# ON THE MODELING OF ACTIVE DEFORMATION IN BIOLOGICAL TRANSVERSELY ISOTROPIC MATERIALS

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Abstract. Many biological materials exhibit the ability to actively deform, essentially due to a complex chemical interaction involving two proteins, actin and myosin, in the myocytes (the muscle cells). While the mathematical description of passive materials is well-established, even for large deformations, this is not the case for active materials, since capturing its complexities poses significant challenges.

This paper focuses on the mathematical modeling of active deformation of biological materials, guided by the important example of skeletal muscle tissue. We will consider an incompressible and transversely isotropic material within a hyperelastic framework. Our goal is to design constitutive relations that agree with uniaxial experimental data whenever possible. Finally, we propose a novel model based on a coercive and polyconvex elastic energy density for a fiber-reinforced material; in this model, active deformation occurs solely through a change in the reference configuration of the fibers, following the mixture active strain approach. This model assumes a constant active parameter, preserving the good mathematical features of the original model while still capturing the essential deformations observed in experiments.

## 1. Introduction

The ability to *actively deform* is one of the key features of most biological materials, first of all muscle tissue [31]. The cardiac cycle, peristalsis, brain activity, lymphatic pumping, and voluntary muscle contractions are all phenomena that result from an interplay between some chemo/electrophysiological reactions and a modification of the mechanical properties of the material, leading to movement or force generation.

The mathematical description of a passive material is a well-established field, thanks to the powerful tools of Continuum Mechanics developed over the last two centuries, which have contributed to the advancements in Civil Engineering [4]. The main innovation in this field lies in the ability of biological materials to undergo large deformations, requiring the use of Nonlinear Elasticity. In Section 3 we describe the passive behavior of the muscle through a hyperelastic energy, which is a function of a the invariants of the deformation gradients. This strategy is customary in literature [4, 7]. After reviewing the main properties, we propose two examples of passive energy which are polyconvex and coercive. More precisely, the first energy is particularly popular in the literature for modeling skeletal muscle behavior [10, 8, 11, 13, 15], while the second one is a new energy proposal for fiber-reinforced materials. The material parameters of these two energies are chosen in such a way that the stress capture the experimental trend reported in [23].

Conversely, a mathematical description of active deformation is more challenging, because the mechanics can vary significantly between materials and is closely linked to their microscopic properties [6]. For example, muscle contraction involves a cyclic interaction between actin and myosin proteins, sustained by ATP supply [9, Ch. 6]. Since the process produces macroscopic effects, it is important to develop simpler and stable mathematical models at the macroscale that can be readily implemented in standard numerical computing applications.

A crucial aspect is establishing a connection between the mathematical features of the passive and active material. Ideally, within a hyperelastic setting, one would prefer to deal with elastic potentials that are polyconvex and coercive, due to their numerical stability and the compatibility with the methods of the Calculus of Variations [2, 5]. However, if active deformation is simply modeled via an additional stress term fitted to experimental data (the so-called *active stress* approach, see Sect. 4.1), this new term might cause the loss of the original mathematical properties. On the other hand, the *active strain* approach (see Sect. 4.2) aims to model active deformation by a change of the reference configuration, without affecting the functional form of the elastic potential; hence, the mathematical features of the model can be preserved [1].

Nevertheless, for better agreement with the experimental data, the change in the reference configuration is sometimes assumed to depend on the actual deformation gradient, which again compromises the good properties of the original model [13]. Therefore, in Sect. 5.2 we propose a new model based on the *mixture active strain* approach [35], where the change in reference configuration is constant and the mathematical properties of the original model are maintained.

## 2. Skeletal muscle tissue and the experiment of Hawkins & Bey

Skeletal muscle tissue produces movement and force, maintains body posture and stabilizes joints. Muscle fibers are the cells of this tissue: they have a preferred alignment and they are composed of myofibrils. The filaments of actin and myosin presented in the fibers are responsible for the contraction. Each individual fiber is surrounded by connective tissue, which is essentially isotropic.

To describe the behavior of the muscle, we take advantage of the well-known paper by Hawkins and Bey [23] which describes the stretch along the fibers and the developed stress of a tetanized rat *tibialis anterior*. Other experimental models are proposed in literature in order to capture the tension-elongation relations, see for instance [21, 26, 36].

The experimental data obtained for the whole muscle in [23] are shown in Fig. 1.

These data were collected in two phases. First, the muscle is stretched in absence of activation, and the *passive* response is measured. The stretching is performed slowly (at a rate of about 1mm/s) in order to minimize viscous effects. Second, the tissue is stimulated isometrically: after stretching the muscle at a given length, the tissue is electrically activated up to its *tetanized* status, keeping the elongation fixed, and then the stress is measured. Since in the activated case actin and myosin in the fibers bind together, the shape of the stress-strain relation (*total curve*) changes significantly compared to the passive curve.

The *active curve* (i.e. the curve due only to the contraction of the sarcomeres and not to the elastic contribution of the tissues) is not directly measured by experiments, but it is obtained by subtracting the passive force from the total one (see Fig. 2).

## 3. Constitutive model

In this section we model the passive behavior of the tissue using standard notions of Continuum Mechanics.

As it is customary, the motion of a body is described by an invertible smooth map from a bounded subset $\Omega \subset \mathbb{R}^3$ into $\mathbb{R}^3$: the function $\boldsymbol{x} = \chi(\boldsymbol{X}, t)$ associates every point $\boldsymbol{X}$ in the reference configuration $\Omega$ with its current placement $\boldsymbol{x}$. The

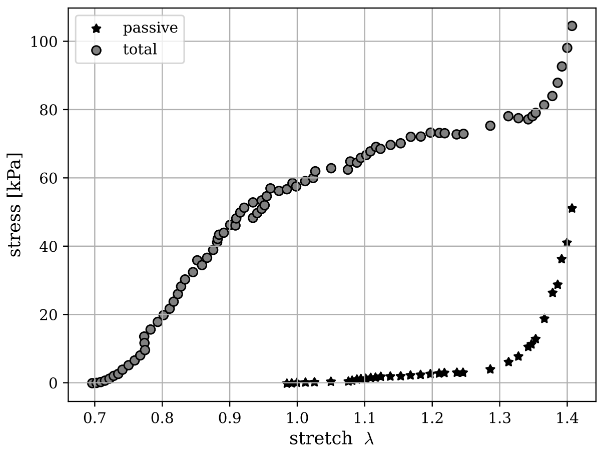


FIGURE 1. Stress-stretch relationship of a rat *tibialis anterior* muscle/tendon complex, as reported in [23]. The stress is computed dividing the measured force by the cross-sectional area of the whole muscle; the stretch is computed dividing the (instantaneous) distance between two markers by the distance between the same markers in a state of zero stress. The compressive passive stress ($\lambda < 1$) is essentially zero and has not been reported in the figure.

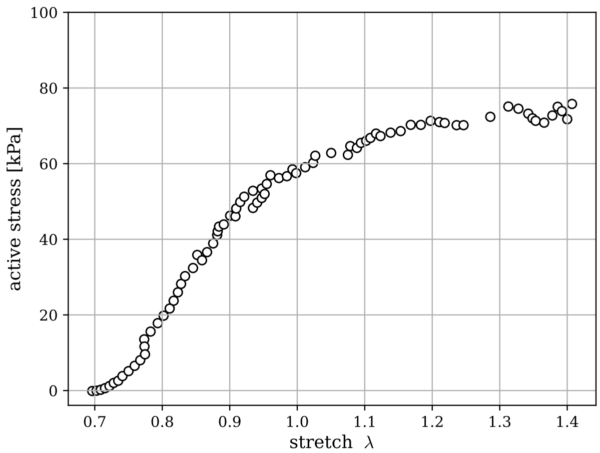


FIGURE 2. Difference between the total stress and the passive data in [23].

*deformation gradient*

$$\mathsf{F} = \mathrm{Grad}\,\chi, \quad F_{ij} = \frac{\partial \chi_i}{\partial X_j}, \quad i,j = 1,2,3$$

belongs to the space of linear operators with strictly positive determinant.

In the following, we set in the frame of *hyperelasticity*. For a hyperelastic material, the first Piola (or nominal) stress tensor $\mathsf{P}$, which describes the tensional state in a continuum medium, is derived from a strain energy density function $W$. By assuming the *principle of material frame indifference*, $W$ is a function of the *right Cauchy-Green tensor* $\mathsf{C} = \mathsf{F}^\mathsf{T}\mathsf{F}$, so that

$$\mathsf{P}\big(\boldsymbol{X}, \mathsf{F}(\boldsymbol{X})\big) = 2\mathsf{F}(\boldsymbol{X})\frac{\partial W}{\partial \mathsf{C}}\big(\boldsymbol{X}, \mathsf{C}(\boldsymbol{X})\big). \tag{1}$$

If the material is *incompressible*, it has to satisfy the constraint $\det \mathsf{F} = 1$ and the expression of the Piola stress has to be written as

$$\mathsf{P}\big(\boldsymbol{X}, \mathsf{F}(\boldsymbol{X})\big) = 2\mathsf{F}(\boldsymbol{X})\frac{\partial W}{\partial \mathsf{C}}\big(\boldsymbol{X}, \mathsf{C}(\boldsymbol{X})\big) - p\mathsf{F}^{-\mathsf{T}}, \tag{2}$$

where $p$ is the Lagrange multiplier of the constraint (the so-called *hydrostatic pressure*). Hence the behavior of the elastic body is described by the hyperelastic strain energy function

$$\int_\Omega W\big(\boldsymbol{X}, \mathsf{C}(\boldsymbol{X})\big) d\boldsymbol{X}.$$

From now on, for the sake of simplicity we assume that the material is *homogeneous*, so that $W$ does not depend explicitly on $\boldsymbol{X}$.

Let us list the additional assumptions that are important when modeling biological tissues such as skeletal muscle.

- **Incompressibility.** In describing biological tissues it is customary to assume that the material is incompressible, due to their typical high content of water (more than 75% of the total volume in the case of skeletal muscle tissue, see [28]). Then we will use (2) as the expression for the Piola stress tensor.
- **Transverse isotropy**. It is due to the local alignment of the muscle fibers. By introducing the direction $\boldsymbol{m}$ of the fibers in the reference configuration and the *structural tensor* $\mathsf{M} = \boldsymbol{m} \otimes \boldsymbol{m}$, we can express the strain energy density as a function of the two invariants

  $$I_1 = \operatorname{tr} \mathsf{C}, \quad I_2 = \frac{1}{2}\left(I_1^2 - \operatorname{tr}(\mathsf{C}^2)\right)$$

  and the two *generalized invariants*

  $$I_4 = \operatorname{tr}(\mathsf{CM}), \quad I_5 = \operatorname{tr}(\mathsf{C}^2\mathsf{M})$$

  which keep into account the transverse isotropy of the material (the third invariant $I_3 = \det \mathsf{C}$ does not play any rôle since the material is incompressible). Due to the Cayley–Hamilton Theorem, the invariant $I_2$ and the generalized invariant $I_5$ can be replaced by

  $$J_2 = \operatorname{tr}(\mathsf{C}^{-1}), \quad J_5 = \operatorname{tr}(\mathsf{C}^{-1}\mathsf{M}),$$

  respectively (see [25]).

Moreover, when dealing with Nonlinear Elasticity, there are some assumptions which are crucial in obtaining a mathematically well-posed model, the main two being the following.

- **Polyconvexity** We recall that an energy density $W(\mathsf{F})$ is polyconvex if there is a convex function $g : \mathbb{R}^{19} \to R$ such that

  $$W(\mathsf{F}) = g(\mathsf{F}, \operatorname{cof} \mathsf{F}, \det \mathsf{F}),$$

  where the cofactor matrix is defined by $\operatorname{cof} \mathsf{F} = \mathsf{F}^{-\mathsf{T}} \det \mathsf{F}$ for any invertible matrix $\mathsf{F}$. Polyconvexity is a suitable generalization of the notion of convexity which is compatible with the usual requirements of Continuum Mechanics.

- **Coercivity** The energy density has to fulfil a growth condition of the form
$$W(\mathsf{F}) \geq \alpha[|\mathsf{F}|^p + |\operatorname{cof}\mathsf{F}|^q + |\det\mathsf{F}|^r] + \beta$$
for some $\alpha > 0$, $\beta \in \mathbb{R}$, $p \geq 2$, $q \geq p/(p-1)$, $r > 1$ (see [5, Section 7.7]).

For a polyconvex and coercive material there is a deep and celebrated existence result, due essentially to John Ball [2], for the equilibrium boundary-value problem of Nonlinear Elasticity.

Several hyperelastic energies satisfy these requirements [4]; we now recall two constitutive models which have been used in the modeling of biological tissues.

3.1. **An example of polyconvex and coercive hyperelastic material.** Typical experiments in muscle tissue show a non-linear J-shaped behavior, which can be successfully described using exponential functions. In [11, 10] the passive behavior of the material is modeled by the strain energy density function

$$W(\mathsf{C}) = \frac{\mu}{4}\left\{\frac{1}{\alpha}\left[e^{\alpha(I_p-1)} - 1\right] + \frac{1}{\beta}\left[e^{\beta(K_p-1)} - 1\right]\right\}, \tag{3}$$

where

$$I_p = \frac{w_0}{3}\operatorname{tr}(\mathsf{C}) + (1-w_0)\operatorname{tr}(\mathsf{CM}), \quad K_p = \frac{w_0}{3}\operatorname{tr}(\mathsf{C}^{-1}) + (1-w_0)\operatorname{tr}(\mathsf{C}^{-1}\mathsf{M}),$$

together with the incompressibility constraint

$$\det\mathsf{C} = 1.$$

Thanks to the notation introduced previously, we can also write

$$I_p = \frac{w_0}{3}I_1 + (1-w_0)I_4, \quad K_p = \frac{w_0}{3}J_2 + (1-w_0)J_5.$$

The tensor $\mathsf{M} = \boldsymbol{m}\otimes\boldsymbol{m}$ is the structural tensor ($\boldsymbol{m}$ being the local orientation of the fibers), $\mu$ is an elastic coefficient, $\alpha > 0$ and $0 \leq w_0 \leq 1$ are dimensionless material constants. The quantities $I_p$ and $K_p$ are weighted combinations of the isotropic and anisotropic components; in particular, $w_0$ measures the ratio of isotropic tissue constituents and $1-w_0$ that of muscle fibers. Moreover, the term $\operatorname{tr}(\mathsf{CM})$ represents the squared stretch in the direction of $\boldsymbol{m}$ and is thus associated with the elongation of the fibers, while the term $\operatorname{tr}(\mathsf{C}^{-1}\mathsf{M})$ describes the change of the cross-sectional area of a surface element which is normal to the direction $\boldsymbol{m}$ in the reference configuration and thus relates to the transverse behavior of the material [39, 8].

Keeping into account that

$$\frac{\partial I_p}{\partial \mathsf{C}} = \frac{w_0}{3}\mathsf{I} + (1-w_0)\mathsf{M}, \quad \frac{\partial K_p}{\partial \mathsf{C}} = \mathsf{C}^{-1}\left[\frac{w_0}{3}\mathsf{I} + (1-w_0)\mathsf{M}\right]\mathsf{C}^{-1},$$

the Piola stress tensor is given by

$$\begin{aligned}\mathsf{P} = 2\mathsf{F}\frac{\partial W}{\partial \mathsf{C}} - p\mathsf{F}^{-\mathsf{T}} = \frac{\mu}{2}\mathsf{F}\Big\{&e^{\alpha(I_p-1)}\left[\frac{w_0}{3}\mathsf{I} + (1-w_0)\mathsf{M}\right] \\ &-e^{\beta(K_p-1)}\mathsf{C}^{-1}\left[\frac{w_0}{3}\mathsf{I} + (1-w_0)\mathsf{M}\right]\mathsf{C}^{-1}\Big\} - p\mathsf{F}^{-\mathsf{T}},\end{aligned} \tag{4}$$

where $p$ is the hydrostatic pressure due to incompressibility.

One of the mathematical features of (3) is that it is polyconvex and coercive [39, 11], hence the equilibrium problem with mixed boundary conditions is well posed. We remark that $\mathsf{C}$ is the identity tensor $\mathsf{I}$ in the reference configuration, so that $I_p = K_p = 1$, *i.e.* we have the energy- and stress-free state of the passive muscle tissue.

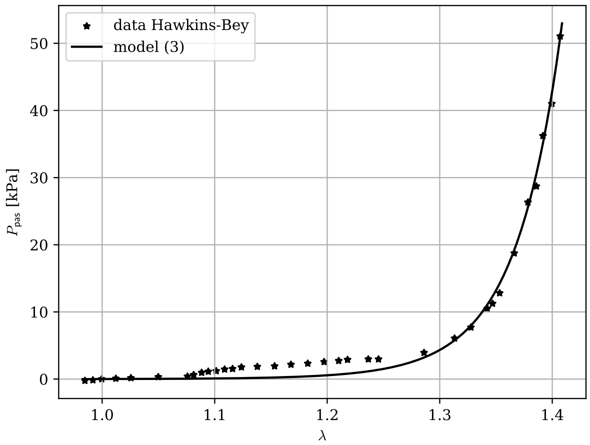


FIGURE 3. Passive stress of Sect. 3.1 for $\mu = 0.1599$ kPa, $\alpha = 19.69$, $\beta = 1.19$, $w_0 = 0.7388$.

The material parameters of the model can be obtained from real data. The experimental data of [23] are collected during a uniaxial deformation along the fibers. Hence we consider the uniform incompressible transversely isotropic deformation

$$\mathsf{F}_\lambda = \lambda \boldsymbol{m} \otimes \boldsymbol{m} + \frac{1}{\sqrt{\lambda}}(\mathsf{I} - \boldsymbol{m} \otimes \boldsymbol{m}), \tag{5}$$

so that $\lambda = \sqrt{I_4}$.

It is now easy to compute $P_{\mathrm{pas}}(\lambda) = P_{mm}(\mathsf{F}_\lambda)$ and, fitting the parameters, we obtain Fig. 3, which is in very good agreement with the experimental data, except for a small discrepancy in the interval between 1.1. and 1.3.

3.2. **Fiber-reinforced materials.** Another possible method is to model the muscle as an additive composition of two phases, the isotropic phase described by the energy $W_{\mathrm{iso}}$ and the transversely isotropic phase described by $W_{\mathrm{ani}}$:

$$W_{\mathrm{frm}} = W_{\mathrm{iso}}(I_1, I_2, I_3) + W_{\mathrm{ani}}(I_4, I_5). \tag{6}$$

The strain energy density $W_{\mathrm{iso}}$ takes into account the isotropic constituents of the tissue, while $W_{\mathrm{ani}}$ describes the fibers and takes into account the contraction of the tissue during the activation process (we will see in Sect. 4.3 why such a specification will be useful in modeling the active deformation of the material).

In this paper we propose a new kind of energy, given by

$$\begin{aligned} W_{\mathrm{iso}}(I_1, J_2) &= \frac{\mu}{4}\left\{\frac{1}{\alpha}\left[e^{\alpha(I_1/3-1)} - 1\right] + \frac{1}{\beta}\left[e^{\beta(J_2/3-1)} - 1\right]\right\}, \\ W_{\mathrm{ani}}(I_4, J_5) &= W_{\mathrm{ani},1}(I_4) + W_{\mathrm{ani},2}(J_5), \\ W_{\mathrm{ani}}(I_4, J_5) &= -\kappa\left[e^{-p(\sqrt{I_4}-s)^2\sqrt{I_4}} + \left(\frac{3-s}{2}\right)e^{-p(\sqrt{J_5}-s)^2}\right], \end{aligned} \tag{7}$$

where $\kappa$, $p$ and $s$ are positive parameters.

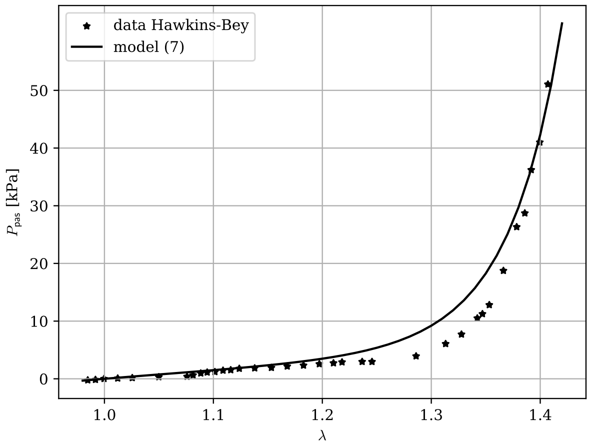


FIGURE 4. Passive stress of Sect. 3.2 for $\mu = 4.94$ kPa, $\alpha = 30.5$, $\beta = 2.08$, $\kappa = 71.81$ kPa, $s = 0.51$, $p = 0.0169$.

Computing again the $\boldsymbol{m}\otimes\boldsymbol{m}$ component of the Piola stress tensor for the uniaxial deformation (5), we obtain $P_{\text{pas}}(\lambda) = P_{\text{iso}}(\lambda) + P_{\text{ani}}(\lambda)$, where

$$
\begin{aligned}
P_{\text{iso}}(\lambda) &= \frac{\mu}{4}\left\{\left[e^{\alpha(I_1/3-1)} - 1\right]\frac{\partial I_1}{\partial\lambda} + \left[e^{\beta(J_2/3-1)} - 1\right]\frac{\partial J_2}{\partial\lambda}\right\}, \\
I_1 &= \frac{1}{3}\left(\lambda^2 + \frac{2}{\lambda}\right), \quad J_2 = \frac{1}{3}\left(\frac{1}{\lambda^2} + 2\lambda\right) \\
\frac{\partial I_1}{\partial\lambda} &= \frac{1}{3}\left(2\lambda - \frac{2}{\lambda^2}\right), \quad \frac{\partial J_2}{\partial\lambda} = \frac{1}{3}\left(-\frac{2}{\lambda^3} + 2\right) \\
P_{\text{ani}}(\lambda) &= \kappa p\left[(\lambda - s)\,(3\lambda - s)\,e^{-p(\lambda-s)^2\lambda} - \left(\frac{3-s}{\lambda^2}\right)\left(\frac{1}{\lambda} - s\right)e^{-p(\frac{1}{\lambda}-s)^2}\right].
\end{aligned}
\tag{8}
$$

We remark that $P_{\text{ani}}(1) = 0$ for any choice of the parameters. Moreover, once the parameters have been chosen as in Fig. 4, the energy is polyconvex.

By tuning the parameters on the experimental data, we obtain Fig. 4. This model, in comparison to the previous one, will have better mathematical features of the active deformation model that we will employ in Sect. 4.3.

## 4. Active deformation

It is now important to include in our mathematical model the mechanical effect of activation. In the case of muscle tissue, the muscle fibers can contract thanks to the sliding of actin and myosin filaments and produce an effect also on the connective tissue. Several methods have been proposed in literature in order to describe the active state of the tissue.

### 4.1. Active stress.

Perhaps the easiest and widely used approach is the *active stress* one: a new term is added in the expression of the stress tensor, which keeps into account the active part of the stress. Hence the total stress is additively decomposed as

$$
\mathsf{P}_{\text{tot}} = \mathsf{P}_{\text{pas}} + \mathsf{P}_{\text{act}}, \tag{9}
$$

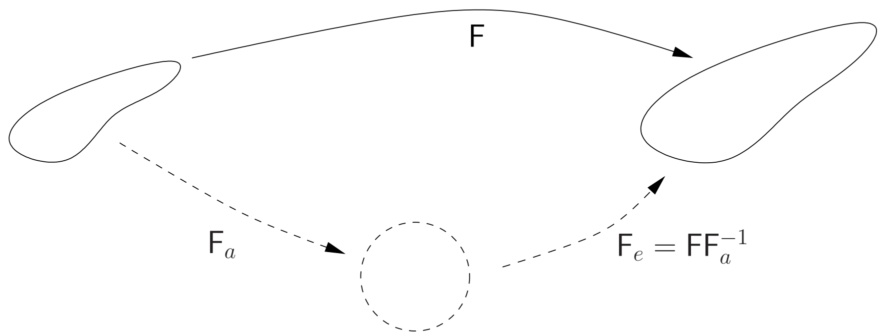


FIGURE 5. Bilby-Kröner-Lee decomposition for the active strain approach.

where $\mathsf{P}_{\mathrm{act}}$ is the active stress, which has to be constitutively provided. This approach has been widely used in the case of cardiac mechanics [32, 20, 34] as well as in the case of skeletal muscle tissue [29, 3, 24].

To remain within the framework of hyperelasticity, the new term must be interpreted as the derivative of a new component of the energy, named *active energy*, so that one has the additive decomposition

$$W_{\mathrm{tot}} = W_{\mathrm{pas}} + W_{\mathrm{act}}.$$

This method is mainly phenomenological and does not account for the mechanics of activation. More importantly, from a mathematical viewpoint the form of the energy changes significantly and the mathematical properties can be lost.

4.2. **Active strain.** In this approach, the form of the strain energy function remains unchanged; conversely, a multiplicative decomposition of the deformation gradient is introduced.

Following the *active strain* approach [13], we rewrite the deformation gradient using the Bilby-Kröner-Lee decomposition

$$\mathsf{F} = \mathsf{F}_e \mathsf{F}_a, \tag{10}$$

where $\mathsf{F}_e$ represents the elastic part and $\mathsf{F}_a$ describes the active contribution (see Fig. 5). The active strain $\mathsf{F}_a$ signifies a change in the reference volume elements due to sarcomere contraction, and therefore it does not store any elastic energy. A reference volume element distorted by $\mathsf{F}_a$ requires further deformation by $\mathsf{F}_e$ to match the actual volume element, which accommodates both the external forces and the active contraction. Note that neither $\mathsf{F}_a$ nor $\mathsf{F}_e$ necessarily represents the gradients of any displacement, meaning that they do not need to fulfill the compatibility condition $\operatorname{curl} \mathsf{F}_a = 0$ or $\operatorname{curl} \mathsf{F}_e = 0$.

The volume elements are modified by the internal active forces without affecting the elastic energy. Therefore, the strain energy function of the active material has to be computed using $\mathsf{C}_e = \mathsf{F}_e^{\mathsf{T}} \mathsf{F}_e$, considering $\mathsf{F}_e = \mathsf{F}\mathsf{F}_a^{-1}$. We then obtain the total hyperelastic energy density

$$W_{\mathrm{tot}}(\mathsf{C}) = (\det \mathsf{F}_a) W(\mathsf{C}_e) = (\det \mathsf{F}_a) W(\mathsf{F}_a^{-\mathsf{T}} \mathsf{C} \mathsf{F}_a^{-1}). \tag{11}$$

Therefore, instead of introducing a new part of the energy, the active part $\mathsf{F}_a$ of the deformation gradient needs to be constitutively modeled. From a mathematical perspective, the active strain approach preserves the desired properties of the energy, namely polyconvexity and coercivity, at least if $\mathsf{F}_a$ is assumed to be independent of the deformation. However, in many cases it is convenient to assume that the active part $\mathsf{F}_a$ changes with the deformation; in such cases the good mathematical properties of the passive energy might be lost (see also the remark below).

The active strain approach was first proposed by Taber and Perucchio [37] for cardiac tissue and it has been developed by several authors (see for example [30, 1, 17, 18, 13]).

*Remark* 1. It is debatable whether the framework of hyperelasticity is appropriate in the context of active materials. Indeed, the mechanics of biological activation usually involves chemical reactions that can alter the energy balance, transforming other forms of energy into elastic energy.

In the case of active strain, another subtle mathematical problem can occur. If $\mathsf{F}_a$ is assumed to change with $\mathsf{F}$, one has

$$W(\mathsf{F};\mathsf{F}_a) = W_{\text{pas}}(\mathsf{F}\mathsf{F}_a^{-1}(\mathsf{F}))$$

where we assumed for simplicity that $\det \mathsf{F}_a = 1$. Hence the Piola stress tensor should be given by

$$\mathsf{P} = \frac{\partial W_{\text{pas}}}{\partial \mathsf{F}}(\mathsf{F}\mathsf{F}_a^{-1})\mathsf{F}_a^{-\mathsf{T}} + \mathsf{F}^{\mathsf{T}}\frac{\partial W_{\text{pas}}}{\partial \mathsf{F}_a}\,\frac{\partial \mathsf{F}_a^{-1}}{\partial \mathsf{F}}.$$

However, for biological tissues the simpler expression

$$\mathsf{P} = \frac{\partial W_{\text{pas}}}{\partial \mathsf{F}}(\mathsf{F}\mathsf{F}_a^{-1})\mathsf{F}_a^{-\mathsf{T}}$$

is often used, as if $\mathsf{F}_a$ were not depending on $\mathsf{F}$. Then, it is no more assured that the Piola stress tensor is the derivative of a potential and the hyperelastic framework can be lost. See [14] for a discussion about this topic.

4.3. **Mixture active strain.** In the case of a fiber-reinforced material (6), it can be assumed that only the anisotropic component of the energy contributes to active deformation. For instance, in the case of skeletal muscle, only the muscle fibers are capable of shortening. Hence, the total strain energy of the active material is expressed as

$$W_{\text{frm}} = W_{\text{iso}}(\mathsf{C}) + (\det \mathsf{F}_a)W_{\text{ani}}(\mathsf{C}_e). \tag{12}$$

If $\det\mathsf{F}_a = 1$, the Piola stress tensor then writes

$$\mathsf{P}_{\text{frm}} = \mathsf{P}_{\text{iso}}(\mathsf{F}) + \mathsf{P}_{\text{ani}}(\mathsf{F}\mathsf{F}_a^{-1})\mathsf{F}_a^{-\mathsf{T}} - \widehat{p}\mathsf{F}^{-\mathsf{T}}. \tag{13}$$

This approach has been considered in [12, 19, 33, 16, 35] and will be used in the important example given in Sect. 5.2.

4.4. **Mixed-active-stress-active-strain approach.** In [27], the Authors propose a new approach where the total stress is obtained in the following way

$$\mathsf{P}_{\text{tot}} = \frac{\partial W_1}{\partial \mathsf{F}} + \frac{\partial W_2}{\partial \mathsf{F}_e}\mathsf{F}_a^{-\mathsf{T}} + \mathsf{P}_a - \widehat{p}\mathsf{F}^{-\mathsf{T}}. \tag{14}$$

In this case, the strain energy $W$ is still divided into an isotropic contribution $W_1$ and an anisotropic part $W_2$, with only the latter contributing to active deformation, as in the mixture active strain approach. Additionally, an active stress $\mathsf{P}_a$ is introduced to account for the coupling with the elastic matrix.

However, we believe that there are few benefits to pursuing this approach, since it introduces an additional term akin to the active stress approach and does not contribute in producing a well-posed mathematical model.

4.5. **Active Fibers.** Finally, it should be mentioned that active deformation has sometimes been described just by changing the zero-strain energy of contracting fibers. More precisely, suppose that the passive energy is a function $W_{\rm pas}(I_1, I_2, I_4)$, then the total energy can be obtained by modifying the influence of the muscle fibers properties through a factor $a$:

$$W = W_{\rm pas}(I_1, I_2, I_4 + a), \qquad 0 \le a < 1.$$

This approach is sometimes called *active fibers* and it has been applied in [10, 14, 22].

## 5. Two proposals for active strain-type models

In this section we focus on the active deformation approaches described in Sect. 4 which involve the multiplicative decomposition of the deformation gradient (10), aiming to model skeletal muscle tissue using the data of Hawkins and Bey [23] as a benchmark.

First of all, a suitable form of $\mathsf{F}_a$ must be chosen in order to apply the Bilby-Kröner-Lee decomposition. A rather popular choice in literature [12, 15, 35] is the following

$$\mathsf{F}_a = (1-a)\boldsymbol{m}\otimes\boldsymbol{m} + \frac{1}{\sqrt{1-a}}(\mathsf{I} - \boldsymbol{m}\otimes\boldsymbol{m}), \tag{15}$$

where $0 \le a < 1$ is a dimensionless parameter representing the relative contraction of activated fibers ($a = 0$ meaning no activation).

This choice aims to take into account some macroscopic aspects of the contraction of the muscle tissue: without entering in the molecular details of the interaction between proteins in the sarcomeres, the main mechanical output is that the activation in the muscle tissue induces a shortening of the muscle fibers, which results in a shortening of the tissue in the direction of the fibers. The model (15) tries to capture this essential physiological feature.

Notice that we assumed that $\det \mathsf{F}_a = 1$, so that we describe a volume-preserving active contraction along the fiber direction. Moreover, (15) and (10) imply that also $\det \mathsf{F}_e = 1$ and the material is elastically incompressible.

Other constitutive choices of $\mathsf{F}_a$ can be made such as an isotropic fibre distribution, a shortening along the compressible fibers [1, 30, 33, 13] or an active deformation induced by shear strains [27].

5.1. **Active strain model.** We start from the exponential passive energy density given in (3) and we apply an active strain approach using $\mathsf{F}_a$ given in (15).

Moreover, in order to accommodate the experimental data of Fig. 1, the activation parameter $a$ cannot be constant [35]. Indeed, it is a key feature of the skeletal muscle tissue that the active part of the stress grows with the stretch until a maximum and then decreases; this behavior is probably due to the molecular structure of the sarcomere, in which the overlap between actin and myosin depends also on the stretch [38, 10]. Hence we assume that the activation parameter $a$ depends on the deformation. A reasonable choice is to take $a$ as a function of the (squared) stretch along the fibers, which is measured by

$$I_4 = \mathrm{tr}\,(\mathsf{CM}),$$

so that $\mathsf{F}_a = \mathsf{F}_a(I_4)$. In that case, taking into account that $\det \mathsf{F}_a = 1$, the corresponding first Piola stress tensor is given by

$$\widehat{\mathsf{P}} = 2\mathsf{F}\frac{\partial \widehat{W}}{\partial \mathsf{C}} - \widehat{p}\mathsf{F}^{-\mathsf{T}} = 2\mathsf{F}\frac{\partial}{\partial \mathsf{C}}\Big[W\left(\mathsf{F}_a^{-\mathsf{T}}(I_4)\mathsf{C}\mathsf{F}_a^{-1}(I_4)\right)\Big] - \widehat{p}\mathsf{F}^{-\mathsf{T}}, \tag{16}$$

where $\widehat{p}$ accounts for the incompressibility constraint $\det \mathsf{C} = 1$.

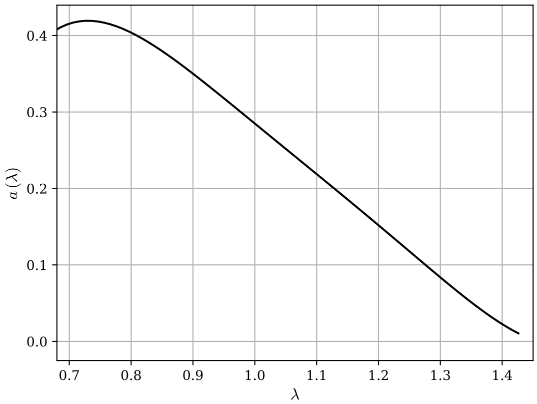


FIGURE 6. The activation function (18) with $p_0 = -11.89, p_1 = 58.23, p_2 = -107.66, p_3 = 98.04, p_4 = -44.46, p_5 = 8.03$.

Taking into account the form of $\mathsf{F}_a$ given in (15) and the expression of the energy (11), substituting in (3) one gets

$$\widehat{W}(\lambda, a(\lambda)) = \frac{\mu}{4}\left[\frac{1}{\alpha}(e^{\alpha(I_e-1)} - 1) + \frac{1}{\beta}(e^{\beta(K_e-1)} - 1)\right], \tag{17}$$

where

$$\lambda = \sqrt{I_4} = \sqrt{\operatorname{tr}\mathsf{CM}},$$

$$\mathsf{C}_e = \frac{\lambda^2}{(1-a)^2}\boldsymbol{m}\otimes\boldsymbol{m} + \frac{1-a}{\lambda}(\mathsf{I} - \boldsymbol{m}\otimes\boldsymbol{m}),$$

$$I_e = \frac{w_0}{3}\operatorname{tr}(\mathsf{C}_e) + (1-w_0)\operatorname{tr}(\mathsf{C}_e\mathsf{M}) = \left(1 - \frac{2}{3}w_0\right)\frac{\lambda^2}{(1-a)^2} + \frac{2w_0}{3\lambda}(1-a),$$

$$K_e = \frac{w_0}{3}\operatorname{tr}(\mathsf{C}_e^{-1}) + (1-w_0)\operatorname{tr}(\mathsf{C}_e^{-1}\mathsf{M}) = \left(1 - \frac{2}{3}w_0\right)\frac{(1-a)^2}{\lambda^2} + \frac{2w_0\lambda}{3(1-a)}.$$

We now look for a polynomial expression of $a(\lambda)$ of the form

$$a(\lambda) = p_5\lambda^5 + p_4\lambda^4 + p_3\lambda^3 + p_2\lambda^2 + p_1\lambda + p_0, \tag{18}$$

where $p_j,\ j = 0, \ldots, 5$ are the fitting parameters.

The profile of $a(\lambda)$ can be obtained numerically by least squares optimization of the equation

$$P_{\text{tot}}(\lambda, a(\lambda)) = \text{total data}\,,$$

where $P_{\text{tot}} = \operatorname{tr}(\widehat{\mathsf{P}}\mathsf{M})$ represents the component along $\mathsf{M}$ of the total first Piola stress tensor (16). We can directly compute $P_{\text{tot}}$ from the corresponding strain energy density (17):

$$P_{\text{tot}}(\lambda, a(\lambda)) = \frac{\partial\widehat{W}}{\partial\lambda}(\lambda, a(\lambda)).$$

where, as is customary in active strain, we neglect the term involving the derivative of $a(\lambda)$ with respect to $\lambda$ (see Remark 1).

The behavior of $a(\lambda)$ is shown in Fig. 6 and the plots of the total and active stress are given in Fig. 7. As one can see, the fitting with experimental data is very good. This is one of the major advantages of choosing a non-constant activation parameter: the achievement of a very accurate fitting of the data.

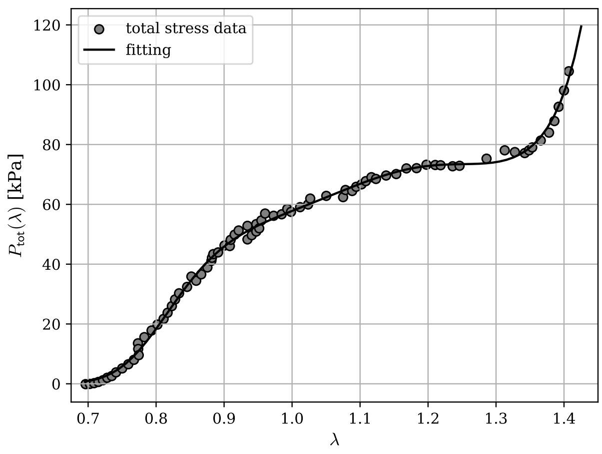


FIGURE 7. Total stress-strain relation with activation function (18). The values of the parameters are given in Fig. 6.

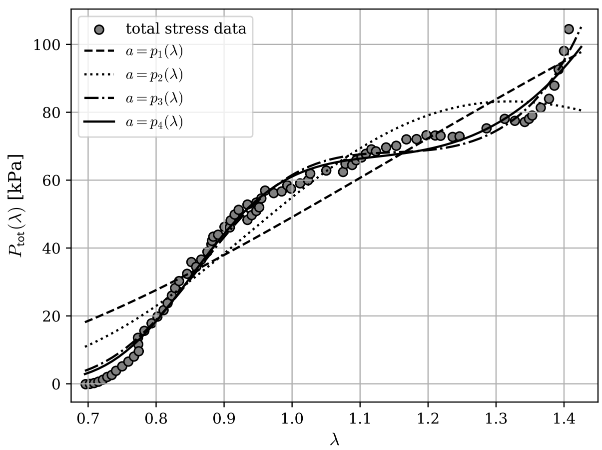


FIGURE 8. Total stress-strain relation with activation function $a(\lambda)$ of polynomial type $p_1, p_2, p_3, p_4$. More precisely: $p_1(\lambda) = -0.65\lambda + 0.93$, $p_2(\lambda) = -0.075\lambda^2 - 0.48\lambda + 0.85$, $p_3(\lambda) = 0.51\lambda^3 - 1.76\lambda^2 + 1.33\lambda + 0.21$, $p_4(\lambda) = -0.5\lambda^4 + 2.69\lambda^3 - 5.28\lambda^2 + 3.82\lambda - 0.45$.

In Fig. 8 we plot the stress by choosing the activation parameter as a polynomial function of the stress with a lower degree than the form proposed in (18). We underline that in order to capture the trend completely it is necessary to have a polynomial of degree 5 and therefore we need to fit six parameters.

5.2. **A mixture active strain model with constant activation parameter.** Referring to Sect. 3.2, we start from the energy density (6) for an incompressible fiber-reinforced material

$$W_{\mathrm{frm}} = W_{\mathrm{iso}}(I_1, J_2) + W_{\mathrm{ani}}(I_4, J_5)$$

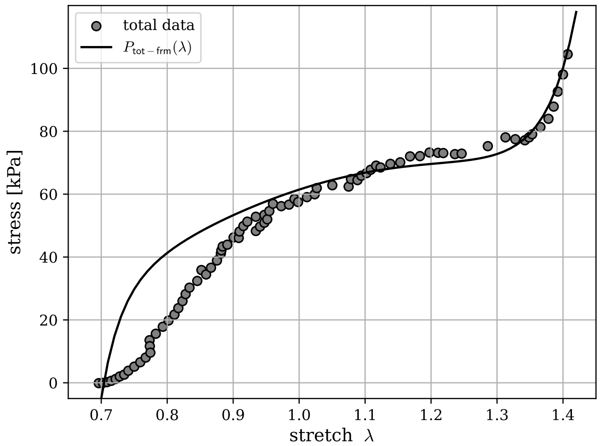


FIGURE 9. Fiber-reinforced material with mixture active strain: the values of the parameters are the same of Fig. 4 and $a = 0.68$.

with the constitutive prescription (7)

$$W_{\text{iso}} = \frac{\mu}{4}\left\{\frac{1}{\alpha}\left[e^{\alpha(I_1/3-1)} - 1\right] + \frac{1}{\beta}\left[e^{\beta(J_2/3-1)} - 1\right]\right\},$$

$$W_{\text{ani}} = -\kappa\left[\exp\left(-p(\sqrt{I_4} - s)^2\sqrt{I_4}\right) + \left(\frac{3-s}{2}\right)\exp\left(-p(\sqrt{J_5} - s)^2\right)\right].$$

Following the procedure as in the previous section, using the mixture active strain approach (12) and the uniaxial deformation (5) we can compute

$$W_{\text{frm}}(\lambda, a) = W_{\text{iso}}(I_1(\mathsf{C}_\lambda), j_2(\mathsf{C}_\lambda)) + W_{\text{ani}}(I_4(\mathsf{C}_{\lambda,e}), J_5(\mathsf{C}_{\lambda,e}))$$

where

$$I_1(\mathsf{C}_\lambda) = \text{tr}(\mathsf{C}) = \left(\lambda^2 + \frac{2}{\lambda}\right), \quad J_1(\mathsf{C}_\lambda) = \text{tr}(\mathsf{C}^{-1}) = \left(\frac{1}{\lambda^2} + 2\lambda\right),$$

$$I_4(\mathsf{C}_{\lambda,e}) = \left(\frac{\lambda}{1-a}\right)^2, \quad J_5(\mathsf{C}_{\lambda,e}) = \left(\frac{1-a}{\lambda}\right)^2.$$

It is important to remark that, unlike in the previous example, the activation parameter remains constant here. This ensures that the total energy density retains its mathematical properties such as polyconvexity and coercivity.

The total stress is then computed by

$$P_{\text{tot}}(\lambda, a) = \frac{\partial W_{\text{iso}}}{\partial \lambda}(\lambda) + \frac{\partial W_{\text{ani}}}{\partial \lambda}(\lambda, a) =: P_{\text{iso}} + P_{\text{ani}}.$$

In particular, the anisotropic part of the total stress is given by

$$\begin{aligned}(19)\quad P_{\text{ani}} = \kappa p\Bigg[&\frac{1}{1-a}\left(\frac{\lambda}{1-a} - s\right)\left(3\frac{\lambda}{1-a} - s\right)e^{-p\left(\frac{\lambda}{1-a}-s\right)^2\left(\frac{\lambda}{1-a}\right)} \\ &- (3-s)\frac{1-a}{\lambda^2}\left(\frac{1-a}{\lambda} - s\right)e^{-p\left(\frac{1-a}{\lambda}-s\right)^2}\Bigg].\end{aligned}$$

The stretch/stress plot is shown in Fig. 9.

Since the activation parameter is constant, it is easy to study the case of a progressive activation of the muscle tissue from the passive case ($a = 0$) to the

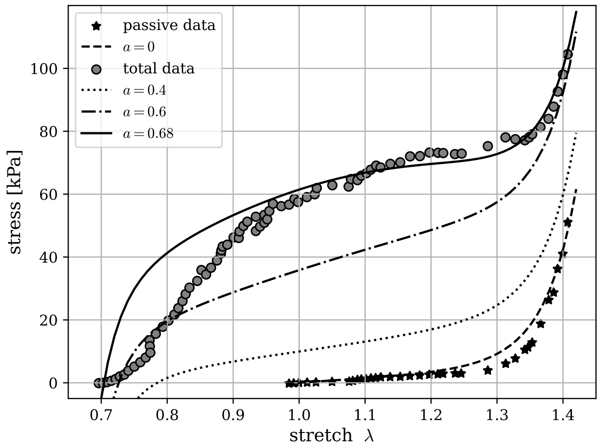


FIGURE 10. Fiber-reinforced material with mixture active strain: the values of the parameters are the same of Fig. 4 and $a = 0, 0.4, 0.6, 0.68$.

tetanized case ($a = 0.68$). In Fig. 10 we compare the passive and tetanized stress with the two intermediate cases $a = 0.4$ and $a = 0.6$.

## 6. Conclusion and discussion of the results

In this paper we focused our attention on "active deformation" of the skeletal muscle tissue and we proposed two hyperelastic models which are able to capture the trend of the experimental data of Hawkins and Bey [23], i.e. the dependence of the stress developed by a fully activated (tetanized) muscle on its imposed extension. Both of these two models fall into the classification of hyperelastic materials as regards the passive part, while to describe active deformation we used the multiplicative decomposition of stress.

First of all, in Sect. 5.1 we used the passive energy proposed in [10] and we followed the typical active strain approach, similar to [13]. The novelty here is that we proposed in (18) a new expression for the active parameter, which has a polynomial shape and needs only 6 fitting parameters. Furthermore, unlike what has been done in [14, 15], the derivative of the activation parameter is not considered here.

The most relevant part is definitely Sect. 5.2, where, inspired by [35], a new hyperelastic model is proposed to describe the behavior on active deformations of skeletal tissue. In this case we used a fiber reinforced material governed by (7) and the active strain $\mathsf{F}_a$ is now constant.

We remark that the two models described in Sect. 5.1 and in Sect. 5.2 involve a different number of parameters. The active strain model developed in Sect. 5.1 considers an energy already proposed in the literature which perfectly captures the trend of passive data on a uniaxial deformation. To obtain the active behavior as well, we therefore need a greater number of parameters in the polynomial that describes the active state, that is in the expression (18). On the contrary, in the other section we tried to build an energy as simple as possible and therefore with as few parameters as possible.

The parameters of the models here studied are obtained to replicate the trend of the data presented in [23]. It would be interesting to have more data on skeletal tetanized muscle in passive and active regimes to further validate our model. Moreover, experiments are typically performed on uniaxial deformations: exploring other types of deformations would be necessary for practical applications [16]. Finally, here we dealt only with time-independent models, where the system is at equilibrium and the viscous effects are negligible. In future work, we aim to enhance our model by considering the variation of stress-strain curves with the external loading rate.

## Acknowledgements

The authors would like to thank the anonymous reviewers for their detailed comments, which have significantly contributed to improve the manuscript.

This work was partially supported by National Group of Mathematical Physics (GNFM-INdAM, "INdAM – GNFM Project", codice CUP_E53C22001930001). This work is partially funded by the EuropeanUnion – NextGenerationEU under the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.1 - Call PRIN 2022 No. 104 of February 2, 2022 of Italian Ministry of University and Research; Project 202249PF73 (subject area: PE - Physical Sciences and Engineering) "Mathematical models for viscoelastic biological matter".

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