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Vorwort

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Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

AN ADJOINT-BASED GRADIENT-TYPE ALGORITHM FOR OPTIMAL FIBER ORIENTATION IN FIBER-REINFORCED MATERIALS

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Abstract. We propose a novel approach to find an optimal fiber orientation in composite materials. Fiber orientation is regarded as a function of space on the macrolevel. The optimization problem is formulated within a function space setting which makes the imposition of smoothness requirements straightforward and allows for rather general objective functionals. The algorithm we use is a one level optimization algorithm which optimizes with respect to the fiber orientation directly. The costly solve of a big number of microlevel problems is avoided using coordinate transformation formulas. We use an adjoint-based gradient type algorithm, but generalizations to higher-order schemes are straightforward. The algorithm is tested for a prototypical numerical example and its behaviour with respect to mesh independence and dependence on the regularization parameter is studied.

Key words. pde constrained optimization, fiber-reinforced materials, fiber orientation, linear elasticity, upscaling, adjoint-based optimization, microstructural optimization

AMS subject classifications. 49K20, 49M29, 65N30, 65K10, 74P10, 74Q05, 90C52, 93B40

1. Introduction. Steadily growing industrial demands on modern materials, such as high stiffness together with minimal weight have led to an increasing interest in composite materials. Combination of different materials yields properties that may differ significantly from the properties of the pure materials. Fiber-reinforced polymers consisting of fibers included in a polymer matrix are used widely in engineering applications, including e.g. aerodynamics or the automotive industry. These materials often show an anisotropic behaviour which highly depends on local concentration and orientation of the fibers inside the matrix (cf. [31], [1], [18], [28]). Using modern technology like the fiber-patch-preforming technique [20] it is nowadays possible to place fiber bundles quite exactly with nearly every desired orientation within the matrix material. Our purpose is to design an optimal fiber-reinforced material in order to minimize a given objective functional. Our design variable is the local fiber orientation. We assume elastic behaviour for the fiber and the matrix material, respectively, and focus on relatively small deformations such that the linear elasticity equations hold. As we are concerned with two different scales (the scale for the fibers is typically in a range of micrometers, while the material we want to study has a scale of millimeters to meters), we can use multiscale theory in order to upscale microscopical properties to the macrolevel ([24], [9], [23]). In this way the effective stiffness tensor A will only depend on the local fiber orientation. For simplicity, we allow only locally unidirectional fibers on the microlevel, but allow fiber orientation to vary locally on the macrolevel. Clearly, this will only be a reasonable approach if we assume scale

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separation and impose certain smoothness requirements on the macrolevel.

A lot of effort has been spent in literature for the design of optimal microstructures with respect to minimizing compliance, i.e., minimizing complementary energy. For an overview on the topic, we refer to the textbooks of Bendsøe and Sigmund [7] and Allaire [2] and the references cited therein. For the case of an orthotropic material the so-called coaxility condition has been derived by different authors, starting from Seregin and Troitskii in [27]. It states that in the optimal state stress and strain have to share common principal axes, which means that fibers should be aligned with these directions. Many results have been published for cases where an optimal tensor can be derived analytically, e.g. via closed-form formulations of optimality conditions (see e.g. [25]) or using Hashin-Shtrikman bounds [15]. These methods have been well-tested for simple geometries, are however restricted to the compliance as objective functional. A numerical approach based on homogenization theory has first been proposed by Bendsøe and Kikuchi in [8]. Since then, a variety of algorithms have been proposed [3], including two-step optimization algorithms using inverse homogenization (e.g. [32], [26]) or stress-based approaches which make use of the coaxility condition [11]. In both approaches, in each macroscopic integration point a local optimization problem has to be solved which each is typically a quite expensive problem for itself in terms of computational cost. This drawback can be circumvented using the Discrete Material Optimization Method (DMO) introduced by Stegmann and Lund [29], [30]. Recent results are even availabel for stochastic loads [13].

Here, fiber angles are restricted to a finite set of angles for which effective tensors can be computed in advance. While this is the natural framework for material optimization problems, i.e. choosing out of a finite set of materials, fiber angles might in principle take every possible value between -90 and +90 degrees and for practical purposes one might be interested in a smooth behaviour of fiber orientation as well, for example allowing only slight changes in a neighborhood of a point x.

In order to be able to deal with different kinds of smoothness requirements we approach the optimization problem via a function space setting regarding the fiber angle distribution as a function of space. Furthermore, minimizing compliance has been the objective of optimization and the extension to more general objective functionals has so far not been considered. Here, we take a different approach which allows for rather general objective functionals. The algorithm we propose is a one-level-optimization which optimizes with respect to the design parameters directly. The calculation of effective stiffness tensors is hereby done using coordinate transformation formulas. In this way, it is sufficient to perform one microlevel calculation in advance to calculate one effective tensor for an appropiate reference configuration. During the algorithm no further microlevel calculations are required.

Finally, we end up with an optimal control problem on the macrolevel which is governed by a semilinear state equation. We refer to the textbook of Tröltzsch [33] and the references cited therein for an overview of known results in this field. Existence and non-existence of solutions for inverse problems have been studied in [21]. To ensure the well-posedness in our case we include a Tikhonov regularization in the objective functional. In this way we can also control the smoothness of the fiber orientation function α.

1.1. The Optimal Control Problem. In three dimensions the local orientation in a point $x \in \Omega$ can be prescribed by two angles $\alpha_1(x), \alpha_2(x)$, e.g., α_1 prescribing the orientation within the x-y-plane which means perpendicular to the z-axis, α_2 the orientation perpendicular to the x-axis. We want to solve the following optimization problem given a convex functional J^u, a body force f, boundary forces g and boundary displacements u^d.

$$\begin{aligned} \min_{(\alpha,u)\in\mathcal{Q}^{\text{ad}}\times\mathcal{U}} \quad & J(\alpha,u) := J^u(u) + \frac{\kappa}{2}\|\alpha\|_{\mathcal{Q}}^2 \\ \text{subject to} \quad & -\operatorname{div}\sigma = f \quad \text{in } \Omega, \\ & \sigma = A(\alpha)e(u) \quad \text{in } \Omega, \\ & u = u^d \quad \text{on } \Gamma \\ & \sigma\cdot n = g \quad \text{on } \partial\Omega\setminus\Gamma, \end{aligned}$$

where Γ denotes the Dirchlet part of the boundary $\partial\Omega$ and n is the outward unit normal along $\partial\Omega$.

Besides compliance the objective functional, J^u might as well be the minimization of certain deformation or stress components or arise from inverse problems (deformation or stress tracking). As for practical purposes a smooth behaviour of the fiber orientations is desirable, we choose an H^1-regularization for our work. Generalizations to stronger or weaker smoothness requirements are possible.

For the discretization we use the finite element method and continuous H^1-conforming finite elements. Both the Tikhonov regularization and conformity are also necessary to ensure convergence of discrete solutions with respect to the mesh size $h \to 0$. A detailed convergence analysis for a similar, but simpler semilinear optimal control problem for finite element discretizations was considered in [19].

1.2. Outline. The outline of the article is as follows: In Section 2, we derive our state equation which couples the control variable α to the resulting deformation u. We start from multiscale theory of scale seperation and derive the constitutive equations on the macrolevel. Furthermore, we analyze the dependence of the stiffness tensor $A(x)$ on the local fiber orientation $\alpha(x)$ and show how to calculate it efficiently using coordinate transformation formulas. The optimal control problem is introduced in Section 3 and we derive the necessary optimality condition as well as the KKT system. In Section 4, we formulate our adjoint-based gradient-type algorithm. Finally, Section 5 is devoted to the presentation a prototypical numerical example to underline the capability of our method. We study its stability and convergence with respect to different regularization parameters κ and different meshes Ω_h.

2. Local Upscaling. In this section, we derive the state equation from multiscale theory. We refer to [23] or [10] for details on upscaling of the linear elasticity equation. Let $\varepsilon \ll 1$ the ratio between micro and macro scale. The linear elasticity equation under consideration reads

$$\begin{aligned} -\operatorname{div}\left(A^\varepsilon e(u^\varepsilon)\right) &= f \quad \text{in } \Omega, \\ u_i^\varepsilon &= u_i^d \quad \text{on } \Gamma_i \quad i = 1...3, \\ (A^\varepsilon e(u^\varepsilon)\cdot n)_i &= g_i \quad \text{on } \partial\Omega\setminus\Gamma_i \quad i = 1,2,3. \end{aligned}$$

Here, $\Omega \subset \mathbb{R}^3$ is assumed to be sufficiently smooth, the Dirichlet parts $\Gamma_i \subset \partial\Omega$ are of positive measure for each $i = 1,2,3$. The vector n denotes the outer unit normal along $\partial\Omega$. We assume $f \in H^{-1}(\Omega)$, $u_i^d \in H^{\frac{1}{2}}(\Gamma_i)$ and $g_i \in H^{-\frac{1}{2}}(\partial\Omega \setminus \Gamma_i)$ and denote by $e(u)$ the symmetric derivative, i.e., the linearized strain tensor

$$e(u) = \frac{1}{2}(\nabla u + \nabla^T u).$$

Let $A^\varepsilon(x) = \tilde{A}(x, \frac{x}{\varepsilon})$ be the fourth-order elasticity tensor. To ensure the unique solvability of our state equation, we assume the following conditions on $A^\varepsilon = (a^\varepsilon_{ijkl})_{1\le i,j,k,l\le 3}$ almost everywhere with positive constants ν and γ

$$a^\varepsilon_{ijkl} \in L^\infty(\Omega) \quad \text{for all } 1 \le i,j,k,l \le 3 \tag{2.1a}$$
$$a^\varepsilon_{ijkl} = a^\varepsilon_{jikl} = a^\varepsilon_{klij} \quad \text{for all } 1 \le i,j,k,l \le 3 \tag{2.1b}$$
$$A^\varepsilon mm \ge \nu \|m\|_F^2 \quad \text{for any symmetric matrix } m \tag{2.1c}$$
$$\|A^\varepsilon m\|_F \le \gamma \|m\|_F. \tag{2.1d}$$

Here, $\|m\|_F = (\sum_{i,j} m_{ij}^2)^{\frac{1}{2}}$ stands for the Frobenius norm of the matrix m.

Let us define the vector-valued function $P^{lm}(y) = (P_k^{lm}(y))_{1\le k\le 3}$ for $1 \le l \le m \le 3$ by

$$P_k^{lm} = y_m \delta_{kl},$$

where δ_{kl} is the Kronecker symbol. We know from multiscale theory [10] that in the limit $\varepsilon \to 0$, an approximation to u^ε is given by the solution u^0 of

$$\begin{aligned} -\operatorname{div}\left(A^0 e(u^0)\right) &= f \quad \text{in } \Omega, \\ u_i^0 &= u_i^d \quad \text{on } \Gamma_i \quad i = 1,2,3. \\ (A^0 e(u^0) n)_i &= g_i \quad \text{on } \partial\Omega \setminus \Gamma_i \quad i = 1,2,3, \end{aligned}$$

where the effective stiffness tensor A^0 is given by

$$a^0_{ijkh}(x) = \frac{1}{|Y|} \int_Y \tilde{A}(x,y)\, e(w^{ij})\, e(w^{kh}) dy$$

and w^{lm} are the solutions of

$$-\operatorname{div}(\tilde{A}(x,y)\, e(w^{lm})) = 0 \quad \text{in } Y, \tag{2.2a}$$
$$\begin{aligned} w_l^{lm} - P_k^{lm} \quad & Y\text{-periodic}, \\ \int_Y w_k^{lm} - P_k^{lm} dy &= 0. \end{aligned} \tag{2.2b}$$

for $1 \le l \le m \le 3$ in a representative volume element (RVE) Y. The remaining functions w^{lm} $(m < l)$ are given by symmetry.

Remark 2.1. *As we are only interested in the macroscopic part of the deformation u^ε, the approximation u^0 is sufficiently accurate for our purposes. We note that for the boundary conditions (2.2b) in the RVE the choice of Dirichlet boundary conditions is also possible. It has been shown that properties (2.1) also hold for the effective tensor A^0 (cf. [10]).*

Here, we consider a unidirectional fiber orientation in every macroscopic point $x \in \Omega$, but which may vary locally over Ω. Considering polar coordinates, the fiber orientation in each point $x \in \Omega$ can be described by two angles $\alpha(x)$ and $\beta(x)$. Let α

be the rotation angle within the x-y-plane. For simplicity, we focus on orientations within this plane and set $\beta = 0$. The generalization to optimizing both α and β is straightforward. With these assumptions, the effective tensor $A^0(x)$ only depends on the local fiber orientation $\alpha(x)$. For better readability we introduce the operator

$$A : L^\infty(\Omega) \to (L^\infty(\Omega))^{3\times3\times3\times3}$$

by the pointwise definition

$$A(\alpha)(x) = A^0(\alpha(x)).$$

and denote the resulting tensor-valued function by $A(\alpha)$. Finally, a simple calculation shows that $Be(u) = B\nabla u$ for each symmetric matrix B satisfying (2.1b). Hence, our state equation reads

$$-\operatorname{div}(A(\alpha)\nabla u) = f \quad \text{in } \Omega, \tag{2.3}$$

$$u_i = u_i^d \quad \text{on } \Gamma_i \quad i = 1,2,3, \tag{2.4}$$

$$(A(\alpha)\nabla u \cdot n)_i = g_i \quad \text{on } \partial\Omega \setminus \Gamma_i \quad i = 1,2,3. \tag{2.5}$$

The weak formulation of (2.5) is given by:
Find $u \in u^d + H_0^1(\Omega;\Gamma)$*, such that*

$$(A(\alpha)\nabla u, \nabla\varphi) = (f,\varphi) - (g,\varphi)_\Gamma \quad \text{for all } \varphi \in H_0^1(\Omega;\Gamma). \tag{2.6}$$

where $H_0^1(\Omega;\Gamma)$ denotes the space of H^1-functions with zero trace along Γ and u^d denotes an appropriate extension of the boundary data. Further, we set

$$(g,\varphi)_\Gamma = \sum_{i=1}^{3} (g_i,\varphi_i)_{\partial\Omega\setminus\Gamma_i}.$$

2.1. The Effective Stiffness Tensor. Next, we want to study the relation $\alpha \to A(\alpha)$ which is essential for our optimization algorithm in detail.

Suppose, the effective stiffness tensor $A^0(0) = (a^0_{ijkl}(0))$, which corresponds to a fiber-matrix configuration with fibers oriented parallel to the x-axis, is given. We can calculate the effective tensor which differs by an angle α in the x-y-plane by a simple coordinate transformation. Two-dimensional rotations in the x-y-plane can be described by the 3x3 matrix

$$Q(\alpha) = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) & 0 \\ \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Denoting its entries by q_{ij}, the fourth-order tensor $A(\alpha) = (a_{ijkl}(\alpha))$ transforms in the following way

$$a_{ijkl}(\alpha) = \sum_{1\le m,n,o,p\le 3} q_{im}(\alpha)q_{jn}(\alpha)q_{ko}(\alpha)q_{lp}(\alpha)a^0_{mnop}(0). \tag{2.7}$$

REMARK 2.2. *This coordinate transformation was already used by Beatty in [6] and has been applied to find optimal stiffness tensors in a variety of works (cf. [22]).*

Note, that due to the periodicity of Q and (2.7) $A(\alpha)$ is Π-periodic with respect to α. Furthermore, the coordinate transformation conserves properties (2.1) such that the state equation (2.6) is uniquely solvable for every $\alpha \in L^2(\Omega)$.

For our optimization algorithm we will need the Frechét-derivative $\frac{d}{d\alpha}A(\alpha)$. We have to analyze the mappings

$$\alpha \mapsto (\sin(\alpha), \cos(\alpha)) \mapsto Q(\alpha) \mapsto A(\alpha).$$

Unfortunately, the operators $\sin(\alpha)$ and $\cos(\alpha)$ are not differentiable from $H^1(\Omega)$ into $H^1(\Omega)$ (see [4]). Hence, we have to make sure that α lies in $L^\infty(\Omega)$, as the Frechét-derivative exists from $L^\infty(\Omega)$ to $L^\infty(\Omega)$. For the sine operator the derivative in the direction $\delta\alpha \in L^\infty(\Omega)$ is then given by

$$\sin'(\alpha)(\delta\alpha) = \cos(\alpha)\delta\alpha.$$

For the cosine operator we have analogously

$$\cos'(\alpha)(\delta\alpha) = -\sin(\alpha)\delta\alpha.$$

The derivatives of Q and A with respect to α read

$$\begin{aligned} Q'(\alpha)(\delta\alpha) &= \begin{pmatrix} -\sin(\alpha)\delta\alpha & -\cos(\alpha)\delta\alpha & 0 \\ \cos(\alpha)\delta\alpha & -\sin(\alpha)\delta\alpha & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ A'(\alpha)(\delta\alpha) &= (a'_{ijkl}(\alpha))_{1\le i,j,k,l\le 3}, \end{aligned}$$

where

$$\begin{aligned} a'_{ijkl}(\alpha)(\delta\alpha) &= \sum_{1\le m,n,o,p\le 3} \tilde{q}_{ijklmnop}(\alpha)\ \delta\alpha\ a^0_{mnop}, \\ \tilde{q}_{ijklmnop} &= q'_{im}(\alpha)q_{jn}(\alpha)q_{ko}(\alpha)q_{lp}(\alpha) + q_{im}(\alpha)q'_{jn}(\alpha)q_{ko}(\alpha)q_{lp}(\alpha) \\ &\quad + q_{im}(\alpha)q_{jn}(\alpha)q'_{ko}(\alpha)q_{lp}(\alpha) + q_{im}(\alpha)q_{jn}(\alpha)q_{ko}(\alpha)q'_{lp}(\alpha). \end{aligned}$$

3. The Optimization Problem.

We are now ready for a precise formulation of the optimization problem. Let $\mathcal{U} = u^d + H^1_0(\Omega;\Gamma)$

$$\min_{(\alpha,u)\in\mathcal{Q}^{\text{ad}}\times\mathcal{U}} J(\alpha,u) := J^u(u) + \frac{\kappa}{2}\|\alpha\|^2_{H^1} \tag{3.1a}$$

$$\text{subject to} \quad (A(\alpha)\nabla u, \nabla\varphi) = (f,\varphi) - (g,\varphi)_\Gamma \quad \text{for all } \varphi \in H^1_0(\Omega;\Gamma). \tag{3.1b}$$

In addition to the notation used above, we suppose $\kappa > 0$ is a constant.

3.1. The Set of Controls.

For the controls, we choose a subset of the Hilbert space $H^1(\Omega)$. There are three main reasons for this choice: First, multiscale theory requires sufficient smoothness of the tensor $A(\alpha)$ to ensure convergence of the two-scale solution u^ε to u^0. Second, we are dealing with a semilinear optimal control problem, which means that we cannot expect further regularity for the optimal control $\overline{\alpha}$ if we use a subset of $L^2(\Omega)$ as ansatz space. Hence, we cannot expect convergence of a discrete solution towards $\overline{\alpha}$ as the grid size tends to zero. And third, due to technical limitations regarding the construction process it might be desirable from an application point of view that the optimal fiber orientation does not change too much from one point to another. Neverthless, we remark that according to the application under consideration different choices of functional spaces are possible.

To ensure $\alpha \in L^\infty(\Omega)$, one could think of imposing the pointwise constraints

$$\mathcal{Q}^{\text{ad}} = \left\{ \alpha \in H^1(\Omega) \;\middle|\; \partial_n \alpha = 0 \text{ on } \partial\Omega,\ 0 \le \alpha(x) \le \Pi \text{ a.e. in } \Omega \right\}$$

as A is Π-periodic with respect to $\alpha(x)$. However, using this control space leads to the following drawback: Suppose for a local minima $\hat{\alpha}$ of the reduced cost functional in $\mathcal{Q}^{\text{ad}}$ the bound $\hat{\alpha}(x) = \Pi$ is active on a subset $\Omega_0 \subset \Omega$ of positive measure, but changing it to $\alpha_\varepsilon = \hat{\alpha} + \varepsilon\delta_x$ for ε sufficiently small and δ_x a smoothened Dirac function, would yield a smaller value of the objective functional. Neverthless, $\hat{\alpha}$ is a local minimum in $\mathcal{Q}^{\text{ad}}$, as $\alpha_\varepsilon \notin \mathcal{Q}^{\text{ad}}$. On the other hand the value $\alpha(x) = \Pi + \varepsilon$ corresponds to the same orientation as $\alpha(x) = \varepsilon$ and from a practical point of view the smoothness requirement is not violated as fiber orientations for Π and $\Pi + \varepsilon$, respectively ε are close. Hence, from a practical point of view it makes no sense not to allow this configuration.

To fix this problem, we use the set of admissible controls

$$\mathcal{Q}^{\text{ad}} = \left\{ \alpha \in H^1(\Omega) \;\middle|\; \partial_n \alpha = 0 \text{ on } \partial\Omega, -c\Pi \le \alpha(x) \le c\Pi \text{ a.e. in } \Omega \right\}$$

for c sufficiently large. In our numerical tests the choice of c=2 was sufficient to ensure that both bounds do not become active.

3.2. Necessary Optimality Conditions. For every $\alpha \in \mathcal{Q}^{\text{ad}}$, we denote the unique solution u of the state equation by $u(\alpha)$. Using this notation, we define the so called reduced cost functional by

$$j(\alpha) = J(\alpha, u(\alpha)).$$

REMARK 3.1. *As the relationship $\alpha \to u(\alpha)$ is highly nonlinear, j defines in general a nonconvex functional on $H^1(\Omega)$, even if J^u is convex. I.e., standard optimization algorithms will in general only converge to a local minimum. In order to find a minimum with good properties from a global point of view, we calculate the functional value of several reference configurations in advance and take the best configuration as a starting value. Furthermore, in practical applications a good initial guess might often be available. For more involved strategies in order to find global minima we refer to [17]. Here, we are only seeking local minima.*

The necessary optimality condition for a local minimum α reads

$$j'(\alpha)(\delta\alpha - \alpha) \ge 0 \quad \text{for all } \delta\alpha \in \mathcal{Q}^{\text{ad}}. \tag{3.2}$$

To calculate the functional derivative $u'(\alpha)$, we use the implicit function theorem. Let

$$E(\alpha, u)(\varphi) := (A(\alpha)\nabla u, \nabla\varphi) - (f, \varphi) + (g, \varphi)_\Gamma.$$

The implicit function theorem ensures us the existence of the Frechét-derivative $\delta u := u'(\alpha)(\delta\alpha)$ given the differentiability of E with respect to both arguments and the boundedness of E_u. Under these assumptions $\delta u \in H^1_0(\Omega; \Gamma)$ solves

$$E_u(\alpha, u(\alpha))(\delta u(\alpha)) = -E_\alpha(\alpha, u(\alpha)),$$

i.e.,

$$(A(\alpha)\nabla\delta u, \nabla\varphi) = -\left(A'(\alpha)(\delta\alpha)\nabla\varphi, \nabla u(\alpha)\right) \quad \forall\varphi \in H_0^1(\Omega;\Gamma). \tag{3.3}$$

We define the adjoint variable $\lambda(\alpha) \in H_0^1(\Omega;\Gamma)$ as solution of

$$(A(\alpha)\nabla\lambda(\alpha), \nabla\varphi) = -\left(\frac{d}{du}J^u(u(\alpha)), \varphi\right) \quad \text{for all } \varphi \in H_0^1(\Omega;\Gamma).$$

Now, we can rewrite j' in the following way

$$\begin{aligned} j'(\alpha)(\delta\alpha) &= \left(\frac{d}{du}J^u(u(\alpha)), \delta u(\alpha)\right) + \kappa(\alpha,\delta\alpha) + \kappa\left(\nabla\alpha, \nabla\delta\alpha\right) \\ &= -(A(\alpha)\nabla\lambda(\alpha), \nabla\delta u(\alpha)) + \kappa(\alpha,\delta\alpha) + \kappa(\nabla\alpha,\nabla\delta\alpha) \\ &= (A'(\alpha)(\delta\alpha)\nabla\lambda(\alpha), \nabla u(\alpha)) + \kappa(\alpha,\delta\alpha) + \kappa(\nabla\alpha,\nabla\delta\alpha). \end{aligned} \tag{3.4}$$

Summarizing, we get the following KKT-system for an optimal control α of (3.1) and its corresponding optimal state $u(\alpha) \in u^d + H_0^1(\Omega;\Gamma)$ and adjoint state $\lambda(\alpha) \in H_0^1(\Omega;\Gamma)$

$$\begin{aligned} (A(\alpha)\nabla u, \nabla\varphi) &= (f,\varphi) - (g,\varphi)_\Gamma \quad \text{for all } \varphi \in H_0^1(\Omega;\Gamma) \\ (A(\alpha)\nabla\lambda(\alpha), \nabla\varphi) &= -\left(\frac{d}{du}J^u(u(\alpha)), \varphi\right) \quad \text{for all } \varphi \in H_0^1(\Omega;\Gamma) \\ (A'(\alpha)(\delta\alpha-\alpha)\nabla\lambda(\alpha), \nabla u(\alpha)) &+ \kappa(\alpha,\delta\alpha-\alpha) \\ &+ \kappa\left(\nabla\alpha, \nabla(\delta\alpha-\alpha)\right) \geq 0 \quad \text{for all } \delta\alpha \in \mathcal{Q}^{\text{ad}}. \end{aligned}$$

4. The Gradient Algorithm. The derivative information derived so far is sufficient to design a steepest descent algorithm for the solution of the minimization problem under consideration.

In particular, we propose the following adjoint based gradient-type algorithm:

1. *Calculate the effective stiffness tensor $A^0(0)$ by numerical upscaling (see Chapter 2) and choose α^0.*

For k=0,1,...:

2. *Calculate $u^k \in u^d + H_0^1(\Omega;\Gamma)$ solving the state equation*

$$(A(\alpha^k)\nabla u^k, \nabla\varphi) = (f,\varphi) - (g,\varphi)_\Gamma \quad \forall\varphi \in H_0^1(\Omega;\Gamma).$$

3. *Calculate $\lambda^k \in H_0^1(\Omega;\Gamma)$ as solution of the adjoint equation*

$$(A(\alpha^k)\nabla\lambda^k, \nabla\varphi) = -\left(\frac{d}{du}J^u(u^k), \varphi\right) \quad \forall\varphi \in H_0^1(\Omega;\Gamma).$$

4. *Calculate the Riesz representation g^k of the gradient $j'(\alpha^k)(\delta\alpha)$ in $H^1(\Omega)$ by solving*

$$\left(\nabla g^k, \nabla\delta\alpha\right) + \left(g^k, \delta\alpha\right) = j'(\alpha^k)(\delta\alpha) \quad \forall\delta\alpha \in H^1(\Omega),$$

where

$$j'(\alpha^k)(\delta\alpha) = (A'(\alpha)(\delta\alpha)\nabla\lambda(\alpha), \nabla u(\alpha)) + \kappa(\alpha,\delta\alpha) + \kappa(\nabla\alpha,\nabla\delta\alpha).$$

5. *Set* $s^k = \frac{g^k}{\|g^k\|_{H^1}}$, *choose a step size* σ^k *and set*

$$\alpha^{k+1} = P_{[-c\Pi,c\Pi]}(\alpha^k - \sigma^k s^k),$$

where $P_{[a,b]}(f) = \min(b, \max(a, f))$ *denotes the pointwise projection to the interval* $[a, b]$.

Remark 4.1. *Of course, instead of the gradient type algorithm proposed, a higher-order acurate scheme, e.g., a Newton-type algorithm in combination with an active set strategy can be used (cf. [16] for different possibilities).*

Remark 4.2. *Note, that in step 2 to 4, we need the stiffness tensor* $A(\alpha)(x)$ *and its derivative* $A'(\alpha)(x)$ *in every Gaussian point* x *of the mesh. These tensors are calculated according to section 2.1 by the coordinate transformation formulas for rotation of* $\alpha(x)$. *In this way the costly subsequent solution of microlevel problems is avoided.*

Remark 4.3. *To find an appropriate step size in step 5 we use the projected Armijo rule [5, 16]. We choose the maximal* $\sigma^k \in \{1, \frac{1}{2}, \frac{1}{4}, ...\}$ *such that*

$$j\left(P_{[-c\Pi,c\Pi]}(\alpha^k - \sigma^k s^k)\right) - j\left(\alpha^k\right) \leq -\frac{\gamma}{\sigma^k}\left\|P_{[-c\Pi,c\Pi]}(\alpha^k - \sigma^k s^k) - \alpha^k\right\|_{H^1}$$

holds.

The algorithm requires in step 2 to 4 the solution of 2 linear systems of linear elasticity type and one system of scalar elliptic type in every iteration. Furthermore, using the Armijo rule, we have to calculate $u(\alpha)$ for several candidates α, which requires to solve the state equation once for every candidate. Hence, typically we end up by solving 3 to 6 systems of linear ellipticity type and one of scalar elliptic type in each iteration. In comparison to solving several microproblems in every iteration the computational cost per iteration is very low. As stopping criterion, we choose

$$\frac{\|g^k\|_{H^1}}{\|g^0\|_{H^1}} \leq \mathrm{TOL}$$

where g^k stands again for the Riesz representation of the gradient of j.

5. Numerical Examples. In this section, we study a prototypical numerical example in order to demonstrate the capabilities of our algorithm. Our objective is to design a material which shows minimal deformation in x-direction under a given stretching in y-direction.

5.1. Model problem. As a model problem, we want to optimize the fiber orientation in a structure consisting of a cube containing a cylindrical hole in the middle

$$\Omega^c = \left\{(x, y, z) \in \mathbb{R}^3 \;\middle|\; -10 < x, y < 10,\ 0 < z < 10,\ \sqrt{(x^2 + y^2)} > 4\right\}.$$

We set the volume force $f = 0$ and prescribe the displacement of the boundary on the lower face and upper face of the cube (cf. Figure 5.1, left side). Furthermore, we impose zero displacement in normal direction on the frontface and backface. As mentioned above, we are interested in the displacement in x-direction u_1. Clearly, the indicated stretching will lead to a deformation u_1 towards the midplane $x = 0$.

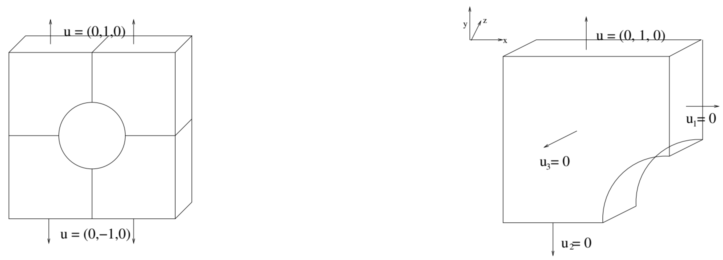


FIG. 5.1. *Model problem*

Due to symmetry reasons, it is sufficient to simulate a quarter of the structure (cf. Figure 5.1, right side).

$$\Omega = \left\{(x,y,z) \,\middle|\, 0 < x,y,z < 10,\ \sqrt{(x^2+y^2)} > 4\right\}.$$

We impose the following Dirichlet boundary conditions $u^d = (u_1^d, u_2^d, u_3^d)$

$$\begin{aligned} u^d &= (0,1,0) \text{ on } \Gamma_{\text{top}}, \\ u_2^d &= 0 \text{ on } \Gamma_{\text{left}}, \\ u_3^d &= 0 \text{ on } \Gamma_{\text{front}} \cup \Gamma_{\text{back}}. \end{aligned}$$

with the intuitive notation for top, front, back and left boundary.

We want to design an optimal material which shows minimal deformation in x-direction under this load, i.e.,

$$\begin{aligned} \min_{(\alpha,u)\in\mathcal{Q}^{\text{ad}}\times\mathcal{U}} \ & J(\alpha,u) := \frac{1}{2}\|u_1\|_{L^2}^2 + \frac{\kappa}{2}\|\alpha\|_{H^1}^2 \\ \text{subject to} \quad & -\operatorname{div}(A(\alpha)\nabla u) = 0 \quad \text{in}\Omega, \\ & u_i = u_i^d \quad \text{on } \Gamma_i \quad i = 1,2,3, \\ & (A(\alpha)\nabla u \cdot n)_i = 0 \quad \text{on } \partial\Omega \setminus \Gamma_i \quad i = 1,2,3, \end{aligned}$$

where

$$\Gamma_1 = \Gamma_{\text{top}},\ \Gamma_2 = \Gamma_{\text{left}} \cup \Gamma_{\text{top}},\ \Gamma_3 = \Gamma_{\text{top}} \cup \Gamma_{\text{front}} \cup \Gamma_{\text{back}}.$$

As material parameters we choose the Young's modulus E and Poisson's ratio ν for fiber and matrix material by

$$E^{\text{mat}} = 0.3, \quad \nu^{\text{mat}} = 0.2 \qquad\qquad E^{\text{fib}} = 100, \quad \nu^{\text{fib}} = 0.3.$$

On the microscale we assume Hooke's law for the fiber and matrix material, respectively, which reads in matrix notation

$$\begin{pmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{pmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{pmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0\\ \nu & 1-\nu & \nu & 0 & 0 & 0\\ \nu & \nu & 1-\nu & 0 & 0 & 0\\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0\\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0\\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{pmatrix} \begin{pmatrix} e_{11}\\ e_{22}\\ e_{33}\\ 2e_{23}\\ 2e_{13}\\ 2e_{12}\end{pmatrix}.$$

FIG. 5.2. *Microstructure for calculating* $A^0(0)$

According to Section 2 we calculate the effective tensor $A^0(0)$ for fibers parallel to the x-axis in a reference structure Y. For the generation of the microstructure, we use the software *GeoDict* [14] and impose a fiber-volume fraction of 5%. The microstructure obtained by GeoDict is shown in Figure 5.2.

5.2. Discretization. Let $\mathcal{T}_h$ be a family of quasiuniform triangulations of Ω into closed tetrahedrons $T_i, i = 1...N$. $\mathcal{P}_1$ the space of H^1-conforming P_1 finite elements on this triangulation. We define the discrete state space by

$$\mathcal{U}_h = \mathcal{U} \cap (\mathcal{P}_1)^3.$$

For the discretization of the control space we set

$$\mathcal{Q}_h^{\mathrm{ad}} = P_1 \cap \mathcal{Q}^{\mathrm{ad}}.$$

5.3. Results. In order to find a good initial value α^0 and to be able to compare the obtained optimal solution, we calculated the functional

$$J^u(u(\alpha)) = \frac{1}{2}\|u_1(\alpha)\|_{L^2}^2$$

for different constant fiber orientations α_i and the corresponding deformations $u(\alpha_i)$ in advance. After calculating $A^0(0)$ we obtain the remaining tensors again using the transformation formulas given in chapter 2.1. We realized calculations for

$$\alpha_k \equiv \frac{5k\,\Pi}{180}, \quad k = 0, ...35.$$

For our simulations we used the finite element software *FeelMath (Finite Elements for elastic Materials and Homogenization [12])*, which has been developed at the Fraunhofer Institute for Industrial Mathematics. The results are shown in Figure 5.3. For further comparison, we also calculated J^u for a random fiber distribution and for

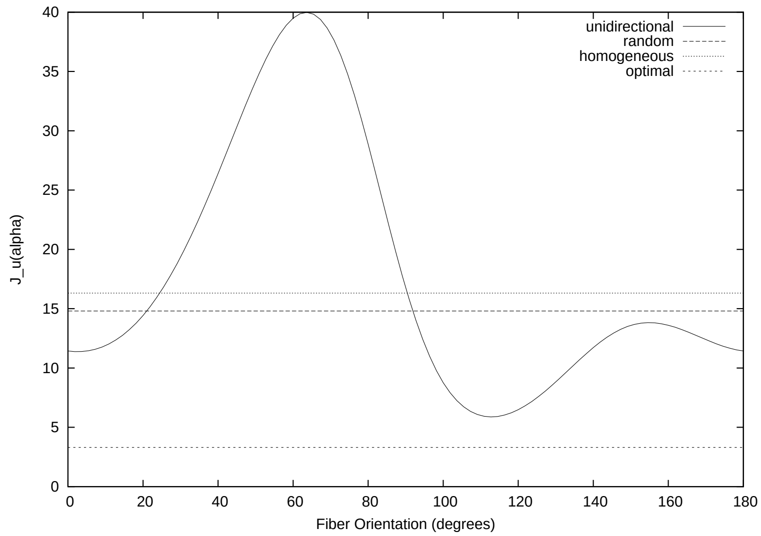


FIG. 5.3. *Values of the objective functional for different constant fiber orientations, random oriented fibers, a homogeneous material without fibers and the optimal orientation found using the algorithm given in section 4*

a pure matrix material without fibers and plotted the respective values as constant dashed lines. As we can see, we get the lowest value for a fiber orientation of 115 degrees ($k = 23$). Thus, we choose $\alpha^0 = \alpha_{23} \equiv \frac{115\Pi}{180}$ as initial control function.

For our optimization algorithm, we set $\kappa = 10^{-5}$ and use a mesh of nearly constant cell size $h = 0.5$ inside the domain, while we impose a cell size of $h = 0.2$ near critical boundaries. The mesh is shown in Figure 5.4. The dependence of the algorithms's convergence on the regularization parameter and mesh will be analyzed in the next subsections.

While the lowest value we get for constant fiber orientation was $J^u(u(\alpha_{23}) = 5.939$, our optimization algorithm converges to $\overline{\alpha}$ with $J^u(u(\overline{\alpha})) = 3.310$. Thus, we were able to reduce the deformation in x-direction by 44, 3% in comparison to the best constant fiber orientation. For comparison, we have included the value of the objective functional for the optimal configuration as another dashed line in Figure 5.4. The optimal fiber orientation $\overline{\alpha}$ is illustrated in Figure 5.4 on the right. Due to the H^1-Tikhonov regularization we observe a sufficiently smooth behaviour of α for practical purposes. We can see that near the right and the lower boundary, a larger angle than 115 degrees is favorable while in the middle of the domain the optimal fiber orientation we found shows an angle smaller than the starting value of 115 degrees.

5.4. Regularization Parameter Studies. To study the dependence of our algorithm on the regularization parameter κ, we realized calculations for $\kappa = 10^{-3}$, 10^{-4}, and 10^{-5} on the mesh introduced in the last section. As initial value we used $\alpha \equiv \frac{\Pi}{2}$ and as stopping criterion, we imposed a reduction factor of TOL=10^{-2} for the H^1-norm of the reduced gradient. The results are shown in Figure 5.5. Figure 5.5 (a)

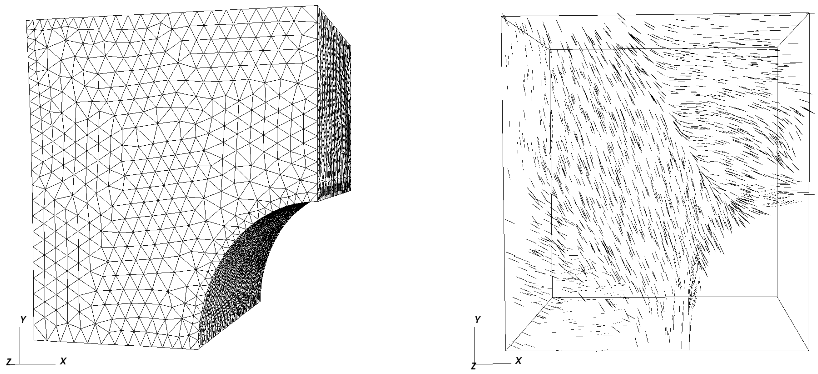


FIG. 5.4. *Used mesh (left) and the optimal fiber orientation (right)*

shows the convergence behaviour of the cost functional

$$J(u(\alpha,\alpha)) = J^u(u(\alpha)) + J_\alpha(\alpha) = \frac{1}{2}\|u_1\|^2 + \frac{\kappa}{2}\|\alpha\|^2_{H^1}.$$

Clearly, a bigger regularization parameter leads to a bigger value in the objective functional as the regularization part increases. Figure 5.5 (b) shows the value of the deformation part

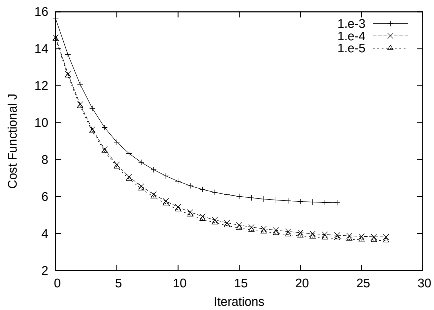
$$J^u(u(\alpha)) = \frac{1}{2}\|u_1(\alpha)\|^2.$$

We get a slightly larger deformation for bigger values of κ. This is because κ is the weight of the regularization part and thus, a bigger κ makes smaller and smoother angle distributions more favourable. In Figure 5.5 (c) we plot the behaviour of the penalty part

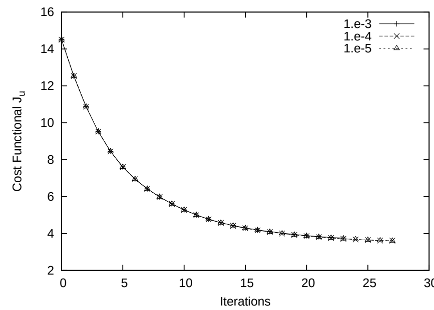
$$J_\alpha(\alpha) = \frac{1}{2}\|\alpha\|^2_{H^1}.$$

As one would expect, the bigger the regularization parameter κ, the smaller gets $\|\alpha\|_{H^1}$. Finally, in 5.5 (d) we plotted the behaviour of the reduced gradient. We observe that the bigger the regularization parameter the faster the decrease of the reduced gradient and hence less iterations are required. Clearly, this is also what we had expected. The initial reduced gradient is reduced by a two orders of magnitude after 23 to 27 iterations.

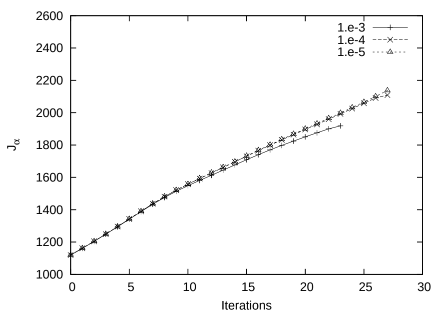
5.5. Dependence on the Mesh. In this section, we fix the regularization parameter to $\kappa = 10^{-5}$ and analyze the convergence behaviour on different meshes.



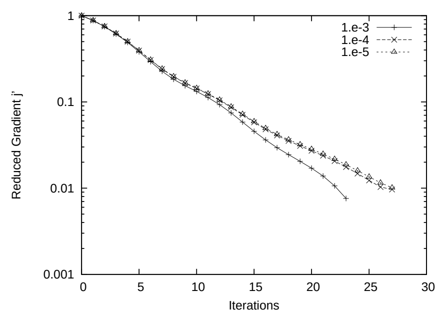
(a) Cost Functional J



(b) Cost functional J^u



(c) Cost Functional J_α/κ



(d) Reduced Gradient j'

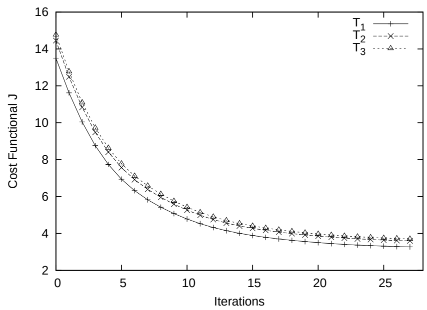
FIG. 5.5. *Influence of the regularization parameter* κ

TABLE 5.1
Discretization

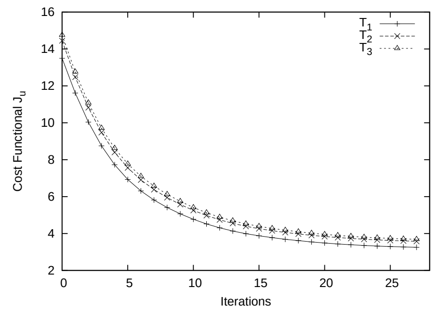
Triangulation	Cell size	Number of Elements
$\mathcal{T}_1$	1	8768
$\mathcal{T}_2$	0.5	69284
$\mathcal{T}_3$	0.25	553145

Therefore, we realized calculations on meshes with nearly constant cell size $h_1 = 1$, $h_2 = 0.5$ and $h_3 = 0.25$. The number of elements and cellsizes are summarized in Table 5.1. In Figure 5.6(a-c), we plot the decrease of the objective functional $J(u(\alpha), \alpha)$ and its components $J^u(u(\alpha))$ and $J_\alpha(\alpha)$. We notice a similar convergence behaviour on all meshes. In Figure 5.6(a) and (b), we see that the functional values on finer grids are larger than those on coarser grids. This is because of the local convexity of our objective functional. Finally, in Figure 5.6(d) we see that the decrease of the reduced gradient shows a very similar behaviour on all meshes. Thus, we have shown that our algorithm is almost independent with respect to grid size and mesh.

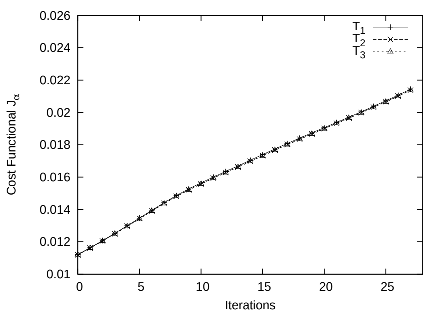
6. Conclusions. We proposed a novel approach to find an optimal fiber orientation in composite materials. Fiber orientation is regarded as a function of space on the



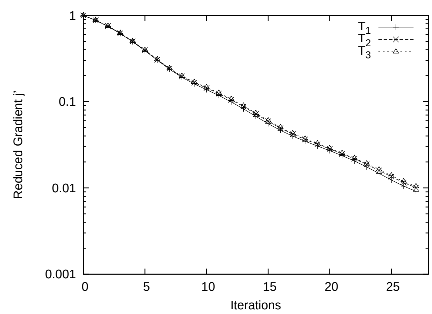
(a) Cost Functional J



(b) Cost functional J^u



(c) Cost Functional J_α



(d) Reduced Gradient j'

FIG. 5.6. *Convergence behaviour on different meshes* T_i

macrolevel which allows for a big class of different fiber orientation distributions and does not restrict orientation to be constant within, e.g., a given layer. The approach is proposed within a function space setting which makes the imposition of smoothness requirements straightforward and allows for rather general objective functionals. In order to guarantee its well-posedness we use a Tikhonov regularization term.

The algorithm we proposed is a one level optimization algorithm which optimizes with respect to the fiber orientation directly. The costly solve of a big number of microlevel problems is avoided using coordinate transformation formulas. Therefore, it is sufficient to do one microlevel calculation in advance. We used an adjoint-based gradient type algorithm, but generalization to higher-order schemes is straightforward. The algorithm was tested for a prototypical example and showed good behaviour with respect to mesh independence and regularization parameter studies.

Furthermore, the framework we developed is clearly not restricted to linearized elasticity. Other applications where anistropy plays an important role can be treated in an analogous way. As an example consider for example the design of an optimal porous media for filter applications.

Within the context of composite materials, optimization with respect to local fiber volume fraction (FVF) might be treated in a similar way. For simultaneous material optimization, we propose a combination of the presented approach with the Discrete Material Optimization Method (DMO, [29], [30]).

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