varepsilon(u^{n,k}_H)(\xi) \) and send \( \varepsilon^{n,k}_{\xi,H} \) to all processes.

Set \( v^{n,k}_{\xi,h} = \sum l \varepsilon^{n,k}_{\xi,H}(\eta_l) w^{n,k-1}_{\xi,h,l} \), \( c^{n,k,0}_{\xi,h} = c^{n,k}_{\xi,h} \), and \( m = 0 \).

S1) Evaluate the micro-strain \( \varepsilon^{n,k,m}_{\xi,h} = \varepsilon^{n,k}_{\xi,H} + \varepsilon(v^{n,k,m}_{\xi,h}) \), the nonlinear material response \( z^{n,k,m}_{\xi,h} = z_{\xi,h,n}(\varepsilon^{n,k,m}_{\xi,h}) \), the micro-stress \( \sigma^{n,k,m}_{\xi,h} = \partial_\varepsilon W(\varepsilon^{n,k,m}_{\xi,h}, z^{n,k,m}_{\xi,h}) \), and the micro-residual

\[
\langle F_h(v^{n,k,m}_{\xi,h}), \delta v_{\xi,h} \rangle = \int_{Y_\xi} \sigma^{n,k,m}_{\xi,h} : \varepsilon(\delta v_{\xi,h}) \, dx, \quad \delta v_{\xi,h} \in V_{\xi,h}.
\]

S2) If the micro-residual \( F_h(v^{n,k,m}_{\xi,h}) \) is small enough, set \( v^{n,k}_{\xi,h} = v^{n,k,m}_{\xi,h} \), \( \sigma^{n,k}_{\xi,h} = \sigma^{n,k,m}_{\xi,h} \) and \( c^{n,k}_{\xi,h} = c^{n,k,m}_{\xi,h} \), and go to N2).

S3) If \( m = m_{\text{max}} \), reduce \( \Delta t_n \) and go to T1).

S4) Evaluate the consistent tangent operator \( c^{n,k,m}_{\xi,h} = c_{\xi,h,n}(\varepsilon^{n,k,m}_{\xi,h}) \) and compute

\[
\int_{Y_\xi} c^{n,k,m}_{\xi,h} \Delta v^{n,k,m}_{\xi,h} : \varepsilon(\delta v_{\xi,h}) \, dx = -\langle F_h(v^{n,k,m}_{\xi,h}), \delta v_{\xi,h} \rangle, \quad \delta v_{\xi,h} \in V_{\xi,h}.
\]

S5) Select a damping parameter \( s^{n,k,m} \in (0,1] \) and set

\[
v^{n,k,m+1}_{\xi,h} = v^{n,k,m}_{\xi,h} + s^{n,k,m} \Delta v^{n,k,m}_{\xi,h}.
\]

If \( s^{n,k,m} \leq s_{\text{min}} \), reduce \( \Delta t_n \) and go to T1).

S6) Set \( m := m + 1 \) and go to S1).
Algorithm 3 Parallel heterogeneous two-scale method for inelastic materials using Alg. 2 in \( \mathcal{Y}_\xi \).

T0) For all points \( \xi \in \Xi_H \) with representative micro-structure compute in parallel the micro-fluctuations \( w^0_{\xi,h,1}, \ldots, w^6_{\xi,h,6} \in V_{\xi,h} \) solving

\[
\int_{\mathcal{Y}_\xi} C(x)[\eta + \varepsilon(w^0_{\xi,h,1})] : \varepsilon(\delta v_{\xi,h}) \, dx = 0, \quad \delta v_{\xi,h} \in V_{\xi,h},
\]

and compute the elastic multiscale tensor

\[
C^0_{\xi,H} = \frac{1}{|\mathcal{Y}_\xi|} \sum_{l=1}^{6} \left( \int_{\mathcal{Y}_\xi} C(x)[\eta + \varepsilon(w^0_{\xi,h,l})] : \eta \right) \eta_l \otimes \eta_j.
\]

Set \( s_h^0 = 0 \), \( t_h = 0 \), and \( n = 1 \).

T1) For given history variable \( z_h^{n-1} \) and time increment \( \Delta t_n = (0, T - t_n-1) \) set \( t_n = t_n-1 + \Delta t_n \) and compute the following steps:

N0) Set \( u_{n,0}^h = u_{n-1,0}^h, z_{n,0}^h = z_{n-1,0}^h, C^{n-1}_{\xi,h} = C^{n-1}_{\xi,h}, w^{n-1}_{\xi,h} = w^{n-1}_{\xi,h}, \) and \( k = 0 \).

N1) Set Dirichlet data \( u_{n,0}^h(x) = u_0(x, t_n) \) on all nodal points \( x \in \partial \Omega_D \) of the macro-space \( V_H \).

N2) Compute the macro-stress

\[
\sigma_{\xi,H}^{n,k} = \frac{1}{|\mathcal{Y}_\xi|} \int_{\mathcal{Y}_\xi} \sigma_{\xi,h}^{n,k} \, dx
\]

and the macro-residual

\[
\langle F_H(u_{n,k}^h), \delta u_H \rangle = \int_{\Xi_H} \sigma_{\xi,H}^{n,k} : \varepsilon(\delta u_H) - \langle \sigma^n, \delta u_H \rangle, \quad \delta u_H \in V_H(0).
\]

N3) If macro-residual small enough, set \( u_{n}^h = u_{n,k}^h, z_{n}^h = z_{n,k}^h, n := n + 1, \) and go to T1.

N4) If \( k = k_{\text{max}} \), reduce \( \Delta t_n \) and go to T1.

N5) Compute the micro-fluctuations \( w^{n,k}_{\xi,h,1}, \ldots, w^{n,k}_{\xi,h,6} \in V_{\xi,h} \) solving in parallel

\[
\int_{\mathcal{Y}_\xi} C^{n,k}_{\xi,h}[\eta + \varepsilon(w_{\xi,h,l}^{n,k})] : \varepsilon(\delta v_{\xi,h}) \, dx = 0, \quad \delta v_{\xi,h} \in V_{\xi,h}.
\]

Then compute the inelastic multiscale tensor

\[
C^{n,k}_{\xi,H} = \sum_{l,j} \left( \frac{1}{|\mathcal{Y}_\xi|} \int_{\mathcal{Y}_\xi} C^{n,k}_{\xi,h}[\eta + \varepsilon(w_{\xi,h,l}^{n,k})] : \eta_j \right) \eta_l \otimes \eta_j.
\]

N6) Compute \( \Delta u_{n,k}^h \in V_H(0) \) solving in parallel

\[
\int_{\Xi_H} C^{n,k}_{\xi,H}[\varepsilon(\Delta u_{n,k}^h)] : \varepsilon(\delta u_H) = -\langle F_H(u_{n,k}^h), \delta u_H \rangle, \quad \delta u_H \in V_H(0).
\]

N7) Select a damping parameter \( s_{n,k} \in (0, 1] \) and set

\[
u_{n,k+1}^h = u_{n,k}^h + s_{n,k} \Delta u_{n,k}^h.
\]

If \( s_{n,k} \leq s_{\text{min}} \) reduce \( \Delta t_n \) and go to T1.

N8) Set \( k := k + 1 \) and go to N1.
5.6 Numerical experiments for inelastic material models

The inelastic two-scale method is now applied to fiber-reinforced polymers, again using the test configuration in Fig. 5.2 with boundary conditions (5.7). The material parameters for the inelastic models are taken from [15]. The damping and yielding point parameter in the damage model for the polymer is set to $H = 0.22702$ and $Y_0 = 0.08692$, and for isotropic plasticity we use yield strength $\sigma_y = 25$ and isotropic linear hardening law with parameters $H_0 = 1$ and $K_\infty - K_0 = 0$.

**The two-scale damage model** In the first experiment we investigate the inelastic uniaxial tensile test with the damage model, using a fiber-reinforced micro-structure with 10% fiber volume fraction and a fiber orientation of $90^\circ$. We use 1024 integration points for the approximation of the macro-solution, and in every RVE a discretization with $\dim V_{\xi,h} = 823,875$ for the representation of the micro-fluctuations $v_{\xi,h}^\nu$ and $\dim Z_{\xi,h} = 2,097,152$ to represent the variable $d_{\xi,h}^n$ at every integration point in the RVE.

At the beginning in step T0) of Alg. 3 corresponding to the 6 symmetric tensor basis $\eta_k$, the representative micro-fluctuations $w_{\xi,h,k}^0$ are computed determining the averaged linear material, see Fig. 5.5.

![Fig. 5.5: Deformation of the periodic micro-fluctuations $w_{\xi,h,k}^0$ corresponding to the basis tensors $\eta_k$ in Sym(3) and stress distribution in the RVE.](image)

Starting with $d^0 = 0$, this is used to compute the elastic material response in every loading step for all RVE until the material response gets inelastic, see Fig. 5.6 for an example at a sample point.
The macroscopic evolution of the averaged stress and damage variable

\[
\sigma^{n}_{\xi,H} = \frac{1}{|Y_{\xi}|} \int_{Y_{\xi}} \sigma^{n}_{\xi,h} \, dx, \quad d^{n}_{\xi,H} = \frac{1}{|Y_{\xi}|} \int_{Y_{\xi}} d^{n}_{\xi,h} \, dx
\]

is shown in Fig. 5.7. Finally, the material response in all RVEs gets inelastic.
Various fiber orientations and filler contents  In the next test we investigate the inelastic material response of the damage model for different fiber orientations and volume fractions, see the stress-strain curves in Fig. 5.8. We clearly observe that the strength of the material is increased by a large volume fraction of the fibers, and the damage process is stronger for a fiber orientation orthogonal to the applied load. The simple damage model is limited to moderate loads, cf. Rem. 5.1, so we stop the incremental test when the overall amount of damage is getting too large so that the algorithmic tangent gets indefinite.

Fig. 5.8: Stress-strain curves of a uniaxial monotonic tensile test for a unidirectional short fiber-reinforced material with different fiber volume fractions and fiber orientations. Here, stress $\sigma_z$ and strain $\varepsilon_z$ are evaluated by (5.8).
Comparison of inelastic two-scale models

The simple damage model is not sufficient for a realistic description of fiber-reinforced polymers. Experimental data \cite{13, Chap. 2.2, Fig. 6} exhibit in addition to the damage process characteristics of an elasto-plastic yield limit and hardening effects. For the numerical investigation of the different inelastic effects we consider cyclic loading using an uniaxial displacement driven load at \( x_3 = 6.5 \) with

\[
\mathbf{u}(t, \mathbf{x}) = \begin{cases} 
(t - T_{k-1})\mathbf{u}_0 & T_{k-1} < t < T_k \text{ loading,} \\
(T_k - t)\mathbf{u}_0 & T_k < t < T_{k+1} \text{ unloading,}
\end{cases}
\]

for the transition points \( T_0 = 0 < T_1 < T_2 < \cdots \) from loading to unloading and from unloading to loading. The scaling factor is set to \( u_0 = 0.01 \).

For the comparison of the different models we compute several load cycles, see Fig. 5.9. The transition points \( T_1, T_3, T_5, \ldots \) are chosen such that the maximal stress is increased in every load cycle, and for complete unloading we set \( T_{2k} = 2T_{2k-1} - T_{2k-2} \). We select an unidirectional micro-structure with 10% fiber volume fraction and orientation aligned to the traction force. In all cases we use on the macro-scale 128 sample points and in each RVE a discretization with \( \dim V_{\xi,h} = 107811 \) and 262144 integration points for the representation of the memory variables \( \mathbf{z}_{\xi,h}^n \).

For the inelastic evolution the simulation of the damage model requires 1 003 loading increments for 4 load cycles with together 457 012 Newton iterations for the computation of the micro-fluctuation, and 73 155 evaluations of the effective material response. Finally, the response in each sample point is inelastic. The load is increased in every load cycle, so that the stress response is more and more reduced, but no permanent deformation remains after unloading, see Fig. 5.9 (a).

In the elasto-plastic model we compute 298 loading increments for 2 load cycles requiring 218 098 Newton iterations for the computation of the micro-fluctuation \( \mathbf{v}_{\xi,h}^n \) and 94 420 evaluations of the material response. Here, the response in 126 of 128 sample points behaves inelastic. Since the equivalent strain is monotone increasing in every inelastic increment, a residual stress remains after unloading, which is clearly observed in Fig. 5.9 (b). Also the yield stress and the linear hardening is characterized by the stress-strain curve: the effective yield stress is linearly increased in every loading cycle, and the elastic unloading is shifted in parallel by the equivalent strain increment.

The results for the combined model are computed with 620 loading increments in 347 296 Newton iterations with 51 691 evaluations for the effective material response, see Fig. 5.9 (c). Here, we observe both defect mechanisms, the shift of the residual stress after unloading caused by hardening effects, and the decreasing stiffness in the elastic unloading since in every load cycle the overall damage is increased.
Fig. 5.9: Stress-strain curve (left) and stress-load step diagram (right) of uniaxial cyclic tensile tests with 10% fiber volume fraction and 90° fiber orientation with respect to the tensile load for a short fiber-reinforced composite using different material models.
Comparing with experimental data [13, Chap. 2.2, Fig. 6] we observe that the two-scale model combining damage and plasticity is suitable for qualitatively correct description of the effective material behavior, and that the coarse resolution on the macro-scale and the moderate resolution on the micro-scale is sufficient to capture these effects correctly.

**Convergence test for the inelastic two-scale method** In order to test whether the characteristic length scale resolution is sufficient, we compare the results of the tensile test for the damage model depending on the sample size $\delta$ and the mesh size $h$ of the RVE, using an isotropic fiber distribution with 10% volume fraction, see Tab. 5.3. Comparing the results with the elastic case in Tab. 5.1 we observe that in the inelastic case the full resolution of the micro-structure is required, since for fractions of the RVE with $\delta/2$ and $\delta/4$ the material response is considerably different. Here, this is tested with fixed approximation on the macro-scale ($\dim V_H = 165$), and for different $\delta$ the convergence with respect to the mesh size $h$ on the micro-scale is considered. From this we can roughly estimate an accuracy of approximately 10% for the stress-strain curves in Fig. 5.9. For a more details on the convergence analysis and the estimation of the extrapolated values for $h \to 0$ we refer to [18, Chap. 7.3].

<table>
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<td>6 440 067</td>
<td>63.955</td>
<td>55.558</td>
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</tr>
</tbody>
</table>

Table 5.3: Numerical results for the macroscopic stress integral for the damage model with RVEs of different size.

A reduced method The full simulation of the cyclic inelastic material behavior is computationally very expensive. So we reduce the computational model by using a full resolution only in a region of interest $\Omega_{ctr} \subset \Omega$ which is also used to evaluate the stress-strain curve by (5.8), see Fig. 5.10. Then, we use a fine resolution $V_{\xi,h}$ and $Z_{\xi,h}$ for $\mathcal{Y}_{\xi} \subset \Omega_{ctr}$, and for $\mathcal{Y}_{\xi} \not\subset \Omega_{ctr}$ coarser spaces $V_{\xi,h}^{red}$ and $Z_{\xi,h}^{red}$.

Fig. 5.10: Region of interest $\Omega_{ctr} = (0,0.5) \times (-0.2,0.2) \times (0,2) \subset \Omega$ with the full resolution of the RVEs.
We evaluate the reduced model for the cyclic loading test with the damage model, see Fig. 5.9 (a), using \( \dim V_{\xi,h}^{\text{red}} = 14\,739 \) and \( \dim Z_{\xi,h}^{\text{red}} = 14\,739 \) for \( \xi \notin \Omega_{\text{ctr}} \). The stress-strain curve is evaluated in the region of interest.

Comparing the results between the full and the reduced model in Fig. 5.11 shows that they differ by less than 1%, i.e., the less accurate approximation in the RVEs outside the region of interest has only a very small influence to the averaged macroscopic solution in \( \Omega_{\text{ctr}} \). The simulation for the reduced model with 938 time increments and together 439,814 Newton iterations in the RVEs requires 45 hours and for the full model approx. 3 days on the IC2 cluster with 256 cores distributed on 16 nodes.

**Conclusion and outlook**

The full inelastic two-scale method of small-strain damage and plasticity models can be realized in an extremely large tensor product finite element space \( V_H \times \prod_{\xi} V_{\xi,h} \), and in case of fine microstructures small mesh sizes \( h \) are required. Since every RVE may have a different evolution, all memory variables \( \prod_{\xi} Z_{\xi,h} \) need to be stored. Thus large parallel machines are required to realize this method and to represent the data well distributed. Here we propose a parallel solution scheme with an efficient parallel data representation and a stable two-stage nonlinear Newton method to determine the minimizer of the incremental loading step.

Nevertheless, on parallel machines which 1024 cores the full simulation of several loading cycles still requires a few days. For the next generation of high performance computers, our method has to be enhanced, see [29] for concepts to a flexible load balancing for a two-scale method applied to dual-phase steel. A further acceleration can be achieved by model reduction [30, 31], where the presented parallel two-scale method can be used in the offline phase in order to compute a suitable reduced basis. Our first test in Fig. 5.11 shows that is approach is promising.

**References**


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