*MAT_295 - Constitutive models

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September 18, 2020

A brief, self-contained theoretical background of *MAT_ANISOTROPIC_HYPERELASTIC, a class of *(an)isotropic, (nearly-in)compressible hyperelastic* material models primarily aimed at describing the mechanical behavior of biological soft tissues is introduced in the present document. The constitutive laws introduced therein are implemented in a modular fashion. Each module may comprise of different models. Consequently, the analyst may easily change models in a module and include additional modules to account for more complex material behavior within the same keyword. A couple of things are worth noting at this point. Firstly, extending an existing module with a new model or even including a new module does not require the developer to add a new material keyword. Secondly, some of the material models may also be used to model a wider class of materials including e.g., fiber-reinforced elastomers or stretchable fabrics.

The remaining part of this document is organized as follows. Relevant concepts of continuum mechanics is summarized in section 1. Hyperelastic (passive) models are outlined in section 2. Electromechanical or active models are discussed in section 3.

1 Fundamentals of nonlinear elasticity

1.1 Kinematics

Let us consider a continuum body $\mathcal{B}$ which is embedded in the three-dimesnional Euclidean space at any given instant of time t. As the continuum body $\mathcal{B}$ moves in space from one instant of a time to another, it occupies a continuous sequence of geometrical regions also known as configurations. The geometric region occupied by the body $\mathcal{B}$ at any fixed reference time $t = t_r$ is known as the *reference configuration* $\mathcal{C}_r$. Similarly, a region at time $t = 0$ is called the *initial configuration* and designated by $\mathcal{C}_0$. In what follows, we assume that the inital and reference configurations coincide, i.e. $\mathcal{C}_0 \equiv \mathcal{C}_r$, and refer to an arbitrary configuration $\mathcal{C} = \mathcal{C}_t$ at $t > 0$ as *current configuration*. Also, let the symbols $\boldsymbol{X}$ and $\boldsymbol{x}$ denote a material point in the reference and current configurations,

respctively.
The *motion* or time-dependent deformation is defined as

$$\boldsymbol{x} = \chi(\boldsymbol{X}, t), \tag{1}$$

where χ is the function describing the motion. The function is invertible at each time instance and assumed to satisfies appropiate regularity conditions. The *deformation gradient* is given by

$$\boldsymbol{F} = \mathrm{Grad}(\boldsymbol{x}) \tag{2}$$

and has components $F_{iJ} = \partial x_i / \partial X_J$, where Grad is the reference gradient operator and the indices $i, J \in \{1, 2, 3\}$. Local invertibility of the deformation requires that the deformation gradient be non-singular, i.e.

$$J := \det(\boldsymbol{F}) > 0. \tag{3}$$

By virtue of the *polar decomposition* theorem, the deformation gradient can be written as

$$\boldsymbol{F} = \boldsymbol{R}\boldsymbol{U} = \boldsymbol{v}\boldsymbol{R}, \tag{4}$$

where $\boldsymbol{R}$ is a proper orthogonal tensor representing a rotation, and $\boldsymbol{U}$ and $\boldsymbol{v}$ are *right* and *left stretch tensors*, both symmetric and positive definite, respectively. The *right* and *left deformation tensors* are introduced as

$$\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F} \equiv \boldsymbol{U}^2, \tag{5}$$

$$\boldsymbol{b} = \boldsymbol{F}\boldsymbol{F}^T \equiv \boldsymbol{v}^2. \tag{6}$$

Furthermore, the following *spectral representations* are recalled

$$\boldsymbol{F} = \sum_{i=1}^{3} \lambda_i \boldsymbol{\phi}_i \otimes \boldsymbol{\Phi}_i, \tag{7}$$

$$\boldsymbol{R} = \sum_{i=1}^{3} \boldsymbol{\phi}_i \otimes \boldsymbol{\Phi}_i, \tag{8}$$

$$\boldsymbol{U} = \sum_{i=1}^{3} \lambda_i \boldsymbol{\Phi}_i \otimes \boldsymbol{\Phi}_i, \tag{9}$$

$$\boldsymbol{v} = \sum_{i=1}^{3} \lambda_i \boldsymbol{\phi}_i \otimes \boldsymbol{\phi}_i, \tag{10}$$

$$\boldsymbol{C} = \sum_{i=1}^{3} \lambda_i^2 \boldsymbol{\Phi}_i \otimes \boldsymbol{\Phi}_i, \tag{11}$$

$$\boldsymbol{b} = \sum_{i=1}^{3} \lambda_i^2 \boldsymbol{\phi}_i \otimes \boldsymbol{\phi}_i, \tag{12}$$

where $\lambda_i > 0$, with $i \in \{1, 2, 3\}$, are the *principal stretches*, while $\boldsymbol{\Phi}_i$ and $\boldsymbol{\phi}_i$ designate the eignevectors of $\boldsymbol{U}$ and $\boldsymbol{v}$ and are also known as the *reference* and *current principal axes*, respectively.

Finally, the Green-Lagrange and Green-Almansi strain tensors are defined as

$$\boldsymbol{E} = \frac{1}{2}\left(\boldsymbol{C} - \boldsymbol{I}\right), \tag{13}$$

$$\boldsymbol{e} = \frac{1}{2}\left(\boldsymbol{I} - \boldsymbol{b}^{-1}\right). \tag{14}$$

1.2 Multiplicative decomposition

The *multiplicative decomposition* of the deformation gradient can be written as

$$\boldsymbol{F} = (J^{1/3}\boldsymbol{I})\bar{\boldsymbol{F}}, \tag{15}$$

where $J^{1/3}\boldsymbol{I}$ is the *dilatational, spherical, or volumetric* part and $\bar{\boldsymbol{F}}$ is the *unimodular, distortional, or isochoric* part of the deformation gradient. Consequently,

$$\bar{\boldsymbol{b}} = J^{-2/3}\boldsymbol{b}, \tag{16}$$

$$\bar{\lambda}_i = J^{-1/3}\lambda_i. \tag{17}$$

2 Hyperelasticity

In the theory of *hyperelasticity*, the existence of a *Helmholtz free-energy* or *strain-energy function* (per unit reference volume) $\Psi := \Psi(\boldsymbol{F}, \boldsymbol{X})$, with $\boldsymbol{X}$ denoting a reference material point, is postulated in order to characterize the properties of an elastic material. The dependence of Ψ on $\boldsymbol{X}$ indicates the spatial dependence on the material properties in an *inhomogeneous material*. For notational brevity, this dependence is omitted henceforth.

The strain-energy function may be written as combination of different strain-energy functions which is commonly referred to as *additive decomposition*. Noting that directional dependent behavior is introduced by a set of collagen fiber families, i.e. n_f with $n_f \geq 1$, ubiquitous in different soft tissues, the general form may be written as

$$\Psi(\boldsymbol{F}) = \Psi_I(\boldsymbol{F}) + \Psi_A(\boldsymbol{F}, \boldsymbol{A}_i), \tag{18}$$

where the subscripts I and A distinguish the isotropic and anisotropic parts, respectively. The symbol $\boldsymbol{A}_i$, with $i \in [1, n_f]$, in equation (18) designates the *unit mean reference direction* of the ith fiber family embedded in the isotopic ground matrix. A couple of things are worth highlighting at this point. Firstly, the pure volumetric part of the strain energy function is included in Ψ_I. Secondly, the term anisotropic is meant in the general sense and Ψ_A also includes transversely isotropic and orthotropic models as special cases.

2.1 Invariants

Hyperelastic constitutive laws, cf. section 2, are often formulated in terms of invariants, i.e. Isotropic models may be defined using the principal invariants of the deformation tensors, i.e. $\Psi_I\left(I_1, I_2, I_3\right)$, given as

$$I_1 := \mathrm{tr}(\boldsymbol{b}) = \sum_{i=1}^{3} \lambda_i^2, \tag{19}$$

$$I_2 := \frac{1}{2}\left[\mathrm{tr}(\boldsymbol{b})^2 + \mathrm{tr}(\boldsymbol{b}^2)\right] = \frac{1}{2}\sum_{\substack{i,j=1 \\ i\neq j}}^{3} \lambda_i^2\lambda_j^2, \tag{20}$$

$$I_3 := \det(\boldsymbol{b}) = J^2 = \prod_{i=1}^{3} \lambda_i^2, \tag{21}$$

and noting that $I_i(\boldsymbol{b}) = I_i(\boldsymbol{C})$ with $i = 1, 2, 3$.
Considering transverse isotropy ($n_f = 1$), $\Psi_A := \Psi_A\left(I_4, I_5\right)$ with invariants

$$I_4\left(\boldsymbol{C}, \boldsymbol{A}\right) = \boldsymbol{A}\cdot\boldsymbol{C}\boldsymbol{A} = \boldsymbol{a}\cdot\boldsymbol{a} = \lambda^2, \tag{22}$$

$$I_5\left(\boldsymbol{C}, \boldsymbol{A}\right) = \boldsymbol{A}\cdot\boldsymbol{C}^2\boldsymbol{A}, \tag{23}$$

where $\boldsymbol{a}$ is the *current mean fiber direction vector*, such that $\boldsymbol{a} = \boldsymbol{F}\boldsymbol{A}$ with $\|\boldsymbol{a}\| \neq 1$ in general, λ is the fiber stretch, and the symbol $(\cdot)$ denotes the generalized inner product henceforth.

Coupling invariants associated with pairs of characteristic material directions may be further invoked to enhance the material model. Consequently, the general form of the strain-energy function may be written as $\Psi_A := \Psi_A\left(I_{4i}, I_{5i}, I_{ij}\right)$, where I_{4i} and I_{5i} are defined for the ith fiber family in equations (22) and (23), and the newly introduced coupling invariants are given as

$$I_{ij}\left(\boldsymbol{C}, \boldsymbol{A}_i, \boldsymbol{A}_j\right) = \boldsymbol{A}_i\cdot\boldsymbol{C}\boldsymbol{A}_j = \boldsymbol{a}_i\cdot\boldsymbol{a}_j \quad \text{with} \quad i, j \in [1, n] \quad \text{and} \quad i \neq j. \tag{24}$$

Notably, the coupling invariants are pseudo- or quasi-invariants in the sense that their value depend on the sense of vectors $\boldsymbol{a}_i$. Also, soft-tissue models are typically characterized by n_f (dispersed) fiber families within a plane. In this case, $n = n_f + 1$ and $\boldsymbol{a}_n$ becomes the normal vector in equation (24), i.e. $\boldsymbol{a}_k\cdot\boldsymbol{a}_n = \delta_{kn}$, with $k = 1, \ldots, n_f$.

The following relations can be established by virtue of the multiplicative decomposition, see equation (15), i.e.

$$\bar{I}_{\mathcal{I}} = J^{-2/3} I_{\mathcal{I}} \quad \text{with} \quad \mathcal{I} = \{1, 4i, ij\}, \tag{25}$$

$$\bar{I}_{\mathcal{J}} = J^{-4/3} I_{\mathcal{J}} \quad \text{with} \quad \mathcal{J} = \{2, 5i\}. \tag{26}$$

2.2 Isotropic hyperelastcicty

Isotropic constitutive laws are defined in the `ISO` module which also includes the definition of a purely *volumetric part of the strain energy function* [8] defined as

$$\Psi_V(J) = \begin{cases} \dfrac{c_v}{\beta^2}\left[\beta \ln(J) + \dfrac{1}{J^\beta} - 1\right] & \text{if } \beta \neq 0 \\ \\ \dfrac{c_v}{2}\left(J-1\right)^2 & \text{if } \beta = 0, \end{cases} \tag{27}$$

where c_v is a material parameter and β is the volumetric response function coefficient. Considering compressible models, cf. 2.2.1, the parameter c_v represents the bulk modulus, i.e. $c_v \leftarrow \kappa$. In case of nearly-incompressible models, cf. 2.2.2, the parameter can be thought of as a penalty factor enforcing the incompressibility constraint, i.e. $J = 1$, in an approximate sense.

2.2.1 Compressible isotropic models

The *compressible Ogden model* (`ITYPE=1`) is formulated as

$$\Psi_I(\lambda_i) = \sum_{m=1}^{M} \frac{\mu_m}{\alpha_m}\left(\lambda_1^{\alpha_m} + \lambda_2^{\alpha_m} + \lambda_3^{\alpha_m} - 3 - \alpha_m \ln J\right) + \Psi_V(J), \tag{28}$$

where μ_m and α_m are material parameters.

Remarks:

(1) The *compressible neo-Hookean model* is obtained as a special case, i.e. $M = 1$ and $\alpha_1 = 2$.

(2) In the limit of infinitesimal deformations, the model is consistent with the linear theory of elasticity, i.e. Hooke's law is recovered with Lamé coefficients $\lambda \equiv c_v$ and $\mu \equiv \dfrac{1}{2}\sum_{m=1}^{M} \mu_m \alpha_m$.

The *compressible Holzapfel-Ogden model* (`ITYPE=3`) is given as

$$\Psi_I(I_1, J) = \frac{k_1}{2k_2}\left[e^{k_2(I_1-3)} - 1\right] - \frac{k_1}{2}\ln J + \Psi_V(J), \tag{29}$$

where k_1 and k_2 are material parameters.

2.2.2 Nearly-incompressible isotropic models

The constrained or *nearly-incompressible Ogden model* (`ITYPE=-1`) is written as

$$\Psi_I(\bar{\lambda}_i, J) = \sum_{i=1}^{3}\sum_{m=1}^{M} \frac{\mu_m}{\alpha_m}\left(\bar{\lambda}_i^{\alpha_m} - 1\right) + \Psi_V(J), \tag{30}$$

where μ_m and α_m are material parameters.

Remarks:

(1) The *nearly-incompressible neo-Hookean* and the *Mooney-Rivlin models* are obtained as a special cases, with $M = 1$, $\alpha_1 = 2$ and $M = 2$, $\alpha_1 = 2$, $\alpha_2 = -2$, respectively.

(2) By setting $\beta = -1$ in equation (27), *MAT_295 yields an identical formulation with *MAT_077_O.

The *nearly-incompressible Yeoh model* (ITYPE=-2) can be written as

$$\Psi_I(\bar{I}_1, J) = c_1 \left(\bar{I}_1 - 3\right) + c_2 \left(\bar{I}_1 - 3\right)^2 + c_3 \left(\bar{I}_1 - 3\right)^3 + \Psi_V(J), \tag{31}$$

where c_i, with $i = 1, 2, 3$, are material parameters satisfying the following conditions: $c_1 > 0$, $c_2 < 0$, and $c_3 > 0$.
The *nearly-incompressible Holzapfel-Ogden model* (ITYPE=-3) takes the following form

$$\Psi_I(\bar{I}_1, J) = \frac{k_1}{2k_2} \left[e^{k_2\left(\bar{I}_1 - 3\right)} - 1\right] + \Psi_V(J), \tag{32}$$

where k_1 and k_2 are material parameters.

2.3 Ansotropic hyperelasticity

2.3.1 Generalized structure tensor

Anisotropy is introduced by collagen fibers embedded within the isotropic ground matrix of soft tissues, e.g. arterial walls, skin, and skeletal muscle. Experimental studies of their micro-structure suggest that the embedded fibers are highly dispersed or, in other words, follow a spatially varying distribution. To this end, accounting for fiber dispersion in the constitutive model is recommended if not imperative.

Generally, there are two methods to incorporate fiber dispersion in continuum constitutive laws, namely the angular integration (AI) [17] and the *generalized structure tensor* (GST) based approaches [5, 10]. It has recently been shown that the two methods yield virtually the same results [12]; however, in view of numerical implementation, accuracy, and efficacy, the latter formulation is more attractive and as a consequence also implemented in LS-DYNA.

The *reference structure tensor* allows us to account for a rotationally non-symmetric fiber dispersion along an arbitrary mean reference fiber direction [10] and is formulated as

$$\boldsymbol{H} = A\boldsymbol{I} + B\boldsymbol{A} \otimes \boldsymbol{A} + C\boldsymbol{N} \otimes \boldsymbol{N}, \tag{33}$$

where the symbols A, B, and $C = 1 - dA - B$, with $d = 2, 3$ denoting the problem dimension, are parameters obtained from experimental data assuming a probability density function that best describes the fiber dispersion. The symbols $\boldsymbol{I}$, $\boldsymbol{A}$, and $\boldsymbol{N}$

designate the second order identity tensor, a unit reference mean fiber direction, and the corresponding unit reference normal, respectively. It is worth noting that equation (33) includes several special cases of fiber dispersion which are summarized in Table 1.

Dispersion	A	B	$\boldsymbol{H}$
no	0	1	$\boldsymbol{A}\otimes\boldsymbol{A}$
isotropic	1/3	0	$1/3\boldsymbol{I}$
transversely isotropic	A	1-3A	$A\boldsymbol{I}+(1-3A)\boldsymbol{A}\otimes\boldsymbol{A}$
planar isotropic	1/2	0	$1/2\boldsymbol{I}$
planar	A	1-2A	$A\boldsymbol{I}+(1-2A)\boldsymbol{A}\otimes\boldsymbol{A}$

Table 1: Special cases of the dispersion model

2.3.2 Anisotropic models

Anisotropic constitutive laws are defined in the `ANISO` module. Currently, one may invoke either a Holzapfel-Ogden model or the frame-invariant Fung formulation. While the former model allows us to exploit the full potential of the generalized structure tensor, the latter formulation relies on its simplified form.

Similarly to the convention invoked in the `ISO` module, the sign of the anisotropic model type, i.e. `ATYPE`, is used to distinguish between nearly-incompressible and compressible formulations. In what follows, the compressible models are shown noting that their nearly-incompressible counterparts are easily obtained by virtue of the multiplicative decomposition, see section 1.2.

The general form of the *Holzapfel-Ogden model* (`ATYPE=`$\pm$`1`) [11] may be written as

$$\Psi_A\left(\boldsymbol{F},\boldsymbol{H}_i,\boldsymbol{H}_{ij}\right)=\sum_{i=1}^{n_f}\Psi_{Fi}\left(\boldsymbol{F},\boldsymbol{H}_i\right)+\sum_{\substack{i,j=1\\ i<j}}^{n}\Psi_{Cij}\left(\boldsymbol{F},\boldsymbol{H}_{ij}\right), \tag{34}$$

where Ψ_{Fi} is the fiber model associated with the ith fiber family, Ψ_{Cij} is the coupling or interaction model between the ith and jth characteristic material directions with the corresponding reference structure tensor defined as

$$\boldsymbol{H}_{ij}=\frac{1}{2}\left(\boldsymbol{A}_i\otimes\boldsymbol{A}_j+\boldsymbol{A}_j\otimes\boldsymbol{A}_i\right). \tag{35}$$

A distinct fiber model may be chosen for each embedded fiber family $i\in[1,n_f]$. The available fiber models include the Holzapfel-Gasser-Ogden and the Freed-Doehring models. The phenomenological *Holzapfel-Gasser-Ogden model* (`FTYPE=1`) [9] for the ith fiber family is given as

$$\Psi_{Fi}\left(\boldsymbol{F},\boldsymbol{H}_i\right)=\chi_i\frac{k_{1i}}{2k_{2i}}\left[e^{k_{2i}E_i^2}-1\right], \tag{36}$$

where k_{1i} is the fiber modulus, k_{2i} is a dimensionless coefficient, and the $E_i=\mathrm{tr}\left(\boldsymbol{h}_i\right)-1$ is Green-Lagrange strain-like quantity defined in terms of the spatial structure tensor

$\boldsymbol{h}_i = \boldsymbol{F}\boldsymbol{H}\boldsymbol{F}^T$. The symbol χ_i in equation (36) designates the tension-compression switch, i.e.

$$\chi_i = \begin{cases} 1 & \text{if } \lambda_i > 1, \\ 0 & \text{otherwise.} \end{cases} \tag{37}$$

The structural *Freed-Doehring model* (`FTYPE=2`) [3] is more complex and therefore will be omitted here. The reader is advised to consult the original publication for more details.

Optionally, one may consider to add the simplified *Holzapfel-Ogden* model (`INTYPE=1`) [9, 2] where a single coupling invariant is introduced between the orthogonal characteristic material directions identifying the fiber and sheet orientations, respectively, i.e.

$$\Psi_{C12}\left(\boldsymbol{F}, \boldsymbol{H}_{12}\right) = \frac{k_1}{2k_2}\left[e^{k_2 I_{12}^2} - 1\right], \tag{38}$$

where k_1 and k_2 is the fiber interaction modulus and a dimensionless coefficient, respectively.

Remarks:

(1) The sign of `ATYPE` also influences the sign of `FTYPE` and `INTYPE` used in the Holzapfel-Ogden models. Consequently, a negative `ATYPE` indicates a pure isochoric formulation such that $\Psi_A\left(\boldsymbol{F}, \boldsymbol{H}_i, \boldsymbol{H}_{ij}\right) \leftarrow \Psi_A\left(\bar{\boldsymbol{F}}, \bar{\boldsymbol{H}}_i, \bar{\boldsymbol{H}}_{ij}\right)$ where by virtue of the multiplicative decomposition, see equation (15),

$$\bar{\boldsymbol{H}}_{\mathcal{K}} = J^{-2/3}\boldsymbol{H}_{\mathcal{K}} \quad \text{with} \quad \mathcal{K} = \{i, ij\}. \tag{39}$$

(3) The type of isotropic and anisotropic models, i.e. `ITYPE` and `ATYPE`, may be controlled separately which enables the use of hybrid formulations, e.g. Nolan *et al.* [19].

(3) There has been a lot of confusion about the tension-compression switch of the fiber model, see equation (37), in the literature [13]. Therefore it is worth noting that the ith fiber model is only activated if $\lambda_i > 1$ and not $\bar{\lambda}_i > 1$, see equation (17), for nearly-incompressible models.

(4) The model proposed by Freed *et al.* [4] is a special case of the general structure tensor-based formulation presented in section 2.3. In there rotational symmetric fiber dispersion is assumed and parameters A_i and B_i $\forall i$ were determined using a normal distribution.

3 Electromechanical models

Electromechanical models describe the contraction of myofibrils within a myofiber (muscle cell) after a wave of electrical activation potential propagates through the myocardium [16]. Contraction of the muscle, in its essence, is regulated by the concentration of calcium ions (Ca^{2+}) within the muscle cell.

3.1 Active models

Active models are defined in the `ACTIVE` module. Active models describe the relationship between the evolution of cytosolic calcium ion concentration and tension developed in the tissue, i.e. the conversion of chemical to mechanical energy.

The *active Kirchhoff stress tensor* is given as

$$\boldsymbol{\tau}_{(A)} = \sum_{i \in \mathcal{A}} \tau \left[\bar{\boldsymbol{a}} \otimes \bar{\boldsymbol{a}} + f \left(\bar{\boldsymbol{t}} \otimes \bar{\boldsymbol{t}} + \bar{\boldsymbol{n}} \otimes \bar{\boldsymbol{n}} \right) \right], \tag{40}$$

where τ is the active fiber stress, $\bar{\boldsymbol{a}}$ is the *unit current mean fiber direction*, i.e. $\bar{\boldsymbol{a}} = \boldsymbol{a}/\|\boldsymbol{a}\|$, $f \in [-1, 1]$ is a scaling factor, $\bar{\boldsymbol{n}}$ is the *unit current normal*, i.e. $\bar{\boldsymbol{n}} = \boldsymbol{n}/\|\boldsymbol{n}\|$ with $\boldsymbol{n} = \boldsymbol{F}\boldsymbol{N}$, and $\bar{\boldsymbol{t}} = \bar{\boldsymbol{n}} \times \bar{\boldsymbol{a}}$ such that $\{\bar{\boldsymbol{a}}, \bar{\boldsymbol{t}}, \bar{\boldsymbol{n}}\}$ forms an orthonormal basis. The symbol $\mathcal{A}$ denotes the index set of fiber families along which active stresses are developed. Active stresses are currently limited to developed either along (and if $f \neq 0$ transverse to) all (`ACDIR` $= 0$) or a predefined mean fiber family direction (`ACDIR` $= i$, with $i \in [1, n_f]$). Furthermore, the stresses are assumed be additive, i.e.

$$\boldsymbol{\tau} := \boldsymbol{\tau}_{(P)} + \boldsymbol{\tau}_{(A)}, \tag{41}$$

where $\boldsymbol{\tau}_{(P)}$ designates the passive stresses which can be derived from the strain energy functions discussed in section 2, see e.g. [8] or [20] for more details, and $\boldsymbol{\tau}_{(A)}$ represents the active stresses as defined in equation (40).

The *modified Hill equation* governing chemical equilibrium is customarily used to compute the active fiber stress, i.e.

$$\tau = c \frac{\left[\mathrm{Ca}^{2+}\right]^n}{\left[\mathrm{Ca}^{2+}\right]^n + \left[\mathrm{Ca}^{2+}_{50}\right]^n} \tau_{max} \tag{42}$$

where τ is the active fiber stress, c is an internal variable, $\left[\mathrm{Ca}^{2+}\right]$ designates the cytosolic calcium concentration, $\left[\mathrm{Ca}^{2+}_{50}\right]$ is the calcium concentration at $\tau = \tau_{max}/2$ often referred to as calcium sensitivity, n denotes the Hill coefficient, and τ_{max} is the maximum isometric tension achieved at the longest sarcomere length and maximum peak intracellular calcium concentration $\left[\mathrm{Ca}^{2+}_{max}\right]$. Dependent on the choice of the internal variable c and calcium concentration $\left[\mathrm{Ca}^{2+}_{50}\right]$, one may distinguish different active phenomenological models.

The *Guccione-Waldman-McCulloch model* (`ACTYPE=1`) [7] accounts for the change in the activation curve due to initial sarcomere length, i.e.

$$\left[\mathrm{Ca}^{2+}_{50}\right] \left[\lambda\left(t\right)\right] = \frac{\left[\mathrm{Ca}^{2+}_{max}\right]}{\left[e^{b(\lambda L - l_0)} - 1\right]^{1/2}}, \tag{43}$$

where b is a shape coefficient, λ desinates the fiber stretch, L is the reference or stress free sarcomere length, and $l_0 > L$ is the sarcomere length at which no active tension

develops. Notice the current sarcomere length, i.e. $l(t) = \lambda(t)L$, in the denominator of equation (43). The internal variable is defines as

$$c\left[\lambda\left(t\right), t\right] = \frac{1 - \cos\left(\omega\right)}{2} \tag{44}$$

with

$$\omega = \begin{cases} \pi \dfrac{t - t_0}{dt_{max}} & \text{if} \quad t_0 \leq t < t_0 + dt_{max} \\ \pi \dfrac{t - (t_0 + dt_{max}) + dt_r}{dt_r} & \text{if} \quad t_0 + dt_{max} \leq t < t_0 + dt_{max} + dt_r \\ 0 & \text{if} \quad t < t_0 \quad \text{and} \quad t_0 + dt_{max} + dt_r \leq t, \end{cases} \tag{45}$$

where t_0 is the time at which active stress development begins, while dt_{max} and dt_r designate the time duration to reach peak tension and relaxation, respectively. The relaxation duration is assumed to take the following linear form

$$dt_r\left[l\left(t\right)\right] = m_r l + t_r, \tag{46}$$

where m_r and t_r denote the slope and time intercept of the relaxation duration-sarcomere length relation.

According to the *Hunter-Nash-Sands model* (`ACTYPE=3`) [15], the calcium sensitivity $\left[\mathrm{Ca}_{50}^{2+}\right]$ is assumed to be constant, i.e. independent of the sarcomere length, in equation (42) and the internal variable is defined as

$$c\left[L, \lambda\left(t\right)\right] = 1 + \eta L\left(\lambda - 1\right), \tag{47}$$

where η is a material parameter. Combining equations (43) and (47) in equation (42) yields the *Guccione-Waldman-McCulloch/Hunter-Nash-Sands model* (`ACTYPE=2`).

The *Hunter-Nash-Sands/Hunter-McCulloch-ter Keurs model* (`ACTYPE=4`) [15, 14], the calcium sensitivity $\left[\mathrm{Ca}_{50}^{2+}\right]$ is constant, the internal variable is defines as in equation (47), and the the evolution of intracellular calcium ion concentration is closely approximated by

$$\left[\mathrm{Ca}^{2+}\right]\left(t\right) = \left[\mathrm{Ca}_0^{2+}\right] + \left(\left[\mathrm{Ca}_{max}^{2+}\right] - \left[\mathrm{Ca}_0^{2+}\right]\right) \frac{t - t_0}{t_{\mathrm{Ca}}} e^{\left[1 - (t - t_0)/t_{\mathrm{Ca}}\right]}, \tag{48}$$

where t_0 and t_{Ca} is the local activation time and a shape parameter, respectively. Note that $t_0 \leq t$ and therefore $t - t_0 = 0$ if $t < t_0$ from the numerical perspective.

Remarks:

(1) Considering implicit dynamics, the active part of the elasticity tensor is formulated in a consistent fashion for all active models except the Guccione-Waldman-McCulloch model (`ACTYPE=1`) where a modified formulation, assuming $\partial\tau/\partial I_4 = 0$, is invoked for increased computational performance.

3.2 Electromechanical coupling

All active models listed in section 3.1 can be used to couple electrophysiology and solid mechanics and ultimately to perform electrophysiology-fluid-structure interaction (EFSI). The coupling between electrophysiology and solid mechanics or fluid-structure interaction (FSI) is currently unidirectional in the sense that material conductivity is independent of the current metric tensor. The mechanical response or it's onset is triggered by either the calcium ion concentration (`ACTYPE=1-3`) or the associated transmembrane potential (`ACTYPE=4`).

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