APPENDIX: Physiological Modeling

[This appendix aims at explaining the physiological muscle modeling with parameter setting in detail. Due to space limitations, this part is not included in our submitted manuscript.]

The strain energy function for a complete muscle is given by:

$$U = U_I + U_J + U_f \tag{1}$$

where U_I, U_J, and U_f are the strain energy densities for muscle matrix, related volume change and muscle fiber respectively. U_I and U_J are described in our paper, they have the following term $U_I(\overline{I}_1, \overline{I}_2) = c_1(\overline{I}_1 - 3) + c_2(\overline{I}_2 - 3)$, $U_J = 1/2K(\ln J)^2$. In this appendix, we would give a detailed description on U_f.

1. strain energy densities for muscle fiber

As mentioned in our paper, a basic Hill three-element model (Fig.1) is constituted of a contractile element (CE), a serial elastic element (SEE) and a parallel elastic element (PE).

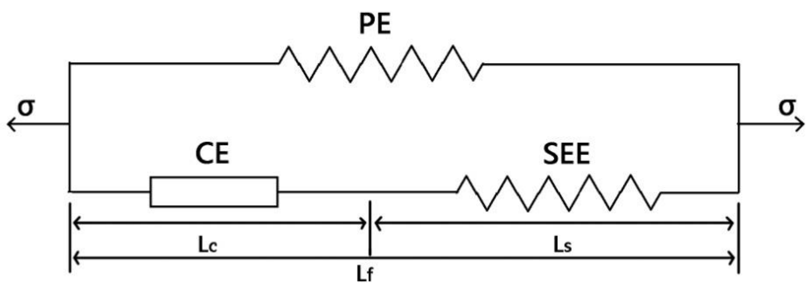

Figure 1: Hill three-element model.

For hyperelastic material, the strain energy function U per unit un-deformed volume can be established as the work done by the stress from the initial to the current position. Thus U_f can be defined as

$$U_f(\lambda_f) = \int_1^{\lambda_f} [\sigma_{PE}(\overline{\lambda}_f) + \sigma_{SEE}(\lambda_s)] d\overline{\lambda}_f \tag{2}$$

where λ_f is the fiber stretch ratio, λ_S is the stretch ratio in the SEE, σ_{PE} is the stress produced in the PE, σ_{SEE} is the stress produced in SEE. λ_S is the function of fiber stretch ration λ_f, which is explained below.

The stress ${}^{t+\Delta t}\sigma_{SEE}$ in SEE can be defined as the function of its stretch ${}^{t+\Delta t}\lambda_s$ at time $t+\Delta t$:

$$ {}^{t+\Delta t}\sigma_{SEE} = \beta[e^{\alpha({}^{t+\Delta t}\lambda_S - 1)} - 1] \tag{3} $$

where α and β are constants in relation to the stiffness of the SEE.

The stress ${}^{t+\Delta t}\sigma_{PE}$ in the PE at time $t+\Delta t$ is given by:

$$ {}^{t+\Delta t}\sigma_{PE} = \sigma_0 {}^{t+\Delta t} f_{PE}(\lambda_f) \tag{4} $$

where σ_0 is the maximum isometric stress, and ${}^{t+\Delta t} f_{PE}(\lambda_f)$ is given by

$$ {}^{t+\Delta t} f_{PE}(\lambda_f) = \begin{cases} 4({}^{t+\Delta t}\lambda_f - 1)^2 & \text{if } {}^{t+\Delta t}\lambda_f > 1 \\ 0 & \text{else} \end{cases} $$

Since having equation 3 and equation 4, as long as λ_S is calculated in function of λ_f, we can calculate the strain energy function stored in the fiber U_f. Here, we begin to explain how we get the value of λ_S.

2. Calculation of λ_S

As Hill model shows, the stress produced in the CE are time $t+\Delta t$ is given by:

$$ {}^{t+\Delta t}\sigma_{CE} = \sigma_0 \cdot {}^{t+\Delta t}a \cdot f_\lambda(\lambda_f) \cdot f_v(\lambda_C) \tag{5} $$

where σ_0 is the maximum isometric stress, ${}^{t+\Delta t}a$ is the muscle activation value at time $t+\Delta t$, $f_\lambda(\lambda_f)$ represent the muscle stress-stretch relationship as shown in equation 6, and $f_v(\lambda_C)$ represent the muscle stress-velocity relationship as shown in equation 7.

$$ f_\lambda(\lambda_f) = \begin{cases} 9({}^t\lambda_f/\lambda_{opt} - 0.4)^2 & \text{if } 0.4 \le {}^t\lambda_f/\lambda_{opt} < 0.6 \\ 1-4(1-{}^t\lambda_f/\lambda_{opt})^2 & \text{if } 0.6 \le {}^t\lambda_f/\lambda_{opt} < 1.4 \\ 9({}^t\lambda_f/\lambda_{opt} - 1.6)^2 & \text{if } 1.4 \le {}^t\lambda_f/\lambda_{opt} < 1.6 \\ 0 & \text{else} \end{cases} \tag{6} $$

where λ_{opt} is the optimal fiber stretch at which the muscle fiber would get the maximum isometric force.

$$ f_v(\lambda_C) = \begin{cases} \dfrac{1+\dot{\lambda}_C/\dot{\lambda}_C^{\min}}{1-k_c\,\dot{\lambda}_C/\dot{\lambda}_C^{\min}} & \text{if } \dot{\lambda}_C \le 0 \\ d-(d-1)\dfrac{1-\dot{\lambda}_C/\dot{\lambda}_C^{\min}}{1+k_c k_e\,\dot{\lambda}_C/\dot{\lambda}_C^{\min}} & \text{if } \dot{\lambda}_C > 0 \end{cases} \tag{7} $$

where k_c, k_e are the shape parameters of the hyperbolic tension force-velocity curve of the CE, d is the parameter quantifying the force offset with respect to the isometric case due to the eccentric movement, $\dot{\lambda}_C$ is the stretch rate of CE which is given by $\dot{\lambda}_C = \Delta\lambda_C / \Delta t$, and $\dot{\lambda}_C^{\min}$ is the minimum stretch rate that corresponds to the maximum isometric force.

In addition, the stress produce in CE is equal to the stress produced in SEE, which is expressed as

$$ {}^{t+\Delta t}\sigma_{CE} = {}^{t+\Delta t}\sigma_{SEE} \tag{8}$$

And it was assumed that k_l is the ratio of the length of SEE to that of CE, thus their geometry relation can be obtained from Fig.1 and expressed as

$$\Delta\lambda_C = \alpha - k_l \Delta\lambda_S \tag{9}$$

where $\alpha = (1+k_l)\,{}^{t+\Delta t}\lambda_f - {}^{t}\lambda_C - k_l\,{}^{t}\lambda_S$, and $\Delta\lambda_C$, $\Delta\lambda_S$ and $\Delta\lambda_f$ are the stretch increments of CE, SEE and muscle fiber respectively.

Therefore, we have got 4 functions (equation 3, equation 5, equation 8 and equation 9) as well as 5 unknown parameters (${}^{t+\Delta t}\sigma_{CE}$, ${}^{t+\Delta t}\sigma_{SEE}$, $\Delta\lambda_C$, $\Delta\lambda_S$ and $\Delta\lambda_f$), thus $\Delta\lambda_S$ can be expressed in function of $\Delta\lambda_f$, in other words, ${}^{t+\Delta t}\lambda_S (= {}^{t}\lambda_S + \Delta\lambda_S)$ can be expressed in function of ${}^{t+\Delta t}\lambda_f (= {}^{t}\lambda_f + \Delta\lambda_f)$. And finally, we can see that U_f is a function of only λ_f. The fiber stretch λ_f in the direction $\boldsymbol{N}$ of the un-deformed fiber is given by

$$\lambda_f = \sqrt{\mathbf{N}^T \bar{\mathbf{C}} \mathbf{N}} = \sqrt{\bar{\mathbf{C}} : (\mathbf{N}^T \otimes \mathbf{N})} \tag{10}$$

where $\bar{\boldsymbol{C}}$ is explained in our paper. The current muscle direction $\mathbf{n}$ after deformation $\mathbf{F}$ occurred is expressed as

$$\mathbf{n} = J^{-1/3} \frac{\mathbf{FN}}{\lambda_f} \tag{11}$$

$\mathbf{N}$ is a constant, while $\mathbf{n}$ is always changing with the change of $\mathbf{F}$. Thus we can see that λ_f is a function of only $\mathbf{F}$.

3. Cauchy stress and constitutive elasticity tensor

Next, by deriving the energy function U for a complete muscle, the Cauchy stress $\boldsymbol{\sigma}$ can be expressed as

$$
\begin{aligned}
\boldsymbol{\sigma} = & \frac{2}{J}[(c_1 + c_2\bar{I}_1^C)\bar{\mathbf{B}} - c_2\bar{\mathbf{B}}^2 - \frac{1}{3}(c_1\bar{I}_1^C + 2c_2\bar{I}_2^C)\mathbf{I}] \\
& + K(J-1)\mathbf{I} \\
& + \frac{1}{J}U_f^{'}[\lambda_f(\mathbf{n}\otimes\mathbf{n}) - \frac{1}{3}\lambda_f\mathbf{I}]
\end{aligned}
\tag{12}
$$

where $\mathbf{I}$ is the second-order unit tensor, $U_f^{'} = \sigma_0 \cdot f_{PEE}(\lambda_f) + \beta\{\exp[\alpha(\lambda_S - 1)] - 1\}$, and $\bar{\mathbf{B}}$ is the left Cauchy stress with the volume change eliminated and is expressed as $\bar{\mathbf{B}} = J^{-2/3}\mathbf{F}\mathbf{F}^T$.

And next, the fourth-order constitutive elasticity tensor $\mathbf{c}$ can be calculated as

$$
\begin{aligned}
\mathbf{c} = & K(J-1)(\mathbf{I}\otimes\mathbf{I} - 2\mathbf{I}\,\underline{\otimes}\,\mathbf{I}) - \tfrac{2}{3}(\mathrm{dev}\sigma\otimes\mathbf{I} + \mathbf{I}\otimes\mathrm{dev}\sigma) \\
& + \tfrac{4}{3J}(c_1\bar{I}_1^C + 2c_2\bar{I}_2^C)(\mathbf{I}\,\underline{\otimes}\,\mathbf{I} - \tfrac{1}{3}\mathbf{I}\otimes\mathbf{I}) \\
& + \tfrac{4c_2}{J}(\bar{\mathbf{B}}\otimes\bar{\mathbf{B}} - \bar{\mathbf{B}}\,\underline{\otimes}\,\bar{\mathbf{B}}) + \tfrac{8c_2\bar{I}_2^C}{9J}(\mathbf{I}\otimes\mathbf{I}) \\
& - \tfrac{4c_2}{3J}[(\bar{I}_1^C\bar{\mathbf{B}} - \bar{\mathbf{B}}^2)\otimes\mathbf{I} + \mathbf{I}\otimes(\bar{I}_1^C\bar{\mathbf{B}} - \bar{\mathbf{B}}^2)] \\
& + \frac{1}{J}[\frac{1}{9}\lambda_f(U_f^{'} + \lambda_f U_f^{''}) + J(U_J^{'} + JU_J^{''})]\mathbf{I}\otimes\mathbf{I} \\
& + \frac{\bar{\lambda}_f^2}{J}(U_f^{'} - \lambda_f^{-1}U_f^{''})(\mathbf{n}\otimes\mathbf{n}\otimes\mathbf{n}\otimes\mathbf{n}) \\
& - \frac{\bar{\lambda}_f^2}{3J}(U_f^{''} + \lambda_f^{-1}U_J^{'})(\mathbf{n}\otimes\mathbf{n}\otimes\mathbf{I} + \mathbf{I}\otimes\mathbf{n}\otimes\mathbf{n}) \\
& + \frac{2}{J}(\frac{1}{3}\lambda_f - JU_J^{'})\mathbf{L}
\end{aligned}
\tag{13}
$$

where $\mathbf{L}$ is the symmetric fourth order unit tensor, and $U_f^{''}, U_J^{''}$ is given by

$$
U_f^{''} = U_{PE}^{''} + U_{SEE}^{''}
$$

$$
U_{PE}^{''}(\lambda_f) = {}'\sigma_0 \begin{cases} 8(\lambda_f - 1) & \text{If } \lambda_f > 1 \\ 0 & \text{else} \end{cases}
$$

$$
U_{SEE}^{''} = \alpha\beta\frac{1+k_l}{k_l}\exp[\alpha(\lambda_S - 1)]
$$

$$
U_J^{''} = K
$$

4. Summary

For our proposed muscle biomechanical model, the material parameters (K , k_l , α , β , k_e , k_c , e_v , σ_0 , λ_{opt} , $\dot{\lambda}_C^{\min}$) are taken from pervious experimental data, the value of these parameters are shown in Tab.1, and activation value a is set according to manual setting or experimental estimation, the initial fiber direction $\mathbf{N}$ is specified by our proposed interactive muscle marking method, which is shown in our paper, the deformation gradient ${}^{t+\Delta t}\mathbf{F}$ at time $t+\Delta t$ served as the input parameters for this muscle model, and finally the Cauchy stress ${}^{t+\Delta t}\boldsymbol{\sigma}$ and constitutive elasticity tensor ${}^{t+\Delta t}\mathbf{c}$ could be computed.

By knowing ${}^{t+\Delta t}\boldsymbol{\sigma}$ and ${}^{t+\Delta t}\mathbf{c}$, the muscle deformation under activation value a can be implemented using a user-defined material subroutine (UMAT) in ABAQUS, or any other Finite-element software package.

Parameter	K	k_l	α	β (N/m^2)	k_e	k_c	e_v (N/m^2)	σ_0 (N/m^2)	λ_{opt}	$\dot{\lambda}_C^{\min}$ (s^{-1})	c_1	c_2
Value	1×10^9	0.3	9.4	1×10^5	5	5	7×10^4	2.2×10^5	1.05	2	10	10
Reference	[2]	[1]	[1]	[1]	[3]	[3]	[1]	[1]	[4]	[1]	[5]	[5]

Table 1. Material parameters.

[1] Kojic M, Mijailovic S, Zdravkovic N. Modelling of muscle behaviour by the finite element method using Hill's three‐element model[J]. International journal for numerical methods in engineering, 1998, 43(5): 941-953.

[2] Simo J C, Taylor R L. Quasi-incompressible finite elasticity in principal stretches. Continuum basis and numerical algorithms[J]. Computer Methods in Applied Mechanics and Engineering, 1991, 85(3): 273-310.

[3] BolM, Reese S. Micromechanical modelling of skeletal muscles based on the finite element method. Comput Methods Biomech Biomed Eng 2008; 11(5): 489–504.

[4] Gordon AM, Huxley AF, Julian FJ. The variation in isometric tension with sarcomere length in vertebrate muscle fibres. J Physiol 1966; 184(1): 170–192.

[5] Weiss J A, Maker B N, Govindjee S. Finite element implementation of incompressible, transversely isotropic hyperelasticity[J]. Computer methods in applied mechanics and engineering, 1996, 135(1): 107-128.