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MUSCLE MODELING IN THE FINITE ELEMENT SOLVER PAK

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Abstract

This paper presents the integration of muscle fatigue modeling into the finite element solver PAK, based on an extended version of Hill’s phenomenological model. While traditional muscle models focus primarily on force generation, this study incorporates fatigue dynamics to provide a more realistic representation of muscle performance over time. By extending Hill’s three-component model to take into account different types of muscle fibers and their distinct fatigue characteristics, we improve the accuracy of computational muscle simulations.

The proposed approach employs functionally graded materials (FGM) to model heterogeneous muscle structures and utilizes an incremental-iterative finite element scheme to calculate equilibrium configurations. The developed model is validated through comparisons with experimental data, demonstrating its ability to capture key aspects of muscle contraction, force production, fatigue progression, and recovery.

The implementation of this model in PAK provides a powerful computational tool for biomechanical research, with potential applications in rehabilitation engineering, sports science, and musculoskeletal system simulations. Future work will focus on refining fatigue mechanisms and extending the model to simulate full musculoskeletal interactions. This study contributes to the advancement of computational biomechanics by enabling more accurate and physiologically relevant simulations of muscle function.

Keywords: muscle, modeling, finite element, fatigue, functionally graded materials

1. Introduction

Muscle modeling plays a crucial role in biomechanics, enabling researchers and engineers to study muscle function, force generation, and fatigue under various physiological and pathological conditions. The complexity of muscle tissue, which exhibits both passive and active mechanical behavior, requires advanced computational methods to capture its nonlinear and time-dependent properties. Among various modeling techniques, phenomenological approaches, such as Hill's three-component model, have been widely used due to their ability to describe muscle contraction dynamics in a computationally efficient manner.

The finite element method (FEM) has emerged as a powerful tool for simulating biomechanical systems, including skeletal muscles (Kojic et al. 2008). By discretizing muscle tissue into finite elements, FEM allows for detailed analysis of muscle deformation, force transmission, and interaction with surrounding structures. However, incorporating muscle-specific constitutive laws and activation dynamics into FEM frameworks poses significant challenges, necessitating the development of specialized computational models and numerical schemes.

PAK (Kojic et al. 1996), a finite element solver developed for complex engineering and biomechanical applications, has been extended to support advanced muscle modeling. In our research, we have implemented muscle constitutive models into PAK, incorporating Hill's three-component model and its extensions to take into account different types of muscle fibers and fatigue effects. These enhancements allow for realistic simulations of muscle function under various loading and activation conditions, improving the accuracy of biomechanical predictions.

This paper presents the implementation of muscle modeling in PAK, detailing the numerical formulations, subroutines, and computational strategies used to simulate skeletal muscle behavior. Additionally, we discuss the integration of fatigue modeling, verification through experimental data, and potential applications of the developed framework. By leveraging these advancements, PAK provides a robust platform for investigating muscle mechanics, contributing to the fields of biomechanics, rehabilitation engineering, and biomedical research.

2. Overview of Muscle Modelling Approaches

The study of muscle mechanics is essential for understanding the physiological behavior of muscles under various loading and activation conditions. Over the years, numerous mathematical models have been developed to describe muscle contraction, ranging from simple empirical models to complex multiscale approaches that account for molecular interactions. Among these, phenomenological models have gained widespread use due to their ability to capture essential mechanical properties of muscles with relatively low computational cost.

2.1. Phenomenological Models of Muscle Contraction

Phenomenological models describe muscle behavior using mathematical functions derived from experimental observations. These models do not explicitly consider the underlying molecular mechanisms of muscle contraction but instead provide macroscopic descriptions of force generation. One of the most well-known phenomenological models is Hill's three-component model, which has been extensively used in muscle modeling due to its simplicity and effectiveness in simulating skeletal muscle mechanics.

2.2. Hill's Three-Component Model

Hill's model, originally proposed in 1938 (Hill, 1938), is based on experimental studies of tetanized frog muscles.

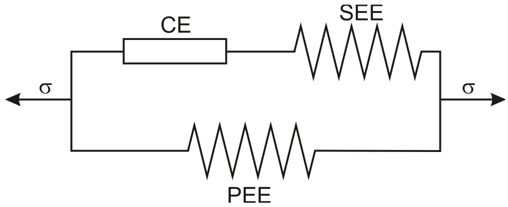

Fig. 1. Hill's mechanical representation of muscle components

The model consists of three key elements:

- **Contractile Element (CE)** represents the active force generation in muscle fibers due to the interaction of actin and myosin filaments. The force output of the CE is velocity-dependent and follows the well-known Hill equation:

$$(v+b)(S+a)=b(S_0+a) \tag{1}$$

  The variable S stands for the muscle tension, v represents the contraction velocity, while a, and b are parameters obtained from the experiment. The constant S_0 represents the maximum isometric force.

- **Series Elastic Element (SEE)** represents the elasticity of tendons and passive structural components within muscle fibers. This element accounts for the force-stretch relationship and is typically modeled using an exponential or linear function.

- **Parallel Elastic Element (PEE)** represents the passive elastic behavior of muscle tissue, including the extracellular matrix and connective tissue. It contributes to muscle stiffness when the muscle is stretched beyond its resting length.

Hill's model has been successfully applied in various biomechanical studies due to its ability to describe the force-velocity and force-length relationships observed in muscle behavior. However, despite its effectiveness, the model has several limitations. It assumes homogeneous muscle properties and does not account for the physiological diversity of muscle fiber types or the effects of fatigue.

2.3. Extensions of Hill's Model

To address the limitations of the classical Hill model, we have introduced several modifications and extensions. These include:

- **Multi-Fiber Hill Models:** Instead of treating muscle as a uniform entity, these models consider different fiber types, such as slow-twitch and fast-twitch fibers, which exhibit distinct mechanical and metabolic characteristics. This way a more realistic simulation of muscle behavior under varying loading conditions is enabled.

- **Fatigue Modeling:** Traditional Hill-based models do not account for muscle fatigue, which significantly affects force production over time. We have made extensions of the Hill model to incorporate fatigue effects by introducing time-dependent changes in force output, based on experimental fatigue curves. These modifications enable a more realistic simulation of prolonged or repetitive muscle contractions.

- **Functionally Graded Material (FGM) Models:** Since real muscles exhibit spatially varying properties due to fiber distribution and metabolic differences, we have introduced functionally graded material models. These models incorporate spatially dependent constitutive properties to more accurately represent muscle heterogeneity.

2.4. Finite Element Implementation of Muscle Models

The finite element method (FEM) provides a powerful computational framework for simulating muscle mechanics, particularly in complex geometries. In FEM-based muscle modeling, muscle tissue is discretized into finite elements, each assigned material properties corresponding to active and passive muscle components. The incorporation of Hill's model and its extensions into FEM enables detailed analysis of muscle function under various loading and activation conditions.

One of the key challenges in FEM-based muscle modeling is the integration of constitutive laws governing muscle contraction. This involves solving nonlinear equations that describe muscle activation, force generation, and interaction with surrounding tissues. The implementation of muscle models within PAK FEM solver allows for simulations that account for large deformations, anisotropic material properties, and realistic muscle activation dynamics.

3. Implementation in PAK

The finite element solver PAK has been extended to support muscle modeling by incorporating phenomenological muscle contraction models, particularly Hill's three-component model and its advanced extensions. The implementation in PAK allows for the simulation of active and passive muscle mechanics, including force generation, fatigue effects, and heterogeneous muscle fiber composition. This section details the numerical formulation, integration of constitutive laws, and specific subroutines developed for muscle modeling in PAK.

3.1. Finite Element Discretization of Muscle Tissue

Muscle tissue is discretized using three-dimensional finite elements where each element is assigned material properties corresponding to both active (contractile) and passive (elastic) muscle components. The primary challenges in muscle modeling using FEM involve:

- **Large deformations and anisotropic behavior** due to the fibrous structure of muscles.
- **Nonlinear force-stretch and force-velocity relationships**, as described by Hill's model.
- **Time-dependent effects**, including fatigue and recovery.

To accurately simulate muscle behavior, PAK employs **functionally graded materials (**FGMs**)** to represent heterogeneous muscle composition. Each finite element is assigned a distribution of fiber types (slow-twitch and fast-twitch), allowing for more precise modeling of muscle mechanics.

3.2. Integration of Hill's Model into PAK

The Hill three-component model is incorporated into PAK through a combination of constitutive equations and incremental-iterative solution schemes. The governing equations for the contractile element (CE), series elastic element (SEE), and parallel elastic element (PEE) are solved within the incremental-iterative framework of nonlinear FEM.

The generation of active muscle force originates from the actomyosin enzymatic cycle, driven by the interactions between myosin molecules and actin filaments. Active tension and muscle stiffness are subsequently computed at each finite element integration (Gaussian) point (Fig. 2b).

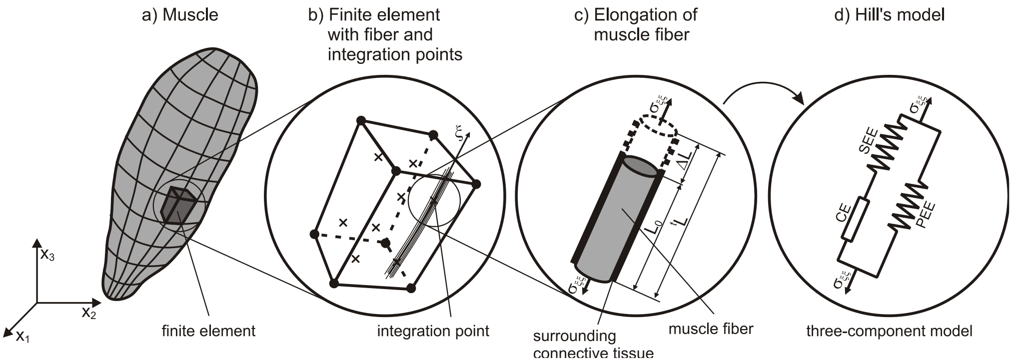

Fig. 2. Schematic representation of muscle finite element (FE) modeling, illustrating the transition from muscle as a deformable body to Hill's model. a) Discretization of the muscle into finite elements; b) A three-dimensional finite element with integration points and embedded muscle fiber; c) Elongation of a muscle fiber under applied stress $\sigma_{\xi\xi}$; d) Hill's three-component model.

At the time $(t+\Delta t)$, the equilibrium equation of a finite element structure in its deformed configuration is expressed as:

$$({}^{t+\Delta t}\mathbf{K}_{pass} + {}^{t+\Delta t}\mathbf{K}_{act})^{(i-1)}\delta\mathbf{U}^{(i)} = {}^{t+\Delta t}\mathbf{F}_{ext} + {}^{t+\Delta t}\mathbf{F}_{pass}^{(i-1)} + {}^{t+\Delta t}\mathbf{F}_{act}^{(i-1)} \tag{2}$$

where ${}^{t+\Delta t}\mathbf{F}_{ext}$, ${}^{t+\Delta t}\mathbf{F}_{pass}^{(i-1)}$, and ${}^{t+\Delta t}\mathbf{F}_{act}^{(i-1)}$ denote the vectors corresponding to external loads, passive internal nodal forces, and active molecular forces, each assembled into the finite element nodal force representation; ${}^{t+\Delta t}\mathbf{K}_{pass}^{(i-1)}$ represents the stiffness matrix associated with the passive components of the muscle, while ${}^{t+\Delta t}\mathbf{K}_{act}^{(i-1)}$ corresponds to the cumulative stiffness arising from actomyosin cross-bridge interactions; the nodal displacement increments at iteration (i) are represented by $\delta U^{(i)}$. At the macroscopic level, the discrete actin–myosin interactions are homogenized into a continuum description, where the resulting active stress is incorporated into the finite element nodal forces, ${}^{t+\Delta t}\mathbf{F}_{act}^{(i-1)}$, and the active muscle stiffness is incorporated into the finite element nodal stiffness matrix, ${}^{t+\Delta t}\mathbf{K}_{act}^{(i-1)}$. A detailed description of nodal force and stiffness matrix calculations within a standard finite element framework can be found in (Kojic et al. 2008, Stojanovic et al. 2007). For muscle modeling, however, the computation of element nodal forces—both passive and active—is carried out as follows:

$$
{}^{t+\Delta t}\mathbf{F}_{pass}^{(i-1)} + {}^{t+\Delta t}\mathbf{F}_{act}^{(i-1)} = \int_{{}^{t+\Delta t}V^{(i-1)}} {}^{t+\Delta t}\mathbf{B}_{L}^{T(i-1)}\ {}^{t+\Delta t}\left[\boldsymbol{\sigma}_{pass}^{(i-1)} + \boldsymbol{\sigma}_{act}^{(i-1)}\right] dV \tag{3}
$$

where ${}^{t+\Delta t}\mathbf{B}_{L}^{T(i-1)}$ denotes the transpose of the geometric linear strain–displacement matrix, $\boldsymbol{\sigma}_{pass}^{(i-1)}$ and $\boldsymbol{\sigma}_{act}^{(i-1)}$ represent the passive and active stress tensors in the form of the second Piola–Kirchhoff measure, and ${}^{t+\Delta t}\mathbf{V}^{(i-1)}$ is the finite element volume. The index $(i-1)$ denotes the most recent muscle configuration obtained during the equilibrium iterations within a given time step.

The material's resistance to deformation is governed by the variable stiffness contributions of actomyosin cross-bridge bonds, ${}^{t+\Delta t}\mathbf{K}_{act}^{(i-1)}$, as well as by the passive component associated with the connective tissue, ${}^{t+\Delta t}\mathbf{K}_{pass}^{(i-1)}$:

$$
{}^{t+\Delta t}\mathbf{K}_{act}^{(i-1)} + {}^{t+\Delta t}\mathbf{K}_{pass}^{(i-1)} = \int_{{}^{t+\Delta t}V^{(i-1)}} \left({}^{t+\Delta t}\mathbf{B}_{L}^{T}\ {}^{t+\Delta t}\mathbf{C}\ {}^{t+\Delta t}\mathbf{B}_{L}\right)^{(i-1)} dV + \int_{{}^{t+\Delta t}V^{(i-1)}} \left({}^{t+\Delta t}\mathbf{B}_{NL}^{T}\ {}^{t+\Delta t}\mathbf{S}\ {}^{t+\Delta t}\mathbf{B}_{NL}\right)^{(i-1)} dV \tag{4}
$$

where ${}^{t+\Delta t}\mathbf{B}_{NL}$ denotes the nonlinear strain–displacement transformation matrix, ${}^{t+\Delta t}\mathbf{C}$ represents the constitutive matrix that defines the stress–strain relationship for both the passive and active components, and ${}^{t+\Delta t}\mathbf{S}$ the assembled matrix of second Piola–Kirchhoff stress components accounting for passive and active parts. It should be emphasized that the formulation in Eq. (4) accounts for both material and geometric nonlinearities, which is crucial for accurately modeling muscle behavior characterized by large strains, displacements, and rotations.

By introducing additional boundary conditions and constraints into the dynamic force equilibrium of Eq. (2), a unique prediction of the mechanical response of muscle tissue can be obtained. Once the element nodal forces and stiffness matrices are computed, the global system of equations (1) is assembled and solved for the entire muscle (Fig. 2a). In order to ensure the equilibrium of $\mathbf{F}_{ext}$, $\mathbf{F}_{pass}$, and $\mathbf{F}_{act}$ at the end of each time step, $t+\Delta t$, the vector of displacements $\mathbf{U}^{(i)}$ is iteratively incremented by $\delta\mathbf{U}^{(i)}$, until the convergence criterion is satisfied ($\delta\mathbf{U}^{(i)} \approx 0$) (Bathe 1996, Kojic and Bathe 2005). The active forces, ${}^{t+\Delta t}\mathbf{F}_{act}^{(i-1)}$, and stiffness, ${}^{t+\Delta t}\mathbf{K}_{act}^{(i-1)}$, are directly influenced by the deformation rate along the principal direction of the muscle fibers (Kojic et al. 2008, Mijailovich et al. 2010). Consequently, the solution of the above equation must account for the effects of shortening velocity on strain-dependent cross-bridge state transitions at the microscale (McMahon, 1984, Smith and Mijailovich, 2008).

The muscle stress $\boldsymbol{\sigma}$ is decomposed into:

- **Active stress** $\boldsymbol{\sigma}_{act}$ is computed using Hill's force-velocity and force-length relationships.

- **Passive stress** $\boldsymbol{\sigma}_{pass}$ accounts for connective tissue elasticity, modeled using nonlinear hyperelastic material laws.

Applying Hill's equation we obtain active stress in the *i*-th fiber type as

$$ {}^{t+\Delta t}\sigma_m^i = {}^t\sigma_0^i \, {}^{t+\Delta t}\alpha_a^i \frac{1+\Delta\lambda_m^i / \Delta\lambda_{m0}^i}{1-c^i\Delta\lambda_m^i / \Delta\lambda_{m0}^i} \tag{5} $$

where ${}^{t+\Delta t}\sigma_m^i$ denotes the stress in the contractile element, $\Delta\lambda_m^i$ and $\Delta\lambda_{m0}^i$ are the stretch increment and the stretch increment under maximal contraction velocity, and $c^i = \sigma_0^i/\alpha^i$. The activation function ${}^{t+\Delta t}\alpha_a^i$ is introduced in order to enable simulate of submaximal fiber activation.

The constitutive relation for the stress of serial elastic element of the *i*-th fiber type is

$$ {}^{t+\Delta t}\sigma_s^i = \left({}^t\sigma_s^i + \beta^i\right)e^{\alpha^i\Delta\lambda_s^i} - \beta^i \tag{6} $$

where α^i and β^i are the material parameters of the fiber, and ${}^t\sigma_s^i$ is calculated as

$$ {}^t\sigma_s^i = \beta^i\left(e^{\alpha^i\left({}^t\lambda_s^i - 1\right)} - 1\right) \tag{7} $$

The stress within the parallel elastic element is determined as follows

$$ {}^{t+\Delta t}\boldsymbol{\sigma}^E = \mathbf{C}^E \, {}^{t+\Delta t}\mathbf{e} \tag{8} $$

where $\mathbf{C}^E$ describing the constitutive elasticity matrix of the connective tissue, while ${}^{t+\Delta t}\mathbf{e}$ corresponds to the strain at a given material point, evaluated on the basis of the displacement field.

3.3. Fatigue and Recovery Modeling in PAK

Muscle fatigue may develop when the tissue is subjected to sustained loading, whether constant or varying. As the ability of the muscle to generate force diminishes, the tetanic stress of a fatigued muscle $\sigma_{0f}(\lambda,t)$ is consistently lower than that of an intact, non-fatigued muscle $\sigma_0(\lambda,t)$. Let $F_0\left(\alpha_a,\lambda\right)$ denote the force produced by an intact muscle under activation α_a and total stretch λ, while $F_f\left(\alpha_a,\lambda,t\right)$ represents the force generated by the fatigued muscle under the same activation α_a. These forces are associated with the tetanized stress states $\sigma_0(\lambda,t)$ and $\sigma_{0f}(\lambda,t)$, respectively. The *fitness level* may then be defined as follows

$$ \alpha_f\left(t\right) = \frac{F_f\left(\alpha_a,\lambda,t\right)}{F_0\left(\alpha_a,\lambda\right)} = \frac{\sigma_{0f}(\lambda,t)}{\sigma_0(\lambda)} \tag{9} $$

Accordingly, the fitness level is defined as the normalized maximal force output of the muscle, with values ranging between 0 and 1. For an intact muscle, the fitness level equals 1, whereas under sustained loading it progressively decreases over time.

The stress generated within the contractile element of a fatigued muscle is expressed as

$$\begin{aligned} {}^{n+1}\sigma_m &= {}^{n+1}\alpha_a \, {}^{n}\sigma_{0f}\left(\lambda_p\right)\frac{1+\Delta\lambda_m/\Delta\lambda_{m0}}{1-c\Delta\lambda_m/\Delta\lambda_{m0}} \\ &= {}^{n+1}\alpha_a \, {}^{n}\alpha_f \, {}^{n}\sigma_0\left(\lambda_p\right)\frac{1+\Delta\lambda_m/\Delta\lambda_{m0}}{1-c\Delta\lambda_m/\Delta\lambda_{m0}} \end{aligned} \tag{10}$$

Because the mechanisms underlying muscle fatigue remain insufficiently understood, no universally reliable model exists to predict the fitness level of a muscle subjected to arbitrary activation over prolonged periods. Nevertheless, several models reported in the cited literature provide approaches for estimating the fitness level $\alpha_f\left(t,...\right)$, which is influenced by time, activation, and a range of physiological and non-physiological factors.

3.5. Verification and Validation

To illustrate the key characteristics of the multi-fiber Hill's muscle model, a simplified representation of the *biceps brachii* is adopted (Fig. 3). The muscle belly is discretized using three-dimensional eight-node hexahedral finite elements, with the fiber orientation aligned along the third local element axis. The tendons linking the muscle to the fixation points are represented by a layer of 3D elements in combination with a bundle of 1D truss elements assigned elastic material properties. The proximal tendon is anchored at the fixation point, whereas the distal tendon is connected to the constrained point via an elastic spring.

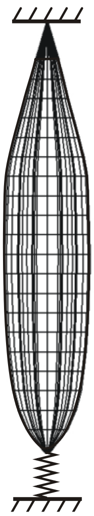

Fig. 3. Simplified finite element model of the human *biceps brachii* muscle

Two numerical simulations were conducted to verify the correct implementation of the multi-fiber Hill's model and the generalized isoparametric element formulation for functionally graded materials within the finite element solver PAK. In the first case, Hill's three-component muscle model was applied, with material properties and the activation function adopted from the literature. In the second case, Hill's multi-fiber model was employed. The muscle was represented with two fiber types: type I (slow) and type II (fast), distributed such that type I fibers comprised 40% of the surface fibers of the biceps brachii and 60% of the deeper fibers, with a linear variation assumed across the cross-sectional radius. To ensure comparability between the two simulations, the properties of both fiber types in the second model were set equal to those used in the first simulation. The resulting muscle force as a function of time is presented in Fig. .

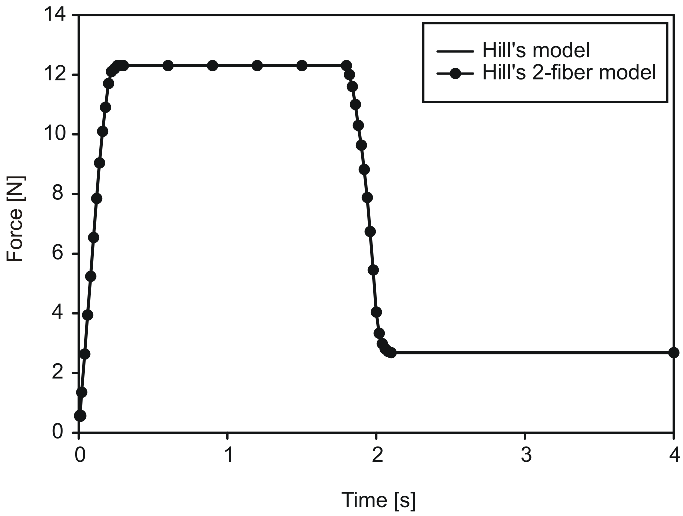

Fig. 4. Comparison between the classical Hill's model and its equivalent two-fiber formulation

As can be seen from Fig. , when identical characteristics are assigned to both fiber types, the two-fiber Hill's model yields results that are indistinguishable from those of the equivalent Hill model. This confirms the correct implementation of both the multi-fiber Hill's formulation and the generalized isoparametric element approach for functionally graded materials.

4. Application in Lingual Deformation Modeling

The finite element solver PAK has been employed to model lingual deformation during swallowing, demonstrating its capability to simulate complex muscle mechanics. This application integrates Hill's three-component phenomenological model into a finite element solver to capture the intricate interactions of intrinsic and extrinsic tongue muscles. By utilizing diffusion tensor imaging (DTI) and tractography, the model aligns finite element meshes with the principal directions of muscle fibers, ensuring anatomically accurate simulations of lingual motion.

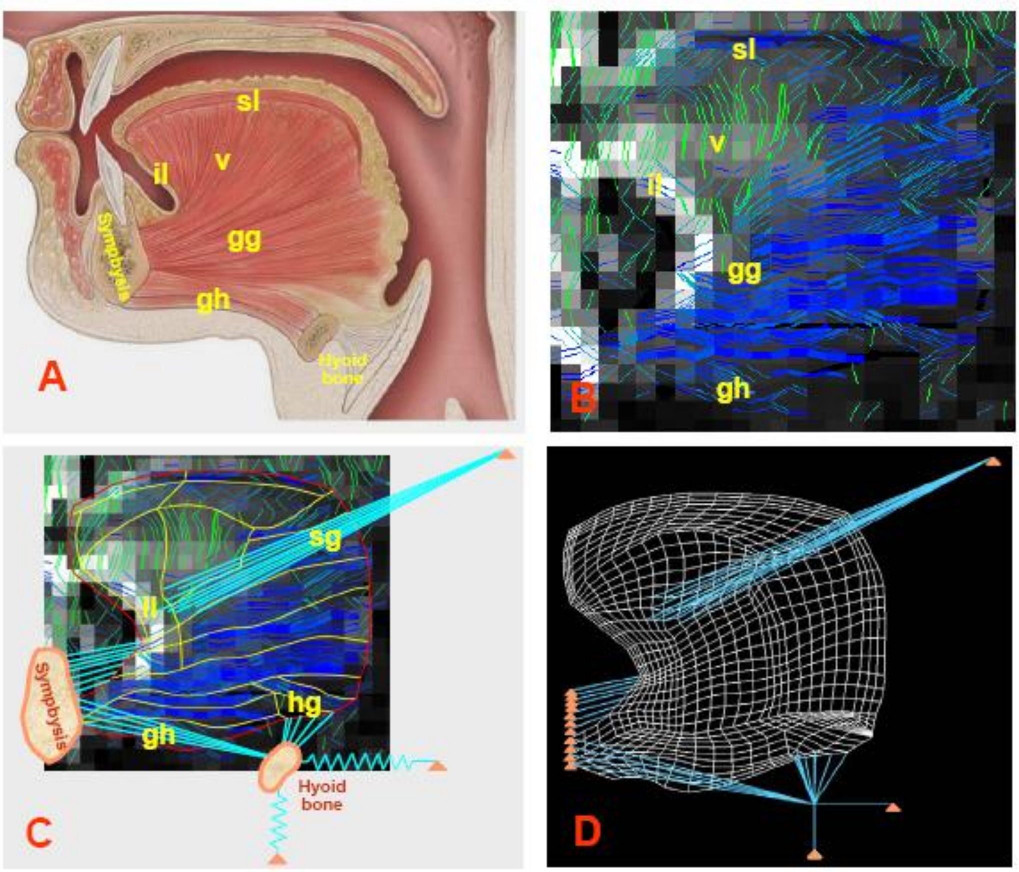

Fig. 5. Finite element mesh generation from diffusion tensor MRI–based tractography of human lingual myofiber tracts.

PAK facilitates a multiscale approach where the tongue is treated as a composite structure comprising anisotropic muscle fibers and isotropic connective tissue. The finite element formulation accounts for both passive and active muscle behaviors, enabling simulations of temporally patterned muscle activation during swallowing. The model incorporates both local and global mechanics by defining activation functions for different muscle groups, capturing the sequential engagement of genioglossus, hyoglossus, and styloglossus muscles in different phases of swallowing.

A significant advancement in this modeling effort is the ability to integrate physiological constraints such as boundary conditions imposed by the hard palate, pharyngeal structures, and hyoid bone movements. This allows for precise simulation of lingual tip elevation, posterior displacement, and rotational deformation observed in normal swallowing. The computed displacement fields, muscle stress distributions, and strain rate evaluations provide valuable insights into both normal and pathological swallowing mechanics.

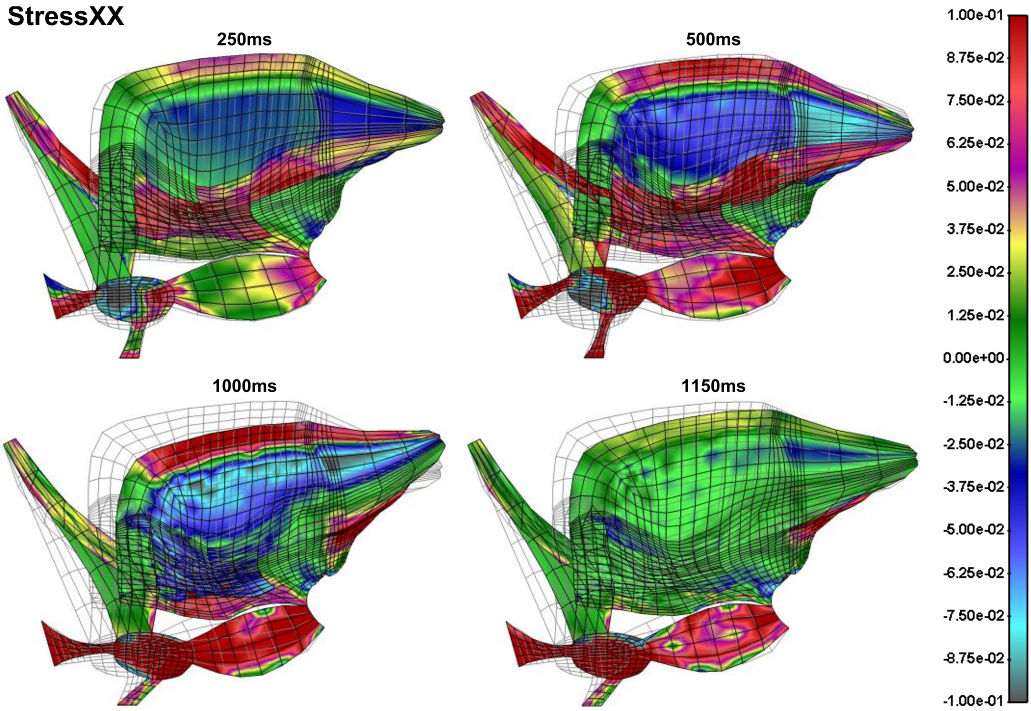

Fig. 6. Total muscle stress (MPa) along the fiber direction during swallowing.

The application of PAK in lingual biomechanics extends beyond basic muscle mechanics. It has potential applications in medical research, particularly in diagnosing and treating swallowing disorders (dysphagia) and speech impairments. The framework also supports surgical planning for procedures affecting tongue mobility and rehabilitation strategies for patients with neuromuscular impairments.

By leveraging the advanced muscle modeling capabilities of PAK, this study demonstrates its effectiveness in capturing the biomechanical complexity of the tongue. This work sets the stage for future research integrating neuromuscular control models and refining muscle activation patterns for improved therapeutic interventions.

5. Conclusion

This study presents a comprehensive computational approach to modeling muscle mechanics by incorporating muscle fatigue within the finite element solver PAK. By generalizing Hill's phenomenological model and extending it to account for different muscle fiber types, we developed a robust framework that enables accurate simulation of muscle behavior under various activation and loading conditions. The integration of fatigue mechanisms into Hill's model allows for a more realistic representation of muscle performance over time, particularly under prolonged or repeated contractions.

The numerical results obtained using PAK demonstrate that the proposed model successfully captures key aspects of muscle contraction, including force generation, fatigue progression, and recovery dynamics. Validation against experimental data and literature confirms the model's accuracy and reliability. Furthermore, the use of functionally graded material (FGM) formulations enables the modeling of heterogeneous muscle structures, enhancing the precision of finite element simulations.

The developed model and its implementation in PAK provide a valuable computational tool for researchers and engineers working in the field of muscle mechanics. Future work may focus on further refining fatigue models by incorporating more detailed biochemical and metabolic aspects, as well as exploring the interactions between muscle fatigue and neuromuscular control.

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