BIPHASIC FIBER-REINFORCED MODELING OF CARTILAGE WITH SAMPLE-SPECIFIC DISTRIBUTED COLLAGEN FIBER ORIENTATIONS

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Summary To model the structural and diffusional response of cartilage we propose a new biphasic, dispersed fiber-reinforced constitutive model which we implement in 3D large-strain finite elements. We complete two simulations of an indentation experiment, one with the sample-specific collagen fiber fabric (from DT-MRI) and one without the fiber contribution. The sample-specific, fiber-dependent permeability acts to maintain fluid pressure beneath the contact surface, enhancing load support and shielding the solid matrix.

INTRODUCTION

Recent publications report that the anisotropic diffusion of fluid in cartilage, e.g., as visualized by Diffusion Tensor Imaging (DTI or DT-MRI), a Magnetic Resonance Imaging (MRI) technique, is largely influenced by the general orientation of the (mainly Type II) collagen fibers, see, e.g., [1]. In fact, two tissue components principally control diffusion of the fluid phase: (i) the proteoglycan gel that gives a baseline isotropic diffusivity, and (ii) the highly anisotropic collagenous fiber network [1]. To model the complex structural and diffusional response of articular cartilage, we propose a new biphasic dispersed fiber-reinforced constitutive model which we implement in 3D large-strain finite elements. As representative numerical examples, we complete two sample-specific finite element (FE) simulations of an indentation experiment, one considering the sample-specific collagen fiber fabric (employing DT-MRI data and the methodology detailed in [2]) and one without considering the fiber contribution.

METHODS AND MATERIALS

Mathematical Model

We propose constitutive relations for the partial Cauchy stress tensors ($\boldsymbol{\sigma}^{\mathrm{S}}$ for solid and $\boldsymbol{\sigma}^{\mathrm{F}}$ for fluid) as

$$\boldsymbol{\sigma}^{\mathrm{S}} = -\, n^{\mathrm{S}}\, p\, \mathbf{I} + 2\, \rho^{\mathrm{S}}\, \mathbf{F}_{\mathrm{S}} \frac{\partial \Psi^{\mathrm{S}}}{\partial \mathbf{C}_{\mathrm{S}}}\, \mathbf{F}_{\mathrm{S}}^{\mathrm{T}} = -\, n^{\mathrm{S}}\, p\, \mathbf{I} + \boldsymbol{\sigma}_{\mathrm{E}}^{\mathrm{S}}\,, \qquad \boldsymbol{\sigma}^{\mathrm{F}} = -\, n^{\mathrm{F}}\, p\, \mathbf{I}\,, \tag{1}$$

where $\boldsymbol{\sigma}_{\mathrm{E}}^{\mathrm{S}}$ is the effective Cauchy stress tensor, see, e.g., [3], n^{α} ($\alpha \in \{\mathrm{S},\, \mathrm{F}\}$) are volume fractions, p is the fluid pressure, $\mathbf{I}$ is the identity tensor, ρ^{S} is the partial density of the solid, $\mathbf{F}_{\mathrm{S}}$ is the deformation gradient of the solid and $\mathbf{C}_{\mathrm{S}}$ is the corresponding right Cauchy-Green tensor. We propose an additive decomposition of the solid Helmholtz free-energy function Ψ^{S} into an isotropic matrix part $\Psi_{\mathrm{IM}}^{\mathrm{S}}$ and a transversely isotropic (fiber fabric) part $\Psi_{\mathrm{FF}}^{\mathrm{S}}$, i.e. $\Psi^{\mathrm{S}} = \Psi_{\mathrm{IM}}^{\mathrm{S}}\,(J_{\mathrm{S}},\, I_1) + \Psi_{\mathrm{FF}}^{\mathrm{S}}\,(I_1,\, I_4)$, where $I_1 := \mathrm{tr}\mathbf{C}_{\mathrm{S}}$, $I_4 := \mathbf{C}_{\mathrm{S}} : \mathbf{M}_0$, with $\mathbf{M}_0 = \mathbf{a}_0 \otimes \mathbf{a}_0$ a (Lagrangian) structural tensor, and the local principal direction of the collagen fibers is characterized by the (reference) direction vector $\mathbf{a}_0$, with $|\mathbf{a}_0| = 1$. We use the Helmholtz free-energy function of [4] for $\Psi_{\mathrm{IM}}^{\mathrm{S}}$, a formulation which includes penalty functions to control material incompressibility and compaction. We capture the nonlinear response of the collagen fiber fabric with a strain-energy function extended to consider dispersion of the collagen fiber orientation as [5]

$$\Psi_{\mathrm{FF}}^{\mathrm{S}}\,(I_1, I_4) = \frac{1}{\rho_{0\mathrm{S}}^{\mathrm{S}}} \left\{ \frac{k_1}{2k_2} \left\{ \exp[k_2 (I_4^{\star} - 1)^2] - 1 \right\} \right\}, \qquad I_4^{\star} = \kappa I_1 + (1 - 3\kappa) I_4\,, \tag{2}$$

where $\rho_{0\mathrm{S}}^{\mathrm{S}}$ is the reference solid density, $k_1 > 0$ and $k_2 > 0$ are material parameters which control the nonlinear fiber fabric response, and $\Psi_{\mathrm{FF}}^{\mathrm{S}} = 0$ for $I_4 < 1$, i.e. the collagen fibers only engage under stretches greater than unity. The parameter $\kappa \in [0, 1/3]$ describes the 'degree of anisotropy' where the limit $\kappa = 0$ represents ideal alignment of collagen fibers, while the limit $\kappa = 1/3$ represents an isotropic distribution of the collagen fabric.
We capture the anisotropic intrinsic permeability of the cartilage solid matrix $\mathbf{K}_{\mathrm{F}}$ as

$$\mathbf{K}_{\mathrm{F}} = \left(\frac{n^{\mathrm{F}}}{1 - n_{0\mathrm{S}}^{\mathrm{S}}} \right)^{m} k_{0\mathrm{S}}\, \mathbf{M}^{\star}\,, \qquad \mathbf{M}^{\star} = \kappa \mathbf{I} + \frac{(1 - 3\kappa)}{I_4} \mathbf{M}\,, \tag{3}$$

where the permeability depends on the deformation, $k_{0\mathrm{S}}$ [m^4/Ns] is the initial Darcy permeability and m is a dimensionless material parameter. Inclusion of the volume fraction n^{F} relates to the change of permeability caused by the change of pore space, where $n_{0\mathrm{S}}^{\mathrm{S}}$ is the reference solid volume fraction. The (spatial) structural tensor $\mathbf{M}$ is defined as $\mathbf{M} = \mathbf{a} \otimes \mathbf{a} = \mathbf{F}_{\mathrm{S}}\, \mathbf{a}_0 \otimes \mathbf{F}_{\mathrm{S}}\, \mathbf{a}_0 = \mathbf{F}_{\mathrm{S}}\, \mathbf{M}_0\, \mathbf{F}_{\mathrm{S}}^{\mathrm{T}}$. Finally, we implement this formulation in 3D large-strain finite elements.

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Analysis of DT-MRI

By careful construction of the FE mesh, a one-to-one mapping from tensors to elements exists within 'inner' regions of the sample [2]. Due to geometrical constraints, this one-to-one mapping breaks down along the sample boundary; here we interpolate tensors in a Log-Euclidean framework [6]. Finally, we have one tensor of estimated diffusion data per finite element. Let $\mathbf{A}$ be one such DTI data tensor for a specific finite element in the mesh, where the unique solution to the eigenproblem $\mathbf{A}\hat{\mathbf{n}}_i = \Lambda_i \hat{\mathbf{n}}_i, i = 1, 2, 3$; no summation, leads to the eigenbasis $\hat{\mathbf{n}}_i$ with corresponding eigenvalues Λ_i.
We take the eigenvector corresponding to the first principal eigenvalue as the principal (reference) fiber direction in the collagen fiber fabric, i.e. $\mathbf{a}_0 = \hat{\mathbf{n}}_1$. Given the principal direction $\mathbf{a}_0$ for a specific element, we estimate the corresponding structure parameter κ using an adjusted set of 'eigenvalues' determined by a normalization condition, i.e.

$$\alpha_i = \frac{\Lambda_i}{\mathrm{tr}\mathbf{A}} = \frac{\Lambda_i}{\Lambda_1 + \Lambda_2 + \Lambda_3}\,, \qquad i = 1, 2, 3\,, \tag{4}$$

such that the normalized values meet the required restriction $\alpha_1 + \alpha_2 + \alpha_3 = 1$. Next, we ensure transverse isotropy, as required by the constitutive model, by a transversely isotropic condition, i.e. $\alpha_{2T} = \alpha_{3T} = (\alpha_2 + \alpha_3)/2$. This mapping to adjusted 'eigenvalues' $\alpha_1, \alpha_{2T}, \alpha_{3T}$ fulfills all normalization requirements of the constitutive model [5], and captures a physically meaningful measure of the fiber dispersion. As a result, κ is directly available as $\kappa = \alpha_{2T} = \alpha_{3T}$ [2].

Representative Numerical Example

In [2], the left patella of a healthy 27-year-old male donor is harvested within 24 hours from death. The sample is cut into a cuboid form to fit into a glass vessel and placed within the vessel under physiologic solution. DT-MRI measurements are first performed on the unindented sample according to the protocol detailed in [2]. After all measurements are completed, the sample is indented ~ 0.50 mm (resulting in a compression of ~ 20 %) using a cylindrical, flat-tipped glass indenter. The sample is allowed to reach thermodynamic equilibrium before measuring it again using the same DT-MRI protocol.
In order to model the experiment, we estimate the geometry of the cartilage, as well as the initial/final location and orientation of the indenter, from the DT-MRI data. The simulations employ 25 194 eight-node brick elements of the Taylor-Hood type, with quadratic shape functions for solid displacements and bi-linear shape-functions for saturation pressure; the Newmark method is used for the time discretization. We specify that the (discretized) cartilage remain within the cylindrical containment vessel using a frictionless rigid-deformable contact algorithm. The contact problem between the cartilage sample and the indenter uses a specialized smooth contact algorithm [7].

RESULTS

By comparison of the representative numerical examples, we are able to draw some conclusions about the role of the collagen fiber fabric on the response of cartilage to indentation. The sample-specific, fiber fabric-dependent permeability modulates the standard behavior of the poroelastic formulation and acts to maintain fluid pressure beneath the contact surface, and thus enhancing load support, shielding the solid matrix and minimizing friction.

DISCUSSION

Our results are consistent with the cartilage mechanics literature wherein researchers note that the arrangement of the collagen fiber network plays an important role in directing fluid flow to optimize tissue function, cf. [8]. (DT-)MRI alone can not yet be used to determine the functional state of cartilage [9]. Given recent advances in in vivo DT-MRI [10], there is hope that a multi-disciplinary combination of DT-MRI and numerical simulation will bring this goal to fruition.

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