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An orthotropic active–strain model for the myocardium mechanics and its numerical approximation

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ABSTRACT

In the wide literature devoted to the cardiac structural mechanics, the strain energy proposed by Holzapfel and Ogden exhibits a number of interesting features: it has suitable mathematical properties and it is based on few material parameters that can, in principle, be identified by standard laboratory tests. In this work we illustrate the implementation of a numerical solver based on such a model for both the passive and active mechanics of the heart. Moreover we discuss its performance on a few tests that can be regarded as preliminary to the adoption of the Holzapfel–Ogden model for a real cardiac simulation.

While the passive behavior of the cardiac muscle is modeled as an orthotropic hyperelastic material, the active contraction is here accounted for a multiplicative decomposition of the deformation gradient, yielding the so-called “active strain” approach, a formulation that automatically preserves the ellipticity of the stress tensor and introduces just one extra parameter in the model.

We adopt the usual volumetric–isochoric decomposition of the stress tensor to obtain a mathematically consistent quasi–incompressible version of the material, then the numerical approximation applies to a classical Hu–Washizu three fields formulation. After introduction of the tangent problem, we select suitable finite element spaces for the representation of the physical fields. Boundary conditions are prescribed by introduction of a Lagrange multiplier.

The robustness and performance of the numerical solver are tested versus a novel benchmark test, for which an exact solution is provided. The curvature data obtained from the free contraction of muscular thin films are used to fit the active contraction parameter.

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1. Introduction

Looking at the heart from a structural point of view, the myocardium can be considered as a hyperelastic orthotropic material, mechanically characterized by two families of mutually orthogonal directions, the fibers and the sheets. In the filling phase of the cardiac cycle, its chambers deform passively because of the venous pressure difference and the suction due to the release of elastic strain energy; in systole the fibers contract, actively produce a strain of the cardiac wall that by contracting the left ventricle determine the ejection of blood through the tricuspid aortic valve.

Among the many material models proposed in the literature, the hyperelastic strain energy model proposed by Holzapfel and Ogden

(2009) to describe the mechanics of the passive myocardium is gaining an increasing popularity. Its simple invariant–based formulation and the small set of material parameters invoked makes it particularly attractive. Even more important, the material parameters of the model can, in principle, be determined on the basis of standard biaxial stress–strain tests (Göktepe et al., 2011; Wang et al., 2013a) without an *ad hoc* fitting in the specific application. While very recent papers have already addressed the use of this model to real geometry simulations (Wang et al., 2013b; Nobile et al., 2012; Rossi et al., 2012), a detailed discussion about the numerical implementation aspects and the performance of the model in test cases is still missing.

In this work we illustrate a step by step implementation of the Holzapfel–Ogden model in a finite element code, where the contractile ability of the muscle is accounted for an active strain approach. In particular, we address some issues that are sometimes overlooked in the literature: the codification of the active contraction in the model, the explicit calculation of the tangent

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problem, the efficient implementation of boundary conditions. The numerical code is then tested on a new benchmark of homogeneous (non-trivial) deformation, for which we provide a semi-explicit solution (up to an algebraic equation). The same test case where the distribution of the fibers orientation is variable in space points out the role of the fibers in dictating the cardiac rotation. The activation of the myocardium introduces, in our modeling framework, only one activation parameter and, coherently with the methodology that characterizes the passive mechanics, we fix such a parameter by an independent lab test. In particular, we fix the activation parameter γ at the value that predicts the correct bending produced by an activated monolayer of cardiomyocytes (Böl et al., 2009; Alford et al., 2010).

2. Background and notation

Given a body \mathfrak{B} that is modeled as a continuum, we consider a reference configuration χ_0 , and a generally unknown actual configuration χ as functions from \mathfrak{B} to \mathbb{R}^3 . The reference and actual placements of the body in \mathbb{R}^3 are $\Omega_0 := \chi_0(\mathfrak{B})$ and $\Omega := \chi(\mathfrak{B})$, respectively; given $p \in \mathfrak{B}$, $\mathbf{X} = \chi_0(p) \in \Omega_0$, and $\mathbf{x} = \chi(p) \in \Omega$, so that a deformation is a map:

$$\varphi = \chi \circ \chi_0^{-1}, \quad \varphi : \Omega_0 \ni \mathbf{X} \mapsto \mathbf{x} = \chi(\chi_0^{-1}(\mathbf{X})) \in \Omega.$$

We assume φ to be a diffeomorphism from Ω_0 into Ω , whose derivative is the tensor gradient of deformation:

$$F(\mathbf{X}) := \frac{\partial \varphi}{\partial \mathbf{X}}, \quad [F_{ij}] = \frac{\partial \varphi_i}{\partial X_j}, \quad i, j \in \{1, 2, 3\}.$$

Denoting by $\text{Lin}^+(\mathbb{R}^3)$ the vector space of all linear transformations from \mathbb{R}^3 to \mathbb{R}^3 with strictly positive determinant, we define the set of admissible configurations as follows:

$$\mathcal{C} = \left\{ \varphi : \Omega_0 \rightarrow \Omega \text{ such that } F(\mathbf{X}) \in \text{Lin}^+ \text{ and } \varphi|_{\partial_b \Omega_0} = \mathbf{X} + \mathbf{g} \right\}, \tag{1}$$

where \mathbf{g} is a given displacement. In what follows we further assume that $\partial_D \Omega_0$ and $\partial_N \Omega_0$ are open subsets (with respect to the induced topology) of the boundary $\partial \Omega_0$ on which essential (Dirichlet) and natural (Neumann) boundary conditions apply, respectively.

As usual, we define the left and right Cauchy–Green and Green strain tensors as follows:

$$C := F^T F, \quad B := F F^T, \quad \text{and} \quad E := \frac{1}{2}(C - I),$$

respectively.

The constitutive relationship is prescribed within the hyperelasticity framework; this means that it exists a function $\mathcal{W} : \Omega_0 \times \text{Lin}^+ \rightarrow \mathbb{R}$, called strain energy density function, which is objective, i.e.

$$\mathcal{W}(\mathbf{X}, F) = \mathcal{W}(\mathbf{X}, QF), \quad \text{for all } Q \in \text{Orth}.$$

A natural way to automatically satisfy objectivity is to prescribe a function $\widehat{\mathcal{W}} : \Omega_0 \times \text{Sym}^+ \rightarrow \mathbb{R}$ and then set $\mathcal{W}(\mathbf{X}, F) = \widehat{\mathcal{W}}(\mathbf{X}, F^T F) = \widehat{\mathcal{W}}(\mathbf{X}, C)$.

The Cauchy stress tensor is $T = (\det F)^{-1} P F^T = (\det F)^{-1} F S F^T$, where the first and the second Piola–Kirchhoff tensors, respectively P and S , are as follows

$$P := \frac{\partial \mathcal{W}}{\partial F}, \quad S := 2 \frac{\partial \widehat{\mathcal{W}}}{\partial C}. \tag{2}$$

For a hyperelastic material, the elastic equilibrium can be characterized as a minimization problem:

$$\min_{\mathbf{u} \in V} \left\{ \int_{\Omega_0} \widehat{\mathcal{W}}(\mathbf{X}, C) dV - \langle \mathbf{f}^{\text{ext}}, \mathbf{u} \rangle \right\} \tag{3}$$

where $\mathbf{u} := \varphi - \mathbf{X}$ is the displacement and \mathbf{f}^{ext} is the linear functional which encodes for the external contributions. We need some extra restriction on the deformations and the functional itself, in order to establish that at least a minimum exists. A typical choice of the function space is $V := \mathcal{C} \cap W^{1,s}(\Omega_0; \mathbb{R}^3)$, with $s > 3/2$, $1/s + 1/q < 4/3$, and q such that $\text{cof } F \in L^q(\Omega_0; \text{Lin}^+)$, while the polyconvexity of the strain energy density function is generally a basic ingredient for the well-posedness of the minimization problem (Hughes and Marsden, 1994; Antman, 2005).

3. Passive mechanics

Given a hyperelastic material with strain energy function $\widehat{\mathcal{W}}(\mathbf{X}, C)$, we suppose that, for a fixed point $\mathbf{X} \in \Omega_0$, the following local invariance property is verified:

$$\widehat{\mathcal{W}}(C) = \widehat{\mathcal{W}}(QCQ^T), \quad \text{for every } Q \in \mathcal{S} \subseteq \text{Orth}.$$

This relation means that the strain energy is the same if we change the reference configuration through the rotation Q , for any given deformation C (and so is the elastic response of the considered material). It is possible to show that \mathcal{S} is a subgroup of Orth , with respect to the usual composition law. In particular, if $\mathcal{S} \equiv \text{Orth}$, the material is *isotropic*; on the other hand, if \mathcal{S} is a proper subgroup of Orth , the material is *anisotropic*.

Given an orthonormal ternary $\{\mathbf{f}_\bullet, \mathbf{s}_\bullet, \mathbf{n}_\bullet\}$, in the reference configuration, for an *orthotropic* material the strain energy is invariant with respect to rotations around any versor of the triplet. This defines (Liu, 1982):

$$\mathcal{S}_{\text{orth}} = \left\{ Q \in \text{Orth} : Q(\mathbf{m} \otimes \mathbf{m})Q^T = \mathbf{m} \otimes \mathbf{m}, \text{ for } \mathbf{m} \in \{\mathbf{f}_\bullet, \mathbf{s}_\bullet, \mathbf{n}_\bullet\} \right\}.$$

In our specific case, \mathbf{f}_\bullet represents the local muscle fiber direction, while \mathbf{s}_\bullet lies within the sheet and is orthogonal to \mathbf{f}_\bullet . The last versor $\mathbf{n}_\bullet = \mathbf{f}_\bullet \wedge \mathbf{s}_\bullet$ is the normal of the local sheet.

If a function $\widehat{\mathcal{W}}(C)$, with $C \in \text{Sym}^+$, is invariant with respect to $\mathcal{S}_{\text{orth}}$, then there exists a representation $\widehat{\mathcal{W}}_{\text{orth}}$ such that:

$$\widehat{\mathcal{W}}(C) = \widehat{\mathcal{W}}_{\text{orth}}(C, \mathbf{f}_\bullet \otimes \mathbf{f}_\bullet, \mathbf{s}_\bullet \otimes \mathbf{s}_\bullet, \mathbf{n}_\bullet \otimes \mathbf{n}_\bullet),$$

for every $C \in \text{Sym}^+$ and with $\widehat{\mathcal{W}}_{\text{orth}}$ isotropic with respect to its arguments. As a matter of fact, the dependency on $\mathbf{n}_\bullet \otimes \mathbf{n}_\bullet$ is redundant, because:

$$\mathbf{f}_\bullet \otimes \mathbf{f}_\bullet + \mathbf{s}_\bullet \otimes \mathbf{s}_\bullet + \mathbf{n}_\bullet \otimes \mathbf{n}_\bullet = I.$$

The function $\widehat{\mathcal{W}}_{\text{orth}}$ can be further specified by accounting for the isotropy requirement with respect to its tensor arguments. The Cayley–Hamilton theorem and the following observation:

$$(\mathbf{a} \otimes \mathbf{b})^k = (\mathbf{a} \cdot \mathbf{b})^{k-1} \mathbf{a} \otimes \mathbf{b}, \quad \text{with } k > 0,$$

restrict the number of possible combinations. Observing that \mathbf{n}_\bullet is redundant and \mathbf{f}_\bullet and \mathbf{s}_\bullet are mutually orthogonal, we have that the invariant set for an orthotropic material is defined as follows:

$$Y_{\text{orth}} = \left\{ \text{tr} C, \text{tr} C^2, \text{tr} C^3, \mathbf{f}_\bullet \cdot C \mathbf{f}_\bullet, \mathbf{s}_\bullet \cdot C \mathbf{s}_\bullet, \mathbf{f}_\bullet \cdot C^2 \mathbf{f}_\bullet, \mathbf{s}_\bullet \cdot C^2 \mathbf{s}_\bullet \right\}. \tag{4}$$

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