

Remodelling in statistically oriented fibre-reinforced materials and biological tissues

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(Article begins on next page)

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Remodelling in Statistically Oriented

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Fibre-Reinforced Materials and Biological Tissues*

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4

Abstract

5

We present a mathematical model of structural reorganisation in a fibre-reinforced composite material in which the fibres are oriented statistically, i.e., obey a probability distribution of orientation. Such a composite material exemplifies a biological tissue (e.g., articular cartilage or a blood vessel) whose soft matrix is reinforced by collagen fibres. The structural reorganisation of the composite takes place as fibres reorient, in response to mechanical stimuli, in order to optimise the stress distribution in the tissue. Our mathematical model is based on the Principle of Virtual Powers and the study of dissipation. Besides incompressibility, our main hypothesis is that the composite is characterised by a probability density distribution that measures the probability of finding a family of fibres aligned along a given direction at a fixed material point. Under this assumption, we describe the reorientation of fibres as the evolution of the most probable direction along which the fibres are aligned. To test our theory, we compare our simulations of a benchmark problem with selected results taken from the literature.

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Keywords: Remodelling, Two-layer dynamics, Dissipation, Statistical composites.

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1 Introduction

One of the properties of biological tissues is the capability of adapting their internal structure in response to the interactions with the environment in which they are placed. In Biomechanics, the evolution of the internal structure of a tissue is sometimes referred to as “remodelling” [26, 60].

We consider a purely mechanical framework, and focus on tissues that can be modelled as fibre-reinforced composite materials with fibres oriented according to a given probability distribution. Examples of tissues of this type are arteries and articular cartilage. Our approximation of these tissues is quite simplified in this work, since we regard them as solid bodies comprising two constituents only: a soft matrix and collagen fibres. The structure of real tissues is much more complicated than that addressed in our work.

The arterial wall comprehends several fibre-reinforced layers, in each of which the fibres are oriented according to rather well defined patterns [35]. Three main strata can be detected. These are referred to as *intima*, *media*, and *adventia*, and represent, respectively, the inner, the middle, and the outer stratum of an artery. The *intima* is the thinnest stratum. It comprises a single layer of endothelial cells located on a basal membrane. The *media* consists of muscle cells and collagen fibrils. It features several fibre-reinforced layers, in each of which the fibres are coiled helically. The direction of the helix in a layer is opposite to that in the consecutive one. Finally, the *adventia* consists of thick bundles of collagen fibres, arranged helically, which have the task of reinforcing the outermost stratum of the arterial wall. More details about the mechanics of arterial walls can be found in the papers by Holzapfel et al. [35] and Gasser et al. [29].

Articular cartilage is a multiphasic, multi-species material. The species can be identified with solid particles, fluids, chemicals and, in particular, ions [42]. The overall mechanical behaviour of the solid phase of articular cartilage is influenced by the presence of inclusions. These are identified with chondrocytes (i.e., the cells that synthesise extra-cellular matrix) and collagen fibres [see, e.g., 49, and references therein]. The latter ones contribute to the tissue overall capability of bearing loads, and are arranged in a way that adapts to the mechanical loading. Given a sample of articular cartilage, three zones can be identified, based on histological features (chondrocyte shape and collagen fibre orientation): the deep zone, which is proximal to the tidemark (bone-cartilage

46 interface), the middle zone, and the superficial zone, which is close to the articular surface. A
47 property of articular cartilage is that the arrangement of collagen fibres depends on the location
48 at which the fibres are placed inside the tissue. The fibres are nearly parallel to the tissue depth
49 in the deep zone, randomly oriented in the middle zone, and parallel to the articular surface in
50 the superficial zone [2, 48]. A linear elastic model of articular cartilage based on a statistical
51 orientation of collagen fibres was proposed by Federico et al. [23], where the tissue was studied as a
52 transversely isotropic, transversely homogenous, multiphasic composite material. The theoretical
53 tools were developed by in a previous work [22] on the basis of Walpole's algebra of fourth-order
54 tensors [63].

55 Under the action of mechanical stimuli, the body deforms and the fibres reorient. While the
56 first process is the standard change of shape of a body subjected to applied loads, prescribed
57 displacements, or combination of both, the second process triggers a reorganisation of the internal
58 structure of the body and, in this sense, represents a type of remodelling.

59 In many cases of interest, the reorientation of the collagen fibres should be investigated in
60 conjunction with the secretion and removal of the fibres themselves. Grillo et al. [31] presented
61 a more comprehensive framework in which growth, interphase mass transfer, and remodelling in
62 fibre-reinforced, multi-constituent materials were studied. This model remained, however, at the
63 theoretical level, since the solution of the determined equations requires a detailed mathematical
64 analysis and is, for this reason, still work in progress. Hence, in order to test the theory presented
65 in the present work by handling quite manageable numerical examples, we focussed here on some
66 aspects of remodelling that are conceptually independent on growth.

67 One reason for studying remodelling is to determine how the effective quantities characterising a
68 tissue evolve in time. Examples of such quantities are the mechanical stiffness and the permeability
69 of the tissue, cf. e.g., [19, 20, 21].

70 In the case of hyperelastic materials undergoing large deformations, the presence of fibres is
71 accounted for by introducing the structure tensor in the list of arguments of the body strain energy
72 function. For example, this approach was adopted by Holzapfel et al. [35] and Menzel [46, 47] for
73 arterial walls. The structure tensor is defined by $\mathbf{a} := \mathbf{m} \otimes \mathbf{m}$, where \mathbf{m} is a unit vector describing

74 the local alignment of a fibre along a prescribed direction of space. If \mathbf{m} follows the deformation
75 of the body, its evolution is determined by $\mathcal{L}_v \mathbf{m} = -\mathbf{d}_m \mathbf{m}$ [9], where \mathcal{L}_v is the Lie-derivative
76 operator, \mathbf{v} is the velocity, $\mathbf{d}_m := \mathbf{m}(\mathbf{d}\mathbf{m})$, and \mathbf{d} is the symmetric part of the velocity gradient.
77 This identity, being purely kinematic, contains neither phenomenological parameters nor material
78 properties.

79 Imatani and Maugin [37] developed a mathematical model of growth and reorientation of fi-
80 bres in anisotropic hyperelastic media in which the Kröner-Lee decomposition of the deformation
81 gradient tensor [5, 38, 40, 56], and the concept of reference crystal [16] were used to modify
82 $\mathcal{L}_v \mathbf{m} = -\mathbf{d}_m \mathbf{m}$.

83 Driessen et al. [15] studied changes in the content and orientation of collagen fibres in soft
84 connective tissues due to mechanical interactions, and related the configuration of the fibres to the
85 macroscopic stress in the tissue. Ohsumi et al. [52] performed simulations of anisotropic collagen
86 gel compaction.

87 Recently, studies on the biomechanical behaviour of biological tissues reinforced by collagen
88 fibres, such as the abdominal aorta, have been performed, e.g., by deBotton and Shmuel [13],
89 Schriefl et al. [58], and Gasser et al. [28]. A review on the subject was written by [62]. In studying
90 the reorientation of fibres in arteries, Olsson and Klarbring [53] proposed a model in which the
91 angles defining the local fibre orientation were treated as additional degrees of freedom of the
92 body, rather than as internal variables, and were determined by solving specific balance laws. A
93 comparison of the results of Olsson and Klarbring [53] with those of Imatani and Maugin [37] was
94 done by Grillo et al. [32].

95 In this work, we propose a model that aims to extend the treatment of remodelling given by
96 Olsson and Klarbring [53] to the case of a composite material featuring a statistical distribution
97 of reinforcing fibres. We assume that the composite material is transversely isotropic with respect
98 to a given symmetry axis, and that the fibres are oriented according to a Gaussian probability
99 density distribution. We denote by Q the angle around which the Gaussian distribution is peaked,
100 and refer to it as to the “remodelling variable”. We treat Q as an additional kinematic descriptor.
101 The implications of this choice and the differences between the work of Olsson and Klarbring [53]

102 and ours are discussed in sections 4 and 8. Other authors who have used the concept of probability
 103 density distribution for modelling fibre-reinforced composite materials are, e.g., [4], and [39].

104 The remainder of this work is organised as follows. In section 2 we introduce the notation.
 105 In section 3, we discuss the composite materials with statistical orientation of fibres. In section
 106 4, we present the Principle of Virtual Powers. In section 5, we study the dissipation and develop
 107 the constitutive theory. In section 6, we present in detail a demonstration problem. Results are
 108 presented in section 7 and summarised in section 8.

109 2 General Notation

110 For the sake of generality, the covariant formalism is adopted throughout this paper and the nota-
 111 tion introduced by Truesdell and Noll [61] and Marsden and Hughes [45], with slight modifications,
 112 is employed.

113 Let \mathcal{B} and \mathcal{E} be a body and the three-dimensional Euclidean space, respectively. The reference
 114 configuration of the body is denoted by $\mathcal{C} \subset \mathcal{E}$. The set $[t_0, t_f] \subset \mathbb{R}$ is the interval of time over
 115 which the evolution of the body is observed. The motion of the body is described by the smooth
 116 function $\chi : \mathcal{C} \times [t_0, t_f] \rightarrow \mathcal{E}$. The set $\mathcal{C}_t = \chi(\mathcal{C}, t) \subset \mathcal{E}$ is the region of space occupied by the body
 117 at time t . It holds that $\chi(X, t) = x$, with $x \in \mathcal{E}$ and $X \in \mathcal{C}$.

118 The spaces $T_x\mathcal{E}$ and $T_X\mathcal{C}$ are said to be the tangent spaces attached, respectively, to \mathcal{E} and \mathcal{C}
 119 at the points x and X . Their dual spaces, $T_x^*\mathcal{E}$ and $T_X^*\mathcal{C}$, are referred to as cotangent spaces. The
 120 tangent and cotangent bundles associated with \mathcal{C} are defined by $T\mathcal{C} := \bigcup_{X \in \mathcal{C}} T_X\mathcal{C}$ and $T^*\mathcal{C} :=$
 121 $\bigcup_{X \in \mathcal{C}} T_X^*\mathcal{C}$, respectively. The tangent and cotangent bundles associated with \mathcal{E} , $T\mathcal{E}$ and $T^*\mathcal{E}$, are
 122 defined in a similar fashion.

123 Let \mathcal{A} be a linear vector space, and let \mathcal{A}^* be its dual space. Then, $\mathcal{A} \otimes \mathcal{A}$ denotes the space
 124 of all real-valued, second-order tensors $\mathbf{a} : \mathcal{A}^* \times \mathcal{A}^* \rightarrow \mathbb{R}$, whereas $(\mathcal{A} \otimes \mathcal{A})_S$ is the subspace of all
 125 symmetric second-order tensors belonging to $\mathcal{A} \otimes \mathcal{A}$. Moreover, given two linear spaces \mathcal{A} and \mathcal{Z} ,
 126 $\mathcal{A} \otimes \mathcal{Z}^*$ represents the space of all two-point tensors $\mathbf{f} : \mathcal{A}^* \times \mathcal{Z} \rightarrow \mathbb{R}$.

127 The spaces $T\mathcal{E}$ and $T\mathcal{C}$ are assumed to be equipped with the metric tensors $\mathbf{g} \in T^*\mathcal{E} \otimes T^*\mathcal{E}$

128 and $\mathbf{G} \in T^*\mathcal{C} \otimes T^*\mathcal{C}$, respectively. For all pairs $(\mathbf{u}, \mathbf{v}) \in T_x\mathcal{E} \times T_x\mathcal{E}$ and $(\mathbf{U}, \mathbf{V}) \in T_X\mathcal{C} \times T_X\mathcal{C}$, the
 129 scalar products $\mathbf{u} \cdot \mathbf{v}$ and $\mathbf{U} \cdot \mathbf{V}$ are defined by $\mathbf{u} \cdot \mathbf{v} = u^a g_{ab}(x) v^b$ and $\mathbf{U} \cdot \mathbf{V} = U^A G_{AB}(X) V^B$.

130 The identities in $T\mathcal{E}$ and $T\mathcal{C}$ are denoted by $\mathbf{i} \in T\mathcal{E} \otimes T^*\mathcal{E}$ and $\mathbf{I} \in T\mathcal{C} \otimes T^*\mathcal{C}$, respectively. It
 131 holds that $\mathbf{i} = \mathbf{g}^{-1}\mathbf{g}$ and $\mathbf{I} = \mathbf{G}^{-1}\mathbf{G}$.

132 The two-point tensor $\mathbf{F} \in T\mathcal{E} \otimes T^*\mathcal{C}$, with components $F^a_A = \partial\chi^a/\partial X^A$ and determinant
 133 $J = \det(\mathbf{F}) > 0$, is the deformation gradient tensor. The Cauchy-Green deformation tensor is
 134 defined as $\mathbf{C} = \mathbf{F}^T \mathbf{g} \mathbf{F} = \mathbf{F}^T \cdot \mathbf{F} \in T^*\mathcal{C} \otimes T^*\mathcal{C}$, with $\mathbf{F}^T \in T^*\mathcal{C} \otimes T\mathcal{E}$. The inverse of \mathbf{C} is denoted by
 135 $\mathbf{B} := \mathbf{C}^{-1} \in T\mathcal{C} \otimes T\mathcal{C}$.

136 The deformation gradient tensor \mathbf{F} can be decomposed into a volumetric and an isochoric
 137 part [25, 51], that is $\mathbf{F} = J^{1/3} \bar{\mathbf{F}}$. The isochoric part, $\bar{\mathbf{F}}$, has unitary determinant, i.e., $\det(\bar{\mathbf{F}}) =$
 138 1. Consequently, the Cauchy-Green deformation tensor becomes $\mathbf{C} = J^{2/3} \bar{\mathbf{C}}$, with $\bar{\mathbf{C}} = \bar{\mathbf{F}}^T \cdot \bar{\mathbf{F}}$.
 139 Furthermore, let $\mathbf{Y}(\mathbf{C}) := [\det(\mathbf{C})]^{-1/3} \mathbf{C} = \bar{\mathbf{C}}$ be an auxiliary function defined for all symmetric,
 140 non-singular tensors of $T^*\mathcal{C} \otimes T^*\mathcal{C}$, and valued in the set of symmetric, unimodular tensors of the
 141 same type. By definition, \mathbf{Y} is homogeneous of degree zero. Its derivative reads

$$\frac{\partial \mathbf{Y}}{\partial \mathbf{C}}(\mathbf{C}) = [\det(\mathbf{C})]^{-1/3} [\mathbb{M}(\mathbf{C})]^T, \quad \mathbb{M}(\mathbf{C}) = \mathbb{I} - \frac{1}{3} \mathbf{B} \otimes \mathbf{C}. \quad (1)$$

142 The fourth-order tensor \mathbb{I} is the identity in $(T\mathcal{C} \otimes T\mathcal{C})_S$ (please, see Appendix).

143 The measures of stress used in this work are the first and the second Piola-Kirchhoff stress
 144 tensors, i.e., $\mathbf{P} \in T\mathcal{E} \otimes T\mathcal{C}$ and $\mathbf{S} = \mathbf{F}^{-1} \mathbf{P} \in (T\mathcal{C} \otimes T\mathcal{C})_S$. The tensor

$$\mathbf{S}_d := \mathbb{M}(\mathbf{C}) : \mathbf{S} = \mathbf{S} - \frac{1}{3} \text{tr}[\mathbf{C}\mathbf{S}] \mathbf{B} \quad (2)$$

145 represents the distortional part of \mathbf{S} and satisfies identically the condition $\text{tr}[\mathbf{C}\mathbf{S}_d] = 0$, i.e., \mathbf{S}_d is
 146 deviatoric with respect to the metric induced by \mathbf{C} . The distortional part of \mathbf{P} is defined by

$$\mathbf{P}_d := \mathbf{F}\mathbf{S}_d = \mathbf{P} - \frac{1}{3} \text{tr}[\mathbf{g}\mathbf{P}\mathbf{F}^T] \mathbf{g}^{-1} \mathbf{F}^{-T}. \quad (3)$$

147 Finally, by introducing the Cauchy stress tensor $\boldsymbol{\sigma} = J^{-1} \mathbf{P}\mathbf{F}^T = J^{-1} \mathbf{F}\mathbf{S}\mathbf{F}^T$, and post-multiplying

148 (3) by \mathbf{F}^T , the expression of the deviatoric part of Cauchy stress

$$\sigma_d := J^{-1} \mathbf{P}_d \mathbf{F}^T = \boldsymbol{\sigma} - \frac{1}{3} \text{tr}[\mathbf{g}\boldsymbol{\sigma}] \mathbf{g}^{-1} \quad (4)$$

149 is arrived at. The tensor $\boldsymbol{\sigma}_d$ is deviatoric with respect to the metric generated by \mathbf{g} .

150 **3 Composite materials with statistical orientation of fibres**

151 The fibre-reinforced composite materials studied in this paper are assumed to comply with the
152 following hypotheses: (a) they can be modelled as saturated biphasic mixtures featuring a matrix
153 (phase m) and several families of fibres (phase f), (b) both phases are constrained to move with
154 the same macroscopic velocity, and (c) each phase is intrinsically incompressible and exhibits
155 hyperelastic material behaviour. Moreover, the fibres are assumed to be oriented in space according
156 to a probability density distribution whose functional form is prescribed from the outset on the
157 basis of experimental data [2, 48].

158 The knowledge of the internal structure of composite materials of the kind described above
159 can be encapsulated into two pieces of information: the volumetric fraction of the fibres and a
160 distribution that measures the probability density of finding a family of fibres aligned along a
161 chosen direction at a given material point. In general, one has to speak of “a family of fibres”
162 rather than of “a fibre”, since fibres with different geometric and/or mechanical properties may be
163 aligned along the same spatial direction.

164 **3.1 Consequences of the hypotheses (a), (b) and (c)**

165 At a sufficiently coarse scale of observation, a composite material of the kind considered in this work
166 can be viewed as a mixture of solids [3]. For the purposes of this article, the mixture is assumed to
167 comprise only two solid phases, which are characterised by different mechanical properties and are
168 separated by an interface. The physical fields that determine the amount of a given phase in the
169 mixture are the true, or intrinsic, mass density and the volumetric fraction of the considered phase.
170 The true mass densities are denoted by ϱ_f and ϱ_m . The volumetric fractions are indicated by φ_f

171 and φ_m . The saturation constraint is expressed by $\varphi_f + \varphi_m = 1$, which must be satisfied at all
 172 times and at all points of the mixture. Moreover, the admissible values of each volumetric fraction
 173 range in the interval $[0, 1]$. The mass density of the composite material as a whole is defined by
 174 $\varrho = \varphi_f \varrho_f + \varphi_m \varrho_m$. All fields are defined here according to the Eulerian (or spatial) description of
 175 Continuum Mechanics.

176 Assuming that matrix and fibres move with the same velocity places the restriction that the
 177 mass balance law of each constituent must comply with the chain of equalities

$$\operatorname{div}(\mathbf{v}) = -\frac{D_t \varphi_f}{\varphi_f} - \frac{D_t \varrho_f}{\varrho_f} = \frac{D_t \varphi_f}{1 - \varphi_f} - \frac{D_t \varrho_m}{\varrho_m}, \quad (5)$$

178 with \mathbf{v} and D_t being the velocity and the convective derivative operator, respectively.

179 Requiring each constituent of the mixture to be incompressible means to set the ratios $D_t \varrho_f / \varrho_f$
 180 and $D_t \varrho_m / \varrho_m$ equal to zero in (5). This yields

$$\operatorname{div}(\mathbf{v}) = 0, \quad (6a)$$

$$D_t \varphi_f = 0. \quad (6b)$$

181 Since (6a) implies $J = 1$, the Piola transformation of φ_f reads $\Phi_f := J \phi_f = \phi_f$, with $\phi_f(\cdot, t) =$
 182 $\varphi_f(\cdot, t) \circ \chi(\cdot, t)$. The quantity Φ_f is the volumetric fraction of the “fibres” as measured in the
 183 reference configuration. It follows from (6a) and (6b) that $\dot{\Phi}_f = 0$. The volumetric fractions Φ_f and
 184 $\Phi_m = 1 - \Phi_f$ may generally depend on the point of \mathcal{C} at which they are evaluated.

185 The condition (6a) can be rephrased as

$$\overline{\ln(J)} = \operatorname{tr}[(\operatorname{Grad} \mathbf{u}) \mathbf{F}^{-1}] = 0, \quad (7)$$

186 with $\mathbf{u} : \mathcal{C} \times [t_0, t_f] \rightarrow T\mathcal{E}$ being defined by $\mathbf{u}(\cdot, t) = \mathbf{v}(\cdot, t) \circ \chi(\cdot, t)$, and $\operatorname{Grad} \mathbf{u}$ being the
 187 material velocity gradient. The conditions (6) also imply $D_t \varrho = 0$.

188 3.2 Probability density distribution (PDD)

189 A fibre-reinforced composite material with statistically oriented fibres is generally an anisotropic
 190 medium. To model anisotropy for materials of this kind, one has to introduce the set of all directions
 191 in space and a probability density distribution (PDD) defined on it. The set of all directions is
 192 locally identified with the unit hemisphere $\mathbb{H}^2 := \{\mathbf{M} \in T_X\mathcal{C} : \|\mathbf{M}\| = 1, \text{ and } \mathbf{M} \cdot \boldsymbol{\Xi} \geq 0\}$
 193 attached to $X \in \mathcal{C}$, where $\boldsymbol{\Xi}$ is the local axis of symmetry of transverse isotropy. If $\{\mathbf{N}_A\}_{A=1}^3 \subset T_X\mathcal{C}$
 194 is an orthonormal vector basis of $T_X\mathcal{C}$, and \mathbf{N}_3 is chosen as the polar axis, the unit vector \mathbf{M}
 195 can be expressed in terms of the co-latitude α from the polar axis and the longitude β from the
 196 \mathbf{N}_1 - \mathbf{N}_2 plane:

$$\mathbf{M} = \sin(\alpha) \cos(\beta) \mathbf{N}_1 + \sin(\alpha) \sin(\beta) \mathbf{N}_2 + \cos(\alpha) \mathbf{N}_3. \quad (8)$$

197 The PDD \wp of finding a fibre locally oriented along the direction \mathbf{M} is defined on the set \mathbb{H}^2 ,
 198 and is determined by a set of parameters that describe the internal structure of the composite.
 199 Depending on the addressed problem and the modelled material, several choices of \wp are possible.
 200 For example, a Gaussian distribution has been proposed by Federico et al. [22, 23], while π -periodic
 201 von Mises distributions have been used by Gasser et al. [29]. Any choice of the PDD has to comply
 202 with the following restrictions: (i) \wp has to fulfill the normalisation condition; (ii) it has to be an
 203 even function of \mathbf{M} ; and (iii) it has to reflect the material symmetries of the composite that it
 204 models.

205 In this work, the composite material is assumed to exhibit transverse isotropy with respect
 206 to the axis determined by \mathbf{N}_3 , which is thus taken as symmetry axis for the whole reference
 207 configuration \mathcal{C} . To be consistent with this feature, \wp cannot depend on the latitude β . Furthermore,
 208 \wp is postulated to be a Gaussian distribution. This requirement implies that \wp depends on two
 209 parameters only, which are the variance, ϖ^2 , and the angle Q defining the most probable direction of
 210 fibres' alignment. In general, both parameters should be regarded as functions of time and position
 211 of material particles. Their dependence on X supplies information about the inhomogeneity with
 212 which the fibres are oriented in the composite, whereas their evolution in time accounts for the
 213 time-dependent structural adaptation of the composite in response to some remodelling force. In

214 the following, however, ϖ shall be regarded as a given constant and assigned from the outset.
 215 Although this is a strong assumption for some practical cases, it allows to keep the model at an
 216 acceptable level of complexity. On the basis of the considerations above, the PDD is taken as

$$\wp(\mathbf{M}, Q) := \frac{g(\mathbf{M}, Q)}{\int_{\mathbb{H}^2} g(\mathbf{M}', Q) dS'}. \quad (9)$$

217 If the re-parameterisation (8) is used, the definition (9) can be reformulated as

$$\wp(\alpha, Q) := \frac{g(\alpha, Q)}{\int_0^{2\pi} \left\{ \int_0^{\pi/2} g(\alpha', Q) \sin(\alpha') d\alpha' \right\} d\beta'}, \quad (10a)$$

$$g(\alpha, Q) := \exp \left[-\frac{(\alpha - Q)^2}{2\varpi^2} \right]. \quad (10b)$$

218 4 Principle of Virtual Powers and Field Equations

219 In the model developed by Olsson and Klarbring [53] for the reorientation of fibres in arteries,
 220 the law governing the time-dependent alignment of the fibres was deduced from the Principle of
 221 Virtual Powers and the Principle of Maximum Dissipation. The model was based on the theories
 222 developed by DiCarlo and Quiligotti [14] for tissue growth, Cermelli et al. [8] for rate-independent
 223 plasticity, and Gurtin [33] for a generalisation of the Allen-Cahn and Cahn-Hilliard models. Al-
 224 though these theories were conceived for quite different modelling purposes, they have common
 225 features and —to the best of our understanding— their most relevant aspects are the treatment of
 226 kinematics and the concept of force (a linear, continuous, real-valued functional defined on the set
 227 of test velocities, cf. DiCarlo and Quiligotti [14]). In summary, a body undergoing both changes of
 228 shape and transformations of internal structure necessitates two types of independent kinematic
 229 descriptors: the first type is given by the velocity \mathbf{v} (or \mathbf{u}); the second type comprehends the
 230 descriptors associated with the body structural changes. In the problem analysed by Olsson and
 231 Klarbring [53], the kinematic descriptors of the second type were the angular velocities with which
 232 the fibres reoriented.

233 It is important to remark that, in the framework outlined above, the structural descriptors

234 are not treated as the rates of internal variables. Rather, they are viewed as generalised velocities
 235 that, as such, must be power-conjugate to properly defined generalised forces. These forces must,
 236 in turn, satisfy balance laws.

237 In the following, a purely mechanical context is considered and only the structural reorganisa-
 238 tion due to the reorientation of fibres is studied. Moreover, the structural change of the composite
 239 material under investigation is characterised by a single kinematic descriptor, which is referred to
 240 as “remodelling variable”, whereas its power-conjugate forces are said to be “remodelling forces”.
 241 These can be both internal and external, and are required to satisfy a balance law. Under suitable
 242 hypotheses, the internal forces are determined constitutively, and it is shown that they feature a
 243 dissipative contribution that is related to the remodelling variable.

244 While the methods discussed above supply the bases for our theory, our paper addresses the
 245 structural reorganisation of statically oriented composites. To this end, the kinematic descriptor of
 246 remodelling chosen in our approach is the generalised velocity $\Omega := \dot{Q}$, i.e., the time derivative of
 247 the angle Q that parameterises the PDD (10a), and determines the most probable direction along
 248 which the fibres are aligned at a given point $X \in \mathcal{C}$ and instant of time $t \in [0, t_f]$.

249 Formally, the set of kinematic descriptors of the body under consideration may be defined as

$$\mathcal{G} := \{(\mathbf{u}, \Omega) : \mathcal{C} \times [t_0, t_f] \rightarrow T\mathcal{E} \times \mathbb{R} \mid \mathbf{u} = \dot{\chi}^a \mathbf{e}_a, \text{ and } \Omega = \dot{Q}\}, \quad (11)$$

250 where $\{\mathbf{e}_a\}_{a=1}^3$ is a vector basis in $T\mathcal{E}$. Here, Ω is assumed to belong to $L^2(\mathcal{C}, \mathbb{R})$, i.e., the Lebesgue
 251 space of real-valued, square-integrable functions over \mathcal{C} , whereas \mathbf{u} is an element of the Sobolev
 252 space $(H^1(\mathcal{C}))^3 := \{\mathbf{w} \in (L^2(\mathcal{C}, T\mathcal{E}))^3 \mid \text{Grad} \mathbf{w} \in (L^2(\mathcal{C}, T\mathcal{E}))^{3,3}\}$, i.e., the set of all vector fields
 253 \mathbf{w} , defined in \mathcal{C} and valued in $T\mathcal{E}$, that are square-integrable over \mathcal{C} and whose first derivatives in
 254 the sense of distribution are square-integrable over \mathcal{C} too [57].

255 The set of generalised virtual (test) velocities is the collection of all admissible realisations

$$\tilde{\mathcal{G}} := \{(\tilde{\mathbf{u}}, \tilde{\Omega}) : \mathcal{C} \times [t_0, t_f] \rightarrow T\mathcal{E} \times \mathbb{R} \mid \tilde{\mathbf{u}}|_{\partial\mathcal{C}_D} = \mathbf{0}\}, \quad (12)$$

256 where $\tilde{\mathbf{u}}|_{\partial\mathcal{C}_D}$ is the restriction of $\tilde{\mathbf{u}}$ to the Dirichlet boundary of \mathcal{C} (i.e., the portion of the boundary

257 where position boundary conditions are imposed). The test velocity $\tilde{\mathbf{u}}$ is an element of the space
 258 $(H_0^1(\mathcal{C}))^3 = \{\tilde{\mathbf{w}} \in (H^1(\mathcal{C}))^3 \mid \tilde{\mathbf{w}}|_{\partial\mathcal{C}_D} = \mathbf{0}\}$.

259 The virtual power done by external forces is defined by the linear functional $\mathcal{P}_e : \tilde{\mathcal{G}} \rightarrow \mathbb{R}$,

$$\mathcal{P}_e(\tilde{\mathbf{u}}, \tilde{\Omega}) := \underbrace{\int_{\mathcal{e}} \mathbf{b} \cdot \tilde{\mathbf{u}} + \int_{\partial\mathcal{C}_N} \mathbf{f} \cdot \tilde{\mathbf{u}}}_{\text{Standard terms}} + \underbrace{\int_{\mathcal{e}} Z_e \tilde{\Omega}}_{\text{Remodelling}}. \quad (13)$$

260 In (13), \mathbf{b} groups together all body forces per unit volume of the reference configuration (i.e., inertia
 261 and long-range interactions), \mathbf{f} denotes contact forces measured per unit area of the Neumann-
 262 boundary $\partial\mathcal{C}_N$, i.e., the portion of the boundary where traction boundary conditions are imposed),
 263 and Z_e comprehends all remodelling forces due to interactions of the body with its environment.
 264 In some biomechanical applications of tissue remodelling, forces of this kind are identified with the
 265 target values of the internal forces that drive the structural reorganisation of the considered tissues.
 266 In some cases, the introduction of these target forces facilitates the determination of the stationary
 267 states of the studied remodelling processes. More details about this issue and its connection with
 268 our work shall be outlined in section 5.

269 The virtual power done by the internal forces is defined by the linear functional $\mathcal{P}_i : \tilde{\mathcal{G}} \rightarrow \mathbb{R}$,

$$\mathcal{P}_i(\tilde{\mathbf{u}}, \tilde{\Omega}) := \underbrace{\int_{\mathcal{e}} \text{tr}[\mathbf{P}(\mathbf{g}\text{Grad}\tilde{\mathbf{u}})^T]}_{\text{Standard term}} + \underbrace{\int_{\mathcal{e}} Z_i \tilde{\Omega}}_{\text{Remodelling}}. \quad (14)$$

270 In (14), \mathbf{P} is the first Piola-Kirchhoff stress tensor, and Z_i is the internal remodelling force. The
 271 physical meaning and the functional form of Z_i are discussed in section 5. The assumption of
 272 incompressibility, as stated in (7), implies that \mathbf{P} takes the form

$$\mathbf{P} = \mathbf{P}_v + \mathbf{P}_d = -Jp\mathbf{g}^{-1}\mathbf{F}^{-T} + \mathbf{P}_d, \quad (15)$$

273 where $\mathbf{P}_v = -Jp\mathbf{g}^{-1}\mathbf{F}^{-T}$ and \mathbf{P}_d are, respectively, the volumetric and distortional parts of \mathbf{P} , and
 274 the hydrostatic pressure p is the Lagrange multiplier associated with (7). Furthermore, the space
 275 $\tilde{\mathcal{P}} \subset L^2(\mathcal{C}, \mathbb{R})$ of virtual pressures \tilde{p} is introduced, and the constrained virtual power $\mathcal{P}_c : \tilde{\mathcal{P}} \rightarrow \mathbb{R}$ is

276 defined as

$$\mathcal{P}_c(\tilde{p}) := - \int_{\mathcal{C}} \text{tr}[J\tilde{p}(\text{Grad}\mathbf{u})\mathbf{F}^{-1}]. \quad (16)$$

277 The Principle of Virtual Powers can be expressed by means of the condition [36]

$$\mathcal{P}_e(\tilde{\mathbf{u}}, \tilde{\Omega}) = \mathcal{P}_i(\tilde{\mathbf{u}}, \tilde{\Omega}) + \mathcal{P}_c(\tilde{p}). \quad (17)$$

278 By substituting (13)–(16) into (17), using the relation $\text{tr}[\mathbf{P}(\mathbf{g}\text{Grad}\tilde{\mathbf{u}})^T] = \text{Div}(\mathbf{P}^T \cdot \tilde{\mathbf{u}}) - \text{Div}(\mathbf{P}) \cdot \tilde{\mathbf{u}}$,
 279 applying Gauss' Theorem, and invoking a well-established localisation argument, one obtains

$$\text{Div}(\mathbf{P}) + \mathbf{b} = \mathbf{0}, \quad \text{in } \mathcal{C}, \quad (18a)$$

$$\mathbf{P} \cdot \mathbf{N} = \mathbf{f}, \quad \text{on } \partial\mathcal{C}_N, \quad (18b)$$

$$\text{tr}[J(\text{Grad}\mathbf{u})\mathbf{F}^{-1}] = 0, \quad \text{in } \mathcal{C}, \quad (18c)$$

$$Z_i = Z_e, \quad \text{in } \mathcal{C}. \quad (18d)$$

280 The equations to be solved are (18a), (18c), and (18d). These constitute a set of five independent
 281 equations. The functional form of the forces \mathbf{b} , \mathbf{f} and Z_e is assumed to be given from the outset,
 282 while \mathbf{P}_d and Z_i should be specified constitutively. By doing so, one obtains a closed mathematical
 283 problem consisting of a system of five equations in the five unknowns $\{\chi^a\}_{a=1}^3$, p , and Q .

284 5 Dissipation and constitutive theory

285 Let $\mathcal{M} \subset \mathcal{C}$ be a fixed part of \mathcal{C} . The dissipation associated with \mathcal{M} is defined by

$$\int_{\mathcal{M}} D = - \overline{\int_{\mathcal{M}} \dot{\Psi}} + \mathcal{P}_n(\mathcal{M}) \geq 0, \quad (19)$$

286 where D and Ψ are, respectively, the dissipation density and stored energy function measured per
 287 unit volume of the reference configuration, and $\mathcal{P}_n(\mathcal{M})$ is referred to as net power, i.e.,

$$\begin{aligned}\mathcal{P}_n(\mathcal{M}) &:= \int_{\partial\mathcal{M}} (\mathbf{P}\cdot\mathbf{N})\cdot\mathbf{u} + \int_{\mathcal{M}} \mathbf{b}\cdot\mathbf{u} + \int_{\mathcal{M}} Z_e\Omega \\ &= \int_{\mathcal{M}} \text{tr}[\mathbf{P}(\mathbf{g}\text{Grad}\mathbf{u})^T] + \int_{\mathcal{M}} Z_i\Omega.\end{aligned}\tag{20}$$

288 Since \mathcal{M} is fixed, it holds true that $\overline{\int_{\mathcal{M}} \dot{\Psi}} = \int_{\mathcal{M}} \dot{\Psi}$. Moreover, by using the chain of identities
 289 $\text{tr}[\mathbf{P}(\mathbf{g}\text{Grad}\mathbf{u})^T] = \text{tr}[\mathbf{P}_d(\mathbf{g}\text{Grad}\mathbf{u})^T] = \frac{1}{2}\text{tr}[\mathbf{S}_d\dot{\mathbf{C}}]$, and localising the result, one obtains

$$D = -\dot{\Psi} + \frac{1}{2}\mathbf{S}_d : \dot{\mathbf{C}} + Z_i\Omega \geq 0.\tag{21}$$

290 The triples $(\mathbf{C}, Q, \Omega) \in (T^*\mathcal{C} \otimes T^*\mathcal{C})_S \times \mathbb{R} \times \mathbb{R}$ are the independent constitutive variables of our
 291 theory. The angle Q describes the changes of the most probable direction of local fibres alignment,
 292 whereas the velocity Ω captures the dissipative aspects of this process.

293 Constitutive functions must comply with the following requirements: (i) objectivity, (ii) locality,
 294 and (iii) criterion of maximum dissipation. Moreover, they are supplied in the form

$$\Psi = \hat{\Psi}(\Phi_f, \mathbf{C}, Q),\tag{22a}$$

$$\mathbf{S}_d = \hat{\mathbf{S}}_d(\Phi_f, \mathbf{C}, Q),\tag{22b}$$

$$Z_i = \hat{Z}_i(\Phi_f, \mathbf{C}, Q, \Omega),\tag{22c}$$

295 In general, (22c) holds true for all $\Omega \neq 0$. It should be remarked that, although the axiomatic
 296 theory of constitutive laws prescribes that all dependent constitutive functionals depend on the
 297 same list of arguments, the elimination of Ω from the list of arguments of $\hat{\Psi}$ and $\hat{\mathbf{S}}_d$ does not affect
 298 the results determined below.

299 To be more specific, $\hat{\Psi}$ and $\hat{\mathbf{S}}_d$ are required to be continuous with respect to the whole list of
 300 their arguments, and $\hat{\Psi}$ is assumed to be smooth in Φ_f , \mathbf{C} , and Q . Moreover, \hat{Z}_i is prescribed to
 301 be bounded and continuous when $\Omega \neq 0$, but it is allowed to be constitutively indeterminate when

302 Ω vanishes.

303 By setting $\Omega \neq 0$, and inserting (22) into (21), the dissipation inequality is rewritten as

$$D = \frac{1}{2} \left[\hat{\mathbf{S}}_d - 2 \frac{\partial \hat{\Psi}}{\partial \mathbf{C}} \right] : \dot{\mathbf{C}} + \left[\hat{Z}_i - \frac{\partial \hat{\Psi}}{\partial Q} \right] \Omega \geq 0. \quad (23)$$

304 Following the prescription $\hat{\Psi}(\Phi_f, \mathbf{C}, Q) = \hat{W}(\Phi_f, \mathbf{\Upsilon}(\mathbf{C}), Q)$, with $\mathbf{\Upsilon}(\mathbf{C}) = \bar{\mathbf{C}}$ [6], the distortional
305 part of the second Piola-Kirchhoff stress tensor is defined constitutively by

$$\mathbf{S}_d = \hat{\mathbf{S}}_d(\Phi_f, \mathbf{C}, Q) = [\det(\mathbf{C})]^{-1/3} \mathbb{M}(\mathbf{C}) : \left(2 \frac{\partial \hat{W}}{\partial \bar{\mathbf{C}}}(\Phi_f, \bar{\mathbf{C}}, Q) \right). \quad (24)$$

306 To obtain the expression of the total second Piola-Kirchhoff stress tensor, the volumetric part
307 $\mathbf{S}_v = -Jp\mathbf{B}$ must be added to \mathbf{S}_d . Since J is equal to unity, it follows that $\mathbf{B} = \bar{\mathbf{B}}$, and \mathbf{S} becomes

$$\mathbf{S} = \mathbf{S}_v + \mathbf{S}_d = -p\bar{\mathbf{B}} + \mathbb{M}(\bar{\mathbf{C}}) : \left(2 \frac{\partial \hat{W}}{\partial \bar{\mathbf{C}}}(\Phi_f, \bar{\mathbf{C}}, Q) \right). \quad (25)$$

308 By introducing the dissipative remodelling force

$$Y := Z_i - \frac{\partial \hat{W}}{\partial Q}, \quad (26)$$

309 the dissipation inequality (23) reduces to $D = Y\Omega \geq 0$, whenever $\Omega \neq 0$. Since dissipation has
310 to vanish when Ω is null, but the force Y might be constitutively indeterminate in this case, one
311 arrives at

$$D = Y\Omega = \begin{cases} \hat{Y}(\Phi_f, \bar{\mathbf{C}}, Q, \Omega) \Omega \geq 0, & \text{if } \Omega \neq 0, \\ 0, & \text{if } \Omega = 0. \end{cases} \quad (27)$$

312 The scope of the study of the residual dissipation inequality is to individuate a constitutive law
313 $Y = \hat{Y}(\Phi_f, \bar{\mathbf{C}}, Q, \Omega)$ that is in harmony with the criterion of maximum dissipation. When this law
314 can be found, the force balance (18d) yields

$$\hat{Y}(\Phi_f, \bar{\mathbf{C}}, Q, \Omega) = Z_e - \frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q). \quad (28)$$

315 Since the functional forms of \hat{Y} and \hat{W} are provided constitutively and the interaction Z_e is known
 316 from the outset, the parameter Q can be determined by solving (28). Once the variables Q and Ω
 317 are known, the remodelling force Z_i can be expressed by means of (26).

318 As remarked by Cermelli et al. [8], when Z_e is zero or negligibly small, the force balance (18d)
 319 implies that the internal force Z_i is zero too, which, in turn, implies that \hat{Y} is given by

$$\hat{Y}(\Phi_f, \bar{\mathbf{C}}, Q, \Omega) = -\frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q). \quad (29)$$

320 5.1 Elastic strain energy function and stress

321 The fibre-reinforced composite material under investigation is assumed to be hyperelastic. Follow-
 322 ing Federico and Grillo [21], the elastic strain energy density of the material is constructed by
 323 superposing the elastic contribution of the matrix to that of the fibres, i.e.,

$$\hat{W}(\Phi_f, \bar{\mathbf{C}}, Q) = (1 - \Phi_f)\hat{W}_m(\bar{\mathbf{C}}) + \Phi_f\hat{W}_f(\bar{\mathbf{C}}, Q), \quad (30)$$

324 where \hat{W}_m and \hat{W}_f denote the stored energy functions of the matrix and fibres, respectively. The
 325 combination (30) is based on the assumption that the matrix consists of an isotropic material
 326 whose mechanical behaviour does not depend on Q . Due to incompressibility, the stored energy
 327 function defined in (30) is taken to be independent of the volumetric part of deformation in order
 328 to ensure that the volumetric part of stress remains constitutively indeterminate [61]. Moreover,
 329 the dependence of \hat{W} on Φ_f and Q accounts for the micro-structural contribution of the composite
 330 to the overall energy.

331 The energy \hat{W}_f is written as the sum of an isotropic and an anisotropic contribution, i.e.,

$$\hat{W}_f(\bar{\mathbf{C}}, Q) = \hat{W}_{fi}(\bar{\mathbf{C}}) + \hat{W}_{fa}(\bar{\mathbf{C}}, Q). \quad (31)$$

332 The energy \hat{W}_{fa} represents the sum of all contributions given by the fibres to the elastic energy of
 333 the composite. Since the fibres are assumed to be oriented statistically, as described by the PDD

334 \wp , \hat{W}_{fa} can be defined as follows

$$\hat{W}_{fa}(\bar{\mathbf{C}}, Q) = \int_{\mathbb{H}^2} \wp(\mathbf{M}, Q) \hat{w}_{fa}(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) dS, \quad (32)$$

335 where $\mathbf{A}(\mathbf{M}) := \mathbf{M} \otimes \mathbf{M}$ is the structure tensor attached at X , and \hat{w}_{fa} is the stored energy
336 function contributed by those fibres that are aligned along \mathbf{M} .

337 If the fibres are regarded to be active only when they are stretched, \hat{w}_{fa} can be written as

$$\hat{w}_{fa}(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) = \mathcal{H}(I_4(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) - 1) \hat{w}_{fb}(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})), \quad (33)$$

338 where \hat{w}_{fb} is the “actual” contribution to the elastic energy of the fibres aligned along \mathbf{M} , the
339 invariant $I_4(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M}))$ is given by $I_4(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) = \text{tr}(\bar{\mathbf{C}}\mathbf{A}(\mathbf{M}))$, and $\mathcal{H}(\cdot)$ is the Heaviside distri-
340 bution (it returns one when its argument is strictly positive, and zero otherwise). In this paper,
341 \hat{W}_m , \hat{W}_{fi} and \hat{w}_{fb} are defined by the expressions

$$\hat{W}_m(\bar{\mathbf{C}}) = \frac{1}{2} c_m [I_1(\bar{\mathbf{C}}) - 3], \quad (34a)$$

$$\hat{W}_{fi}(\bar{\mathbf{C}}) = \frac{1}{2} c_{fi} [I_1(\bar{\mathbf{C}}) - 3], \quad (34b)$$

$$\hat{w}_{fb}(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) = \frac{1}{4} c_{fb} [I_4(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) - 1]^2, \quad (34c)$$

342 where c_m , c_{fi} , and c_{fb} are material constants, and $I_1(\bar{\mathbf{C}}) = \text{tr}(\mathbf{G}^{-1}\bar{\mathbf{C}})$. Thus, the differentiation of
343 \hat{W} with respect to \mathbf{C} yields the distortional part of the second Piola-Kirchhoff stress tensor, i.e.,

$$\begin{aligned} \mathbf{S}_d &= c(\Phi_f) [\mathbf{G}^{-1} - \frac{1}{3} I_1(\bar{\mathbf{C}}) \bar{\mathbf{C}}^{-1}] \\ &+ \int_{\mathbb{H}_0^2(\bar{\mathbf{C}})} \wp(\mathbf{M}, Q) \zeta(\Phi_f, \bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) \hat{\mathbf{A}}_d(\mathbf{M}, \bar{\mathbf{C}}) dS, \end{aligned} \quad (35)$$

344 where the following notation has been introduced:

$$c(\Phi_f) := (1 - \Phi_f)c_m + \Phi_f c_{\bar{v}}, \quad (36a)$$

$$\zeta(\Phi_f, \bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) := \Phi_f c_{fb} [I_4(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) - 1], \quad (36b)$$

$$\hat{\mathbf{A}}_d(\mathbf{M}, \bar{\mathbf{C}}) := \mathbf{A}(\mathbf{M}) - \frac{1}{3} I_4(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) \bar{\mathbf{B}}, \quad (36c)$$

$$\mathbb{H}^2 \supset \mathbb{H}_0^2(\bar{\mathbf{C}}) := \{\mathbf{M} \in \mathbb{H}^2 \mid I_4(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) > 1\}. \quad (36d)$$

345 5.2 Principle of Maximum Dissipation

346 The results reported in this section follow closely the theory developed by Hackl and Fischer[34].

347 In the residual dissipation inequality (27), D is assumed to admit the constitutive form

$$D = \hat{D}(\Lambda, \Omega) \geq 0, \quad (37)$$

348 where $\Lambda := (\Phi_f, \bar{\mathbf{C}}, Q)$ collects all variables other than Ω . Our hypotheses are that $\hat{D}(\Lambda, \Omega)$ is zero
 349 at $\Omega = 0$, that \hat{D} is continuous for all Λ and for all real values of Ω , but differentiable only for
 350 $\Omega \neq 0$, and that \hat{D} can be expressed as a homogeneous function of degree $n \in \mathbb{N}$ with respect to
 351 Ω , i.e., $\hat{D}(\Lambda, \alpha\Omega) = \alpha^n \hat{D}(\Lambda, \Omega)$ for all values of Ω , and for all $\alpha > 0$.

352 If the requisite $\Omega \neq 0$ is fulfilled, an expression defining Y constitutively, i.e., $Y = \hat{Y}(\Lambda, \Omega)$, is
 353 sought for. This expression maximises the dissipation over the space of all admissible velocities Ω .
 354 To achieve this result under the condition that \hat{D} maintains the structure $\hat{D}(\Lambda, \Omega) = Y\Omega$ (cf. (27)
 355 and Hackl and Fisher [34] for explanations about this issue), a constrained optimisation problem
 356 has to be solved. This is done by setting equal to zero the partial derivatives of

$$\hat{L}(\Lambda, \Omega, \gamma) := \hat{D}(\Lambda, \Omega) + \gamma[\hat{D}(\Lambda, \Omega) - Y\Omega], \quad (38)$$

357 where \hat{L} is the Lagrangian function of the constrained optimisation problem, and γ is an unknown

358 Lagrangian multiplier. This procedure leads to:

$$\frac{\partial \hat{L}}{\partial \Omega}(\Lambda, \Omega, \gamma) = (1 + \gamma) \frac{\partial \hat{D}}{\partial \Omega}(\Lambda, \Omega) - \gamma Y = 0, \quad (39a)$$

$$\frac{\partial \hat{L}}{\partial \gamma}(\Lambda, \Omega, \gamma) = \hat{D}(\Lambda, \Omega) - Y\Omega = 0. \quad (39b)$$

359 Solving the set (39) for γ and Y yields

$$\gamma = \gamma_n = \frac{n}{1-n}, \quad n \neq 1, \quad (40a)$$

$$Y = \hat{Y}_n(\Lambda, \Omega) = \frac{1}{n} \frac{\partial \hat{D}}{\partial \Omega}(\Lambda, \Omega). \quad (40b)$$

360 When the degree of homogeneity of the dissipation function is unitary (e.g., for rate-independent
361 materials), the multiplier γ_n is not defined. In this case, (40b) is valid as long as $\Omega \neq 0$ holds true,
362 since Y is constitutively indeterminate at $\Omega = 0$.

363 5.3 Rate-dependent remodelling

364 We assume here that the dissipation function (37) admits the form

$$\hat{D}(\Lambda, \Omega) = \hat{Y}(\Lambda, \Omega)\Omega \geq 0, \quad (41)$$

365 where $\hat{Y}(\Lambda, \Omega)$ is constitutively determinate at $\Omega = 0$. Moreover, we require that $\hat{Y}(\Lambda, \Omega)$ vanishes
366 for vanishing Ω , which implies the even stronger condition $\hat{Y}(\Lambda, 0) = 0$, for all Λ . Conditions
367 of this type can be found in the derivation of Fourier's law of heat conduction, e.g., [17]. These
368 derivations meet the characterisation of thermodynamic equilibrium of Glansdorff and Prigogine
369 [30] and Rajagopal and Srinivasa [54], which requires both flux-like variables and affinities to be
370 zero. In the theory presented in our work, the flux-like variable is the remodelling force Y , while
371 the affinity is the velocity Ω .

372 In the cases in which a linearisation of the constitutive function $\hat{Y}(\Lambda, \Omega)$ in a neighbourhood of

373 $\Omega = 0$ is physically acceptable, the force Y may be assigned through the constitutive expression

$$\hat{Y}(\Lambda, \Omega) = \Gamma(\Lambda)\Omega, \quad (42)$$

374 where $\Gamma(\Lambda)$ is a positive function of Λ . Substitution of (42) into (41) leads to define the dissipation
 375 as a positive definite quadratic function of Ω , i.e., $\hat{D}(\Lambda, \Omega) = \Gamma(\Lambda)\Omega^2$. Since a function of this type
 376 is homogeneous of degree two with respect to Ω , the formula (40b) yields (42).

377 Substituting (42) into the force balance (28) leads to the evolution equation for Q , i.e.

$$\Gamma(\Phi_f, \bar{\mathbf{C}}, Q)\Omega = Z_e - \frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q). \quad (43)$$

378 Equations (43), (18a) and (18b), equipped with initial conditions, describe the problem of remod-
 379 elling in a fibre-reinforced material. When Z_e is identically zero, the condition $\Omega = 0$, which implies
 380 the vanishing of the left-hand side of (43), is attained for those physically meaningful values of Q
 381 solving the stationary problem

$$-\frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q) = 0. \quad (44)$$

382 For given Φ_f and $\bar{\mathbf{C}}$, the existence of stationary points of $\hat{W}(\Phi_f, \bar{\mathbf{C}}, \cdot)$ restricts the choice of the
 383 admissible forms of the strain energy function.

384 5.4 Remodelling force

385 In order to evaluate the evolution of the remodelling variable Q according to (43), we have to
 386 compute the derivative of the Helmholtz free energy density \hat{W} with respect to Q . Looking at the
 387 definition of \wp given in (10a) and at the form of \hat{W} given in (34), we notice that \hat{W} depends on Q
 388 through \wp .

389 By plugging (10b) into (30), we obtain

$$\frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q) = \Phi_f \int_{\mathbb{H}_0^2(\bar{\mathbf{C}})} \frac{\partial \wp}{\partial Q}(\mathbf{M}, Q) \hat{w}_{fb}(\bar{\mathbf{C}}, \mathbf{A}(\mathbf{M})) d\mathbf{S}, \quad (45)$$

390 where

$$\frac{\partial \wp}{\partial Q}(\alpha, Q) = \wp(\alpha, Q) \frac{\alpha - \langle \alpha \rangle(Q)}{\varpi^2}, \quad (46)$$

391 and $\langle \alpha \rangle$ denotes the directional (statistical) average of α . For any function \mathbf{f} defined on the unit
 392 hemisphere, the directional average of \mathbf{f} is defined by:

$$\langle \mathbf{f} \rangle(Q) := \int_{\mathbb{H}^2} \wp(\mathbf{M}, Q) \mathbf{f}(\mathbf{M}) dS. \quad (47)$$

393 With this notation, the derivative (45) can be written in compact form as

$$\frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q) = \Phi_f \frac{\langle \alpha \hat{w}_{fa} \rangle(\bar{\mathbf{C}}, Q) - \langle \alpha \rangle(Q) \langle \hat{w}_{fa} \rangle(\bar{\mathbf{C}}, Q)}{\varpi^2}. \quad (48)$$

394 6 Study of a benchmark problem

395 In order to test the approach proposed above, we propose a modified version of the benchmark
 396 problem solved by Olsson and Klarbring [53]. The problem, originally conceived for studying re-
 397 modelling in arteries, considered a fibre-reinforced, thick-walled, growing cylindrical body made of
 398 hyperelastic material and subjected to pure inflation. The problem was axial symmetric and was
 399 solved under the constraint of isochoric elastic deformations.

400 We made four main modifications to the original problem. The first one deals with the general
 401 approach to remodelling, since our composite material is reinforced by statistically oriented fibres,
 402 whereas the composite material studied by Olsson and Klarbring [53] features a given pattern
 403 of fibre orientation. Secondly, we do not consider growth here. Thirdly, we do not specifically
 404 study remodelling in blood vessels (we recall that the PDD defined in (10), on which the following
 405 calculations are based, was introduced for studying articular cartilage [22, 23]). Finally, we set the
 406 external remodelling force equal to zero (this choice and its consequences are discussed below).

407 In the present framework, the body forces \mathbf{b} are disregarded, and the equation that governs
 408 remodelling is given by (43), with Γ being a known, strictly positive constant. An essential differ-
 409 ence with respect to the paper by Olsson and Klarbring [53] is that, in our approach, the external

410 remodelling force Z_e is switched off from the outset (i.e., $Z_e = 0$). Because of the balance of remod-
 411 elling forces (18d), this amounts to say that the internal remodelling force Z_i vanishes identically
 412 too and, consequently, the dissipative force, which is constitutively determined by (42), is compen-
 413 sated by the derivative of the stored energy function with respect to Q (cf. (29)). In this case, the
 414 balance laws (18a)–(18d), augmented with an initial condition for Q , become

$$\text{Div}(\mathbf{P}) = \mathbf{0}, \quad \text{in } \mathcal{C}, \quad (49a)$$

$$\mathbf{P} \cdot \mathbf{N} = \mathbf{f}, \quad \text{on } \partial\mathcal{C}_N, \quad (49b)$$

$$J = 1, \quad \text{in } \mathcal{C}, \quad (49c)$$

$$\Gamma \dot{Q} = -\frac{\partial \hat{W}}{\partial Q}, \quad \text{in } \mathcal{C}, \quad (49d)$$

$$Q(X, 0) = Q_0(X), \quad \text{in } \mathcal{C}. \quad (49e)$$

415 6.1 Deformation under the incompressibility constraint

416 The coordinates parameterising the reference configuration, \mathcal{C} , are denoted by (R, Θ, Z) , with
 417 $R \in [R_i, R_o]$, $\Theta \in [0, 2\pi]$ and $Z \in [0, L]$. Here, R_i and R_o are the values of the inner and outer
 418 radius of the cross-section of the body, and L is the axial length of the cylinder. The coordinates
 419 associated with the current configuration are indicated by (r, ϑ, z) . Since the deformation is assumed
 420 to be a pure inflation, we obtain

$$(R, \Theta, Z) \mapsto (r, \vartheta, z) = (\chi^r(R, t), \Theta, Z). \quad (50)$$

421 For notational convenience, it is set $\chi^r \equiv \xi$ from here on, and ξ' denotes the derivative $\partial\chi^r/\partial R$.

422 With respect to the orthonormal bases $\{\mathbf{E}_R, \mathbf{E}_\Theta, \mathbf{E}_Z\}$ and $\{\mathbf{e}_r, \mathbf{e}_\vartheta, \mathbf{e}_z\}$, which are associated
 423 with the reference and current configuration, respectively, the deformation gradient is expressed
 424 by

$$\mathbf{F} = \xi' \mathbf{e}_r \otimes \mathbf{E}^R + \frac{\xi}{R} \mathbf{e}_\vartheta \otimes \mathbf{E}^\Theta + \mathbf{e}_z \otimes \mathbf{E}^Z. \quad (51)$$

425 Because of incompressibility, the radial deformation ξ has to comply with the constraint $\det(\mathbf{F}) = 1$,

426 which results into the differential equation with separable variables

$$\xi'(R, t)\xi(R, t) = R. \quad (52)$$

427 This condition determines ξ up to an unknown function of time K , i.e.,

$$\xi(R, t) = \sqrt{R^2 + K(t)}. \quad (53)$$

428 6.2 Boundary conditions

429 The boundary of the current configuration is given by $\partial\mathcal{C}_t = \partial\mathcal{C}_{to} \cup \partial\mathcal{C}_{ti}$, where the subscripts “o”
 430 and “i” define the “outer” and “inner” surface of the inflated cylinder, respectively. The boundary
 431 conditions are written as

$$\boldsymbol{\tau}|_o = -\lambda_o \mathbf{n}_o \quad \text{on } \partial\mathcal{C}_{to}, \quad \boldsymbol{\tau}|_i = -\lambda_i \mathbf{n}_i \quad \text{on } \partial\mathcal{C}_{ti}, \quad (54)$$

432 where $\boldsymbol{\tau}$ denotes the distribution of imposed contact forces, $\mathbf{n}_o \equiv \mathbf{e}_r(r_o, t)$ and $\mathbf{n}_i \equiv -\mathbf{e}_r(r_i, t)$
 433 are the unit vectors normal to the outer and inner walls, respectively, and λ_o and λ_i are scalar
 434 constants having the physical dimensions of pressure. With these boundary conditions, $\partial\mathcal{C}_t$ and
 435 $\partial\mathcal{C}$ are entirely Neumann boundaries.

436 The force \mathbf{f} featuring in (49b), and defined per unit surface of the reference configuration
 437 of the body, is given by $\mathbf{f} = \boldsymbol{\tau} J \sqrt{\mathbf{N} \cdot \mathbf{C}^{-1} \cdot \mathbf{N}}$ [6], where the factor $J \sqrt{\mathbf{N} \cdot \mathbf{C}^{-1} \cdot \mathbf{N}}$ accounts for the
 438 change of area when passing from the boundary of the current configuration to that of the reference
 439 placement, and $\boldsymbol{\tau}$ is the contact force defined per unit area of $\partial\mathcal{C}_t$. Using Nanson’s formula, and
 440 accounting for incompressibility yield

$$\mathbf{P} \cdot \mathbf{N}|_o = -\lambda_o \mathbf{g}^{-1} \mathbf{F}^{-T} \cdot \mathbf{N}, \quad \text{on } \partial\mathcal{C}_o, \quad (55a)$$

$$\mathbf{P} \cdot \mathbf{N}|_i = -\lambda_i \mathbf{g}^{-1} \mathbf{F}^{-T} \cdot \mathbf{N}, \quad \text{on } \partial\mathcal{C}_i. \quad (55b)$$

441 Under the assumption that the components of the stress tensor do not depend on the coordinates

442 Θ and Z , the boundary conditions (55a) and (55b) as well as the symmetry requirement of the
 443 Cauchy stress tensor, $\mathbf{PF}^T = \mathbf{FP}^T$, are sufficient to ensure that the only nonzero components of
 444 \mathbf{P} are P^{rR} and $P^{\vartheta\Theta}$. Therefore, conditions (55a) and (55b) can be reformulated as

$$p(R_o, t) = \lambda_o + \frac{R_o^2}{R_o^2 + K(t)} S_d^{RR}(R_o, t), \quad \text{on } \partial\mathcal{C}_o, \quad (56a)$$

$$p(R_i, t) = \lambda_i + \frac{R_i^2}{R_i^2 + K(t)} S_d^{RR}(R_i, t), \quad \text{on } \partial\mathcal{C}_i. \quad (56b)$$

445 6.3 Pressure and time-dependent integration constant K

446 Pressure can be determined by solving the balance of momentum

$$\frac{\partial P^{rR}}{\partial R} + \frac{P^{rR} - P^{\vartheta\Theta}}{R} = 0 \quad (57)$$

447 together with (56a) and (56b). Indeed, direct integration of (57) leads to

$$p(R, t) = \left[\frac{R}{\xi(R, t)} \right]^2 S_d^{RR}(R, t) + \lambda_i(t) - \int_{R_i}^R \frac{1}{\xi(A, t)} \eta(A, t) dA, \quad (58)$$

448 where η is the auxiliary function defined by

$$\eta(A, t) := \frac{\xi(A, t)}{A} S_d^{\Theta\Theta}(A, t) - \left[\frac{A}{\xi(A, t)} \right]^3 S_d^{RR}(A, t). \quad (59)$$

449 Equation (58) defines pressure up to the (still unknown) function of time K . To determine K ,
 450 the pressure is evaluated at $R = R_o$, and the boundary condition (56a) is enforced. Under the
 451 simplifying assumption $\lambda_o = 0$, the following consistency condition is arrived at

$$\lambda_i(t) = \int_{R_i}^{R_o} \frac{1}{\xi(R, t)} \eta(R, t) dR. \quad (60)$$

6.4 Initial-boundary-value problem and numerical implementation

The benchmark problem investigated in our work considers a thick-walled cylinder reinforced by fibres, and subjected to a uniformly distributed hydrostatic load applied to the inner wall of the cylinder. At each material point X , identified by the triple (R, Θ, Z) , the direction of the most probable fibre orientation is represented by the unit vector $\mathbf{M}_p := \sin(Q)\mathbf{E}_R + \cos(Q)\mathbf{E}_Z$, with Q being the angle that the symmetry axis of the cylinder (parallel to \mathbf{E}_Z) forms with \mathbf{M}_p . In order to preserve the axial symmetry of the problem, the angle Q is required to be independent of the tangential coordinate. At the same material point, a generic fibre is aligned along the direction specified by the unit vector $\mathbf{M} = \sin(\alpha)\cos(\beta)\mathbf{E}_R + \sin(\alpha)\sin(\beta)\mathbf{E}_\Theta + \cos(\alpha)\mathbf{E}_Z$, where α is the angle that \mathbf{M} forms with \mathbf{E}_Z , and β is the angle that the projection of \mathbf{M} onto the plane \mathbf{E}_R - \mathbf{E}_Θ forms with \mathbf{E}_R . The set of all space directions emanating from X , \mathbb{H}^2 , is obtained by varying $\alpha \in [0, \pi/2]$ and $\beta \in [0, 2\pi)$. Furthermore, the directional distribution of the fibres is governed by the PDD defined in (10), with the parameter Q satisfying the evolution law (49d). In (49e), the initial distribution $Q_0(X) = \pi/4$, for all $X \in \mathcal{C}$, is used.

We remark that, in order to simulate the pattern of fibre orientation in an artery, Olsson and Klarbring [53] considered, at each material point X , two unit vectors \mathbf{M}_1 and \mathbf{M}_2 lying on the plane \mathbf{E}_Θ - \mathbf{E}_Z . According to the description given above, the directional distribution of the fibres assumed in our work is different from that considered by Olsson and Klarbring [53].

The initial-boundary value problem (IBVP), given by (49a)–(49e), is reformulated and put in terms of the system of equations (53), (58), (60) and (49d), which determine ξ , p , K , and Q . Equations (53) and (58) can be decoupled from (60) and (49d). Thus, the deformed radius ξ and the remodelling angle Q can be determined by solving the subsystem resulting from (60) and (49d). Once ξ and Q are known, K is found by inverting (53), and the pressure p is provided by (58).

Equations (53), (58), (60) and (49d) are solved numerically for a given initial distribution of the remodelling variable Q . The solution is based on the remodelling equation (49d), with the angle Q being treated as primary unknown. Thus, stress, energy, and deformed radius are viewed as functions of Q . The external remodelling force Z_e was set equal to zero in our calculations. This ensured that there was no external influence on the remodelling of the system, and that remodelling

480 was purely driven by internal forces.

481 From the numerical point of view, a difficulty arises because the right-hand-side of (49d) ne-
 482 cessitates, at each time step, the evaluation of the integral given in (45), which, in turn, requires
 483 the knowledge of the integration set $\mathbb{H}_0^2(\overline{\mathbf{C}})$. To specify $\mathbb{H}_0^2(\overline{\mathbf{C}})$, we have to detect the subset of the
 484 unit hemisphere in which the argument of the Heaviside distribution is strictly positive, i.e., we
 485 have to look for the directions and deformations that satisfy the condition

$$f(\overline{\mathbf{C}}, \mathbf{M}) := I_4(\overline{\mathbf{C}}, \mathbf{A}(\mathbf{M})) - 1 > 0. \quad (61)$$

486 By accounting for (53), and noting that the unit vector \mathbf{M} depends on the angles α and β , we can
 487 rephrase (61) as

$$f(K(t), R, \alpha, \beta) = K \frac{[\sin(\alpha)]^2 [\cos(\beta)]^2}{R^2} \left\{ [\tan(\beta)]^2 - \frac{R^2}{R^2 + K(t)} \right\} > 0. \quad (62)$$

488 If K is strictly positive (which is consistent with the assumption that the cylinder is being inflated),
 489 and α is different from zero, the condition (62) is respected when

$$\beta \in (\beta_0, \pi/2) \cup (\pi/2, \pi - \beta_0) \cup (\pi + \beta_0, 3\pi/2) \cup (3\pi/2, 2\pi - \beta_0), \quad (63)$$

490 with $\beta_0(R, t) = \arctan[R/\xi(R, t)]$. Furthermore, we introduce the auxiliary quantity

$$\mathfrak{J}(R, t) := \int_{R_i}^R \frac{1}{\xi(A, t)} \eta(A, t) dA. \quad (64)$$

491 Since ξ depends on time through K , while the stresses S_d^{RR} and $S_d^{\Theta\Theta}$ depend on time through both
 492 K and Q , we may write

$$\mathfrak{J}(R, t) = \hat{\mathfrak{J}}_{A=R_i}^R(K(t), Q(A, t), R), \quad (65)$$

493 where $\hat{\mathfrak{J}}_{A=R_i}^R$ is a functional of Q .

494 The material parameters used in our simulations are listed in Table 1. The implementation of

495 the mathematical problem was performed in MATLAB[®]. The algorithm is presented in Table 2,
496 and amounts to apply the explicit Euler method to the system of equations (53), (58), (60) and
497 (49d). To proceed, we denote by t_f the final time of observation of the system, and discretize
498 the interval $[0, t_f]$, with $t_f < +\infty$, by selecting $(N + 1)$ time instants $\{t_0, t_1, \dots, t_N\}$, such that
499 $t_0 = 0$, $t_N = t_f$ and, for $n = 0, \dots, (N - 1)$, $t_{n+1} = t_n + \Delta t_n$, where $\Delta t_n > 0$ is the length of
500 the subinterval $\mathcal{J}_{n,n+1} = [t_n, t_{n+1}]$. In an analogous fashion, the interval $[R_i, R_o]$ is discretized
501 with a one-dimensional grid of $(M + 1)$ nodes $\{R_0, R_1, \dots, R_M\}$, such that $R_0 = R_i$, $R_M = R_o$.
502 The intervals $\mathcal{J}_{k,k+1} := [R_k, R_{k+1}]$, with $k = 0, \dots, (M - 1)$, are disjoint and cover $[R_i, R_o]$. The
503 length of $\mathcal{J}_{k,k+1}$ is denoted by $\Delta R_k > 0$. If ψ denotes a function that depends on time and radial
504 coordinate, we use the notation $\psi(R_k, t_n) \equiv \psi_{k,n}$. We write $\psi(t_n) \equiv \psi_n$, when ψ depends on time
505 only, and $\psi(R_k) \equiv \psi_k$, when ψ depends on the radial coordinate only.

Table 1: Material parameters used in the implementation of the model for the reorientation of fibres in the benchmark problem. The fibres are oriented statistically. To allow for a direct comparison, the parameters were selected to closely approximate the model of Olsson and Klarbring [53]. The parameter Γ was selected equal to unity in order make the evolution speed computable.

Parameter	Value or range	Units
R_i	1.0	mm
R_o	2.0	mm
α	$\in (0, \pi/2)$	rad
β	$\in (0, 2\pi)$	rad
Φ_m	0.8	—
Φ_f	0.2	—
c_m	0.03574	MPa
c_{fi}	0.03574	MPa
c_{fb}	0.35740	MPa
λ_i	0.02000	MPa
ϖ	0.5	rad
Γ	1	$\text{N} \cdot \text{m}^{-2} \cdot \text{rad}^{-2} \cdot \text{s}$
Z_e	0	$\text{N} \cdot \text{m}^{-2} \cdot \text{rad}^{-1}$
Q_0	$\pi/4$	rad

Table 2: The algorithm used for the implementation of the remodelling constitutive model for the remodelling of the fibres in the benchmark problem, with a statistically oriented fibre distribution. The model was implemented in MATLAB[®] due to simplicity of the implementation and the flexibility with array manipulations.

GIVEN:	
Discretized radial profile $R_i \leq R_k \leq R_o, k = 0, \dots, M$	
Inner boundary pressure λ_i	
Initial value Q_0	
DO: $n = 1, \dots, N$	
Use the boundary constraint to find $K(t_n)$	Eq. (60)
Find the deformed radius for all values of R	Eq. (53)
Find the hydrostatic pressure p_n	Eq. (58)
Find the first Piola–Kirchhoff stress P_n^{rR}	
Find the first Piola–Kirchhoff stress $P_n^{\vartheta\Theta}$	
Find the next time step value of Q_{n+1}	Eq. (69)
END DO	

506 In discretized form, the system of equations (60), (53), (58), and (49d) become

$$\lambda_i(t_n) = \hat{\mathcal{J}}_{j=0}^M(K_n, Q_{j,n}, R_o), \quad (66)$$

$$\xi_{k,n} = \sqrt{R_k^2 + K_n}, \quad (67)$$

$$p_{k,n} = \left[\frac{R_k}{\xi_{k,n}} \right]^2 (S_d^{RR})_{k,n} + \lambda_i(t_n) - \hat{\mathcal{J}}_{j=0}^k(K_n, Q_{j,n}, R_k), \quad (68)$$

$$Q_{k,n+1} = Q_{k,n} + \frac{\Delta t_n}{\Gamma} \left[(Z_c)_{k,n} - \frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}_{k,n}, Q_{k,n}) \right]. \quad (69)$$

507 For a given distribution $Q_{k,n}$, the code computes the integration constant K_n , the deformed radius
508 $\xi_{k,n}$ and the radial profile of the hydrostatic pressure by solving (66), (67), and (68), respectively.
509 Determining these quantities allows to calculate the radial profiles of the stresses, $(S_d^{RR})_{k,n}$ and
510 $(S_d^{\Theta\Theta})_{k,n}$. The computed values of $\xi_{k,n}$ are then substituted into (69) in order to determine $Q_{k,n+1}$.
511 Then, the whole procedure is iterated.

512 All integrals were calculated by using the trapezoidal rule. This could be done because the
513 integral functions were separable. The deformed radius was calculated by applying a “brute-force”
514 approach to (66). Even though it would be possible to use the “brute-force” approach for deter-
515 mining K_n (rather than $\xi_{k,n}$) from (66), and compute then $\xi_{k,n}$ analytically from (67), we decided

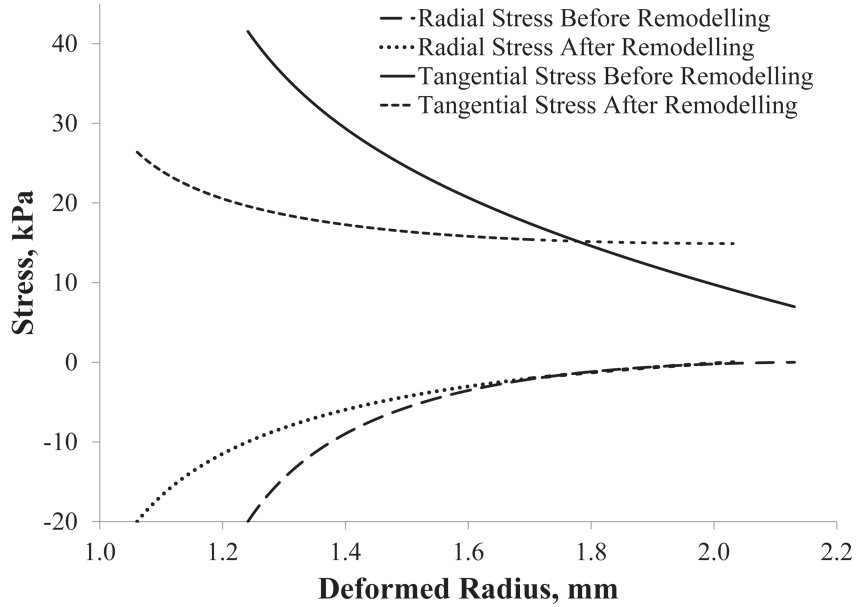


Figure 1: The first Piola–Kirchhoff stress in the radial and tangential directions for the initial loaded configuration and the remodelled configuration.

516 to implement the inverse path because it is more versatile and easy to extend to more difficult
517 cases without essential modifications to the algorithm.

518 7 Results

519 The state of stress at each radial point is an important parameter to consider when dealing with
520 remodelling of biological tissues. In the case of the benchmark problem addressed in this paper, the
521 change in both the radial and tangential stresses, before and after remodelling, is plotted versus
522 the deformed radius as depicted in Figure 1. The change in the radial stress is not significant,
523 due to the boundary conditions and the thin profile of the radial geometry. The tangential stress,
524 on the other hand, changes significantly. We observed that, due to the evolution of Q at different
525 radii, the tangential stress changes non-uniformly with respect to the radius and, in fact, becomes
526 more constant. This is in good agreement with the results of Olsson and Klarbring [53], but

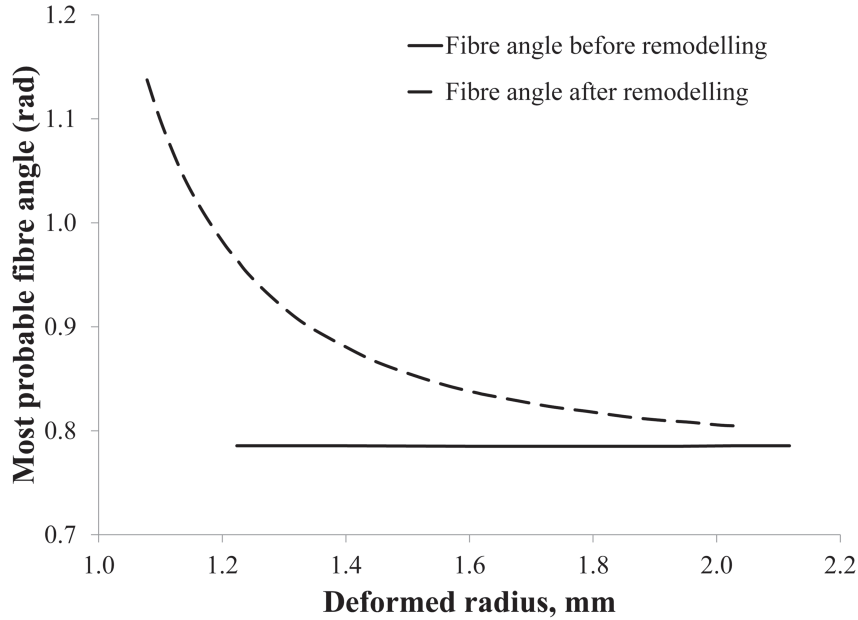


Figure 2: The fibre distribution as a function of the deformed radius, where this angle is formulated as the angle between the fibre direction vector and the axis of symmetry.

527 there are several differences. Since Olsson and Klarbring [53] modelled growth in addition to fibre
 528 remodelling, they observed a slightly different state of tangential stress after remodelling.

529 Figure 2 depicts Q as a function of the current radius before and after remodelling. Since
 530 the initial value of the most probable angle is constant, Q is homogeneous before remodelling
 531 has occurred. This feature changes when Q is observed after remodelling, since it becomes quite
 532 inhomogeneous. It can be observed that Q is maximum at the inner surface, and minimum at the
 533 outer surface of the hollow cylinder. Since the most probable fibre angle is measured from the
 534 symmetry axis, this behaviour might be explained by the fact that, in order to compensate for the
 535 higher state of stress at the inner surface, the fibres reorient in a manner that results in higher
 536 fibre engagement.

537 In order to observe the remodelling of the composite material as governed by the remodelling
 538 equation, it is important to observe how the most probable fibre angle changes over time. This is
 539 shown in Figure 3, which illustrates Q as a function of time for three different points on the radius:

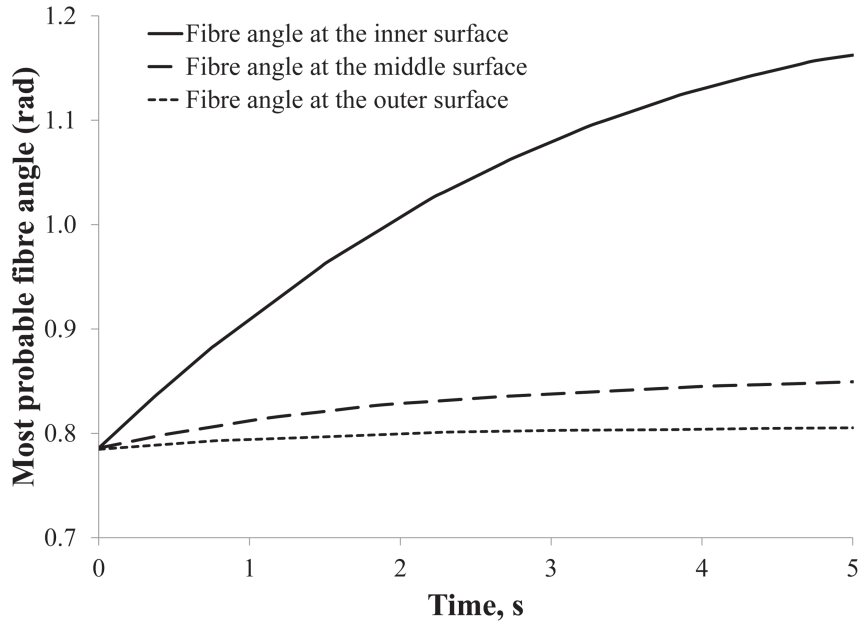


Figure 3: The evolution of the fibre angle over time for three different radii: the inner radius, the outer radius, and the middle radius.

540 at the inner surface, midway between the inner and the outer surface, and at the outer surface.

541 The initial value of Q is the same for all three points on the radius, and that angle was set
542 equal to $\pi/4$. As time progresses, the fibre angle evolves differently at each radial point. This can
543 be attributed to the different states of stress at each point, as the stress is one of the driving forces
544 of remodelling. In fact, the tangential stress is highest on the inner surface of the artery studied
545 by Olsson and Klarbring [53], and this is the point at which the mean fibre angle changes the
546 most. Thus, it could be concluded that the fibres attempt to optimise the state of stress through
547 remodelling.

548 It is also important to note that the mean fibre angle at each radial point is supposed to reach
549 a steady state value, as illustrated in Figure 3. This steady state value represents the optimal fibre
550 orientation. In Figure 3, it can be observed that Q at the inner surface reaches the steady state
551 the slowest, and this could be attributed to the magnitude of the stress at this material point. In
552 other words, the variation of the most probable fibre angle takes a longer time to reach a steady

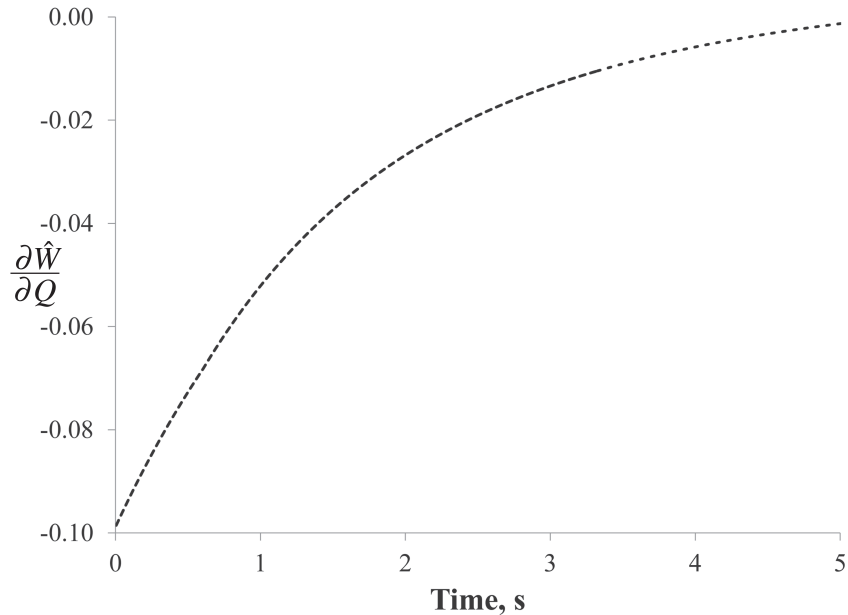


Figure 4: The evolution of the derivative $\partial \hat{W} / \partial Q$ of the strain energy potential with respect to the remodelling parameter, Q , over time.

553 state when there is a large change in the driving force behind remodelling, which is, in this case,
 554 stress.

555 8 Discussion and outlook

556 We studied the structural reorganisation of an incompressible composite material, in which the
 557 reinforcing fibres were oriented according to a Gaussian probability distribution. The variance of
 558 the Gaussian was given from the outset and assumed to be constant, whereas the angle Q was
 559 taken as the only remodelling variable of the problem. The geometry of the system was taken to
 560 be a hollow, thick-walled cylinder.

561 In addition to the standard balance of momentum, equipped with boundary conditions and
 562 the incompressibility constraint, we exploited the Principle of Virtual Powers and the Principle of
 563 Maximum Dissipation to determine an admissible constitutive expression for the dissipative force

564 that drives the reorientation of the fibres. Then, we retrieved the same type of evolution law for
 565 the remodelling variable as that found by Olsson and Klarbring [53] and solved numerically the
 566 mathematical problem, closed by the specification of the initial distribution of the remodelling
 567 variable, according to the scheme presented in equations (66)–(69) and in Table 2.

568 Beyond the choice of the remodelling variable, the treatment of the external remodelling force
 569 features a relevant difference with respect to that done by Olsson and Klarbring [53], who expressed
 570 the external remodelling force Z_e (with the notation adopted here) as

$$Z_e := \frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q_T), \quad (70)$$

571 where Q_T represents a *target angle*. Substituting (70) into (43) yields

$$\dot{Q} = \frac{1}{\Gamma} \left(\frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q_T) - \frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q) \right), \quad (71)$$

572 which means that the choice (70) of Z_e leads to a stop of fibre reorientation when Q reaches the
 573 target value Q_T . In our study, we do account for the external force Z_e in the presentation of the
 574 mathematical model, but we set it equal to zero in numerical simulations. Since this amounts to
 575 describing the case in which the interaction with the environment is either switched off or so weak
 576 that the contribution of external forces is fairly negligible, we are actually solving

$$\dot{Q} = \frac{1}{\Gamma} \left(- \frac{\partial \hat{W}}{\partial Q}(\Phi_f, \bar{\mathbf{C}}, Q) \right). \quad (72)$$

577 Still, looking at (48), which defines the right-hand-side of (72), and at its evolution over time
 578 (cf. Figure 4), we see that the force triggering structural reorganisation, i.e., $-\partial \hat{W} / \partial Q$, tends
 579 towards zero as time progresses. Thus, granted the balance of internal forces, our system naturally
 580 tends towards a stationary value of Q , which depends only on deformation and volumetric fraction
 581 of the fibres. One might argue that the result (72) is closely related to the choice of \hat{W} , whereas
 582 using an appropriate Z_e (e.g., as in (70)) supplies a criterion that, independently on the choice of
 583 \hat{W} , determines the conditions under which remodelling ceases, i.e., when Q approaches one of all

584 the physically meaningful solutions of the stationary equation $Z_e = \partial \hat{W} / \partial Q$. However, if we rely
 585 on such a criterion, we must be always able to compute a physically sound Z_e .

586 Another concern addresses the hypotheses that the dissipation function is differentiable for
 587 all Ω , and homogeneous of degree two in this variable. Although these hypotheses are usually
 588 dictated by computational simplicity, the resulting model may be too restrictive, for it leads to
 589 (42), meaning that $\hat{Y}(\Lambda, \Omega)$ vanishes with vanishing Ω , and that remodelling starts as soon as Y
 590 is different from zero. Perhaps, in some circumstances, a more realistic assumption could be to
 591 assume that remodelling starts when the dissipative force reaches a positive target value $Y_0(\Lambda)$,
 592 which plays the role of a yield “stress”. In this case, much inspiration can be taken from the theory
 593 of rate-independent plasticity [59]. By doing so, it can be shown that, if the mechanical behaviour
 594 of a material is independent on Ω , neither \hat{W} nor \hat{S}_d may depend on Ω (cf., e.g., [8]), and the
 595 force \hat{Y} depends on the sign of Ω rather than on Ω itself. To this end, the dissipation can be
 596 specified constitutively as a homogeneous function of degree one, i.e., $\hat{D}(\Lambda, \Omega) = Y_0(\Lambda)|\Omega|$ (as in
 597 perfect rate-independent plasticity), with \hat{D} being smooth in Λ , continuous for all values of Ω , but
 598 non-differentiable at $\Omega = 0$. Hence, applying (40b) in the regions of differentiability of \hat{D} leads to

$$Y = \hat{Y}(\Lambda, \text{Sign}(\Omega)) = \begin{cases} Y_0(\Lambda), & \text{if } \Omega > 0, \\ -Y_0(\Lambda), & \text{if } \Omega < 0, \end{cases} \quad (73)$$

599 and the reorientation of fibres, i.e., $\Omega \neq 0$, occurs as long as the condition

$$y(Y, \Lambda) := |Y| - Y_0(\Lambda) = 0 \quad (74)$$

600 is satisfied. Since the sign of Ω is the same as the sign of Y , one can write

$$\Omega = \kappa \frac{\partial y}{\partial Y} = \kappa \text{Sign}(Y), \quad Y \neq 0, \quad \kappa \geq 0, \quad (75)$$

601 together with the Karush-Kuhn-Tucker conditions $\kappa \geq 0$, $y(Y, \Lambda) \leq 0$, and $\kappa y(Y, \Lambda) = 0$. The
 602 multiplier κ is then determined by means of the consistency condition $\kappa \dot{y}(Y, \Lambda) = 0$. Equation (74)

603 defines a “yield”-criterion, with y being the yield-function, and $Y_0(\Lambda)$ being the target value of Y
604 that determines the onset of fibre re-orientation. If Ω is zero, the dissipation vanishes identically,
605 Y belongs to the subdifferential of \hat{D} at $\Omega = 0$, i.e., $Y \in]-Y_0(\Lambda), Y_0(\Lambda)[$ [55, 8], and $y(Y, \Lambda) < 0$.
606 Using models of fibres reorientation inspired by formal analogies with the Theory of Plasticity is
607 still part of our current investigations.

608 The main limitation of our model is that the functional form of the PDD is assumed to be
609 known from the outset. Thus, given φ at the instant of time t_0 , the structural reorganisation of the
610 material preserves the functional form of the original distribution throughout the whole remodelling
611 process. This could be too restrictive for some applications. In order to solve this problem, we are
612 currently investigating the feasibility of a model of structural reorganisation in which the PDD
613 itself plays the role of the remodelling variable, and is determined by an appropriate balance law.

614 A natural generalisation of the results presented in this paper could be achieved by studying the
615 reorientation of fibres in a growing medium, while considering the structural remodelling induced
616 by growth. The resulting framework could be extended to a constitutive description involving the
617 second gradient of deformation and/or the gradient of the tensor of inelastic distortions due to
618 growth. Such a programme requires the formulation of constitutive models featuring higher-order
619 tensors. To handle these, the tools and suggestions presented by Auffray et al. [1] and Ferretti et
620 al. [24] should be considered and perhaps adequately further developed.

621 It should be remarked that second gradient theories have been recently proposed, for example,
622 by Lekszycki and dell’Isola [41], Madeo et al. [43, 44] for different purposes. Synthesis and resorption
623 phenomena in bone reconstructed with bio-resorbable material have been investigated by Lekszycki
624 and dell’Isola [41]. The biomechanical interactions between living bone and a bio-resorbable graft
625 after reconstructive surgery have been studied by Madeo et al. [43]. Finally, Madeo et al. [44], by
626 means of Hamilton’s Principle of Stationary Action, deduced a set of equations for deformable,
627 second gradient porous media partially saturated by compressible fluids. A relevant aspect of
628 their results is that the evolution of the volumetric fractions of the fluids are neither prescribed
629 constitutively (cf., for example, [50]) nor computed by solving balance laws in the sense of [64].
630 Rather, the volumetric fractions are regarded as “Lagrangian parameters” of a suitably defined

631 Lagrangian density function and, as such, must satisfy the Euler-Lagrange equations obtained by
 632 means of Hamilton's Principle.

633 In addition to growth, a careful thermodynamic study of tissue damage should be performed.
 634 Studies in this direction have been recently done by Gasser [27] with application to abdominal
 635 aneurysms, whereas some theoretical tools have been proposed by Cuomo and Contraffatto [11]
 636 and Contraffatto and Cuomo [10] within the framework of Elastoplasticity and Damage. To tackle
 637 biomechanical problems in which a tissue is viewed as a multi-phasic mixture featuring solids
 638 and fluids, these concepts should be re-formulated in the context of Mixture Theory in order
 639 to account for solid-fluid interactions and a treatment of the related dissipative effects. To this
 640 end, it is perhaps interesting to remark that the dissipative dynamics of a system regulated by a
 641 scalar quantity (such as Q in our work) satisfying an evolution equation of the type (43) could be
 642 generalised as done by Carcaterra and Akay [7].

643 A Appendix. Fourth-order tensors

644 Let $\mathbf{a} \in (T\mathcal{E} \otimes T\mathcal{E})_S$ and $\mathbf{A} \in (T\mathcal{C} \otimes T\mathcal{C})_S$. Then, the fourth-order tensors

$$\mathbb{I} := \frac{1}{2}(\mathbf{i} \underline{\otimes} \mathbf{i} + \mathbf{i} \overline{\otimes} \mathbf{i}), \quad \mathbb{I}^{ab}_{mn} = \frac{1}{2}(\delta^a_m \delta^b_n + \delta^a_n \delta^b_m), \quad (76)$$

$$\mathbb{II} := \frac{1}{2}(\mathbf{I} \underline{\otimes} \mathbf{I} + \mathbf{I} \overline{\otimes} \mathbf{I}), \quad \mathbb{II}^{AB}_{MN} = \frac{1}{2}(\delta^A_M \delta^B_N + \delta^A_N \delta^B_M) \quad (77)$$

645 define the identities in $(T\mathcal{E} \otimes T\mathcal{E})_S$ and $(T\mathcal{C} \otimes T\mathcal{C})_S$, respectively. Indeed, it holds that $\mathbb{I} : \mathbf{a} = \mathbf{a}$,
 646 for all $\mathbf{a} \in (T\mathcal{E} \otimes T\mathcal{E})_S$ and $\mathbb{II} : \mathbf{A} = \mathbf{A}$, for all $\mathbf{A} \in (T\mathcal{C} \otimes T\mathcal{C})_S$. The notation “:” means double-
 647 contraction of indices, i.e., $[\mathbb{I} : \mathbf{a}]^{ab} = \mathbb{I}^{ab}_{mn} a^{mn}$ and $[\mathbb{II} : \mathbf{A}]^{AB} = \mathbb{II}^{AB}_{MN} A^{MN}$. The symbols $\underline{\otimes}$ and
 648 $\overline{\otimes}$ were introduced by Curnier et al. [12]. The tensors \mathbb{I} and \mathbb{II} admit the decompositions

$$\mathbb{I} = \mathbb{K} + \mathbb{M}, \quad \mathbb{K} := \frac{1}{3}(\mathbf{g}^{-1} \otimes \mathbf{g}), \quad \mathbb{M} := \mathbb{I} - \mathbb{K}, \quad (78)$$

$$\mathbb{II} = \mathbb{K} + \mathbb{M}, \quad \mathbb{K} := \frac{1}{3}(\mathbf{C}^{-1} \otimes \mathbf{C}), \quad \mathbb{M} := \mathbb{II} - \mathbb{K}. \quad (79)$$

649 Here, \mathbb{K} and \mathbb{M} extract, respectively, the volumetric and deviatoric parts of \mathbf{a} with respect to \mathbf{g} , i.e.,

$$\mathbf{a}_v = \mathbb{K} : \mathbf{a} = \frac{1}{3} \text{tr}[\mathbf{g}\mathbf{a}]\mathbf{g}^{-1}, \quad (80a)$$

$$\mathbf{a}_d = \mathbb{M} : \mathbf{a} = \mathbf{a} - \frac{1}{3} \text{tr}[\mathbf{g}\mathbf{a}]\mathbf{g}^{-1}, \quad (80b)$$

650 whereas \mathbb{K} and \mathbb{M} determine, respectively, the volumetric and deviatoric parts of \mathbf{A} with respect
651 to the *pulled-back* metric induced by \mathbf{C} (which is the pull-back of \mathbf{g}), i.e.,

$$\mathbf{A}_v = \mathbb{K} : \mathbf{A} = \frac{1}{3} \text{tr}(\mathbf{C}\mathbf{A})\mathbf{B}, \quad (81a)$$

$$\mathbf{A}_d = \mathbb{M} : \mathbf{A} = \mathbf{A} - \frac{1}{3} \text{tr}(\mathbf{C}\mathbf{A})\mathbf{B}. \quad (81b)$$

652 The tensors \mathbb{K} and \mathbb{M} are orthogonal, i.e., $\mathbb{K} : \mathbb{M} = \mathbb{M} : \mathbb{K} = \mathbb{0}$ ($\mathbb{0}$ is the zero in the space of fourth-order
653 tensors), and idempotent, i.e., $\mathbb{K} : \mathbb{K} = \mathbb{K}$ and $\mathbb{M} : \mathbb{M} = \mathbb{M}$. Analogous properties are satisfied by \mathbb{K}
654 and \mathbb{M} . The transposed tensors

$$\mathbb{I}^T := \frac{1}{2}(\mathbf{I}^T \otimes \mathbf{I}^T + \mathbf{I}^T \bar{\otimes} \mathbf{I}^T), \quad \mathbb{K}^T := \frac{1}{3} \mathbf{C} \otimes \mathbf{B}, \quad (82a)$$

$$\mathbb{M}^T := \mathbb{I}^T - \mathbb{K}^T \quad (82b)$$

655 are applied on second-order tensors of the type $\mathbf{Z} \in (T^*\mathcal{C} \otimes T^*\mathcal{C})_S$ and have properties analogous
656 to those shown above. The notations \mathbb{K} and \mathbb{M} correspond to \mathbb{K}^* and \mathbb{M}^* introduced by Federico
657 [18] in order to emphasise that these tensors are the pull-back of the spatial *true* volumetric (or
658 spherical) and deviatoric operators \mathbb{K} and \mathbb{M} , respectively (cf. (80a) and (80b)).

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