Supporting Material

Long Range Force Transmission in Fibrous Matrices Enabled by Tension-Driven Alignment of Fibers

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A: Discrete fiber simulations

We developed a finite element based 2D discrete fiber model that captures all aspects of network mechanics including non-affine stiffening, fiber alignment and bending-stretching transitions following our earlier work on crosslinked biopolymer networks (1). The 2D random fiber networks representing collagen gels are created with linear elastic fibers and rigid crosslinks (Fig. 1a). Fibers are uniformly distributed in the computational domain and a crosslink is formed when two fibers intersect. Collagen fibers have diameter in the range of few 100 nanometers to few microns and moduli of few 100 kPa (2–4). As the persistence length of collagen fibers is in the range of few microns, these fibers are typically modeled as linear elastic. Fibers are modeled using shear flexible Timoshenko beam elements in the finite element package, ABAQUS (5). Collagen gel considered in experiments is converted into a computational network (with equivalent fiber density) using the approach of Stein, Andrew M., et al (6). For the given concentration and volume of the gel, fiber radius is given by

$$r = \sqrt{\frac{V_g \rho_c v_c}{\pi L_{Tot}}} \qquad (A1)$$

where V_g $(\mu m^3)$is the volume of the gel, $\rho_c(= 1 - 5\ mg/ml)$ is the mass density of collagen, $v_c = 0.73\ ml/g$ is the specific volume of collagen, r (μm) is the radius of the fibers and L_{Tot} (μm) is the total length of collagen in the gel. The 3D variables converted into equivalent the 2D ones by transforming quantities per unit volume to quantities per unit area. Fiber radius is assumed to be $250\ nm$ and from the above relation, the total length of fiber in the gel is calculated for varying collagen concentrations. The fibers have both flexural and stretching rigidities and the crosslinks are assumed to be rigid (7). A parametric study for various collagen concentrations ($2, 3, 4\ and\ 5\ mg/ml$), simulating simple shear deformation shows good agreement with the experimentally observed strain sweep results (8). Increasing gel concentration reduces the collagen mesh size (distance between two crosslinks) leading to a stiffer response. The reduction in the length of the fiber between the crosslinks affects the bending characteristics and leads to an increase in the initial stiffness and a decrease the knee strain.

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B: Finite element implementation of the fibrous constitutive law

All simulations were performed in a finite deformation setting. The matrices are modeled using 4-node bilinear axisymmetric quadrilateral elements. The axisymmetric constitutive law, the equilibrium condition, $\partial\sigma_{ij}/\partial dx_j = 0$, and the boundary conditions constitute a well-posed boundary value problem. We implemented the constitutive equation in a user material model in the finite element package ABAQUS (5). The tangent modulus tensor in the material description $\boldsymbol{C}^{SC}$, the tangent modulus tensor for the convected rate of the Kirchhoff stress $\boldsymbol{C}^{\tau C}$, the tangent modulus tensor for the Jaumann rate of the Kirchhoff stress $\boldsymbol{C}^{\tau J}$, and the material Jacobin $\boldsymbol{C}^{MJ}$ (needed for the user material model) can be expressed as (9, 10)

$$C^{SC}_{mnpq} = 4\frac{\partial^2 W}{\partial C_{nm}\partial C_{pq}}$$

$$C^{\tau C}_{ijkl} = F_{im}F_{jn}F_{kp}F_{lq}C^{SC}_{mnpq} \tag{B1}$$

$$C^{\tau J}_{ijkl} = C^{\tau C}_{ijkl} + \delta_{ik}\tau_{jl} + \tau_{ik}\delta_{jl}$$

$$C^{MJ}_{ijkl} = C^{\tau J}_{ijkl}/J$$

Here the second Piola–Kirchhoff stress $\boldsymbol{\tau} = \boldsymbol{\sigma}/J$,

$$C^{MJ}_{ijkl} = C^{b}_{ijkl} + C^{f}_{ijkl}$$

$$C^{b}_{ijkl} = \frac{\mu}{J}\left(\frac{1}{2}\left(\delta_{ik}\bar{B}_{jl} + \bar{B}_{ik}\delta_{jl} + \delta_{il}\bar{B}_{jk} + \bar{B}_{il}\delta_{jk}\right) - \frac{2}{3}(\delta_{ij}\bar{B}_{kl} - \bar{B}_{ij}\delta_{kl}) + \frac{2}{9}\delta_{ij}\delta_{kl}\bar{B}_{mm}\right) + \kappa(2J-1)\delta_{ij}\delta_{kl} \tag{B2}$$

$$\boldsymbol{C^f} = \frac{1}{J}\sum_{a=1}^{3}\frac{\partial}{\partial\lambda_a}\left(\frac{\partial f(\lambda_a)}{\partial\lambda_a}\frac{1}{\lambda_a}\right)\lambda_a^3\boldsymbol{n_a}\otimes\boldsymbol{n_a}\otimes\boldsymbol{n_a}\otimes\boldsymbol{n_a} + \sum_{\substack{a,b=1\\a\neq b}}^{3}\frac{\sigma_b{\lambda_a}^2 - \sigma_a{\lambda_b}^2}{{\lambda_b}^2 - {\lambda_a}^2}(\boldsymbol{n_a}\otimes\boldsymbol{n_b}\otimes\boldsymbol{n_a}\otimes\boldsymbol{n_b} + \boldsymbol{n_a}\otimes\boldsymbol{n_b}\otimes\boldsymbol{n_b}\otimes\boldsymbol{n_a}) + \boldsymbol{I}\overline{\otimes}\boldsymbol{\sigma^f} + \boldsymbol{\sigma^f}\overline{\otimes}\boldsymbol{I}$$

Here we have adopted the abbreviations $(A\otimes B)_{ijkl} = A_{ij}B_{kl}$ and $(A\overline{\otimes}B)_{ijkl} = A_{ik}B_{jl}$. We define

$$\sigma_a = \frac{1}{J}\frac{\partial f(\lambda_a)}{\partial\lambda_a}\lambda_a \tag{B3}$$

If $\lambda_b \to \lambda_a$, $\frac{\sigma_b{\lambda_a}^2 - \sigma_a{\lambda_b}^2}{{\lambda_b}^2 - {\lambda_a}^2}$ gives us $0/0$ and must be determined using the limiting conditions (9),

$$\lim_{\lambda_b\to\lambda_a}\frac{\sigma_b{\lambda_a}^2 - \sigma_a{\lambda_b}^2}{{\lambda_b}^2 - {\lambda_a}^2} = \frac{1}{2}\frac{d\sigma_a}{d\lambda_a}\lambda_a - \sigma_a \tag{B4}$$

Integrating Eq. 4, the energy function $f(\lambda_a)$ can be expressed as,

$$f(\lambda_a) = \begin{cases} 0, & \lambda_a < \lambda_1 \\ \dfrac{E_f \left(\dfrac{\lambda_a - \lambda_1}{\lambda_2 - \lambda_1}\right)^n (\lambda_a - \lambda_1)^2}{(n+1)(n+2)}, & \lambda_1 \le \lambda_a < \lambda_2 \\ E_f \left[\dfrac{(1 + \lambda_a - \lambda_2)^{m+2} - 1}{(m+1)(m+2)} + \dfrac{\lambda_2 - \lambda_a}{m+1} + \dfrac{(\lambda_a - \lambda_2)(\lambda_2 - \lambda_1)}{n+1} + \dfrac{(\lambda_2 - \lambda_1)^2}{(n+1)(n+2)}\right], & \lambda_a \ge \lambda_2 \end{cases} \quad \text{(B5)}$$

The second derivative of Eq. 4 can be expressed as,

$$\frac{\partial^2 f(\lambda_a)}{\partial {\lambda_a}^2} = \begin{cases} 0, & \lambda_a < \lambda_1 \\ E_f \left(\dfrac{\lambda_a - \lambda_1}{\lambda_2 - \lambda_1}\right)^n, & \lambda_1 \le \lambda_a < \lambda_2 \\ E_f (1 + \lambda_a - \lambda_2)^m, & \lambda_a \ge \lambda_2 \end{cases} \quad \text{(B6)}$$

Here $\lambda_1 = \lambda_c - \lambda_t/2$, $\lambda_2 = \lambda_c + \lambda_t/2$.

C: Analytical linear solution for the spherically symmetric case

We further introduce Green-Lagrange strain tensor $\boldsymbol{\varepsilon} = (\boldsymbol{C} - \boldsymbol{I})/2$**.** For infinitesimal strains $\boldsymbol{\varepsilon}$ with $|\varepsilon_{\boldsymbol{ij}}| \ll 1$,

$$J = 1 + \mathrm{tr}(\boldsymbol{\varepsilon})$$

$$\overline{\boldsymbol{B}} = \boldsymbol{I} + 2\boldsymbol{\varepsilon} \quad \text{(C1)}$$

$$\lambda_a = (1 + 2\varepsilon_a)^{1/2} = 1 + \varepsilon_a$$

Substituting Eq. C1 into Eq. 2

$$\boldsymbol{\varepsilon} = \sum_{a=1}^{3} \varepsilon_a \boldsymbol{n}_{\mathbf{a}} \otimes \boldsymbol{n}_{\mathbf{a}} \quad \text{(C2)}$$

The fiber energy function in Eq. 1 can also be expressed as $f(\lambda_a) = U(\varepsilon_a)$,

$$\frac{\partial f(\lambda_a)}{\partial \lambda_a} = \frac{\partial U(\varepsilon_a)}{\partial \varepsilon_a} \frac{\partial \varepsilon_a}{\lambda_a} = \frac{\partial U(\varepsilon_a)}{\partial \varepsilon_a} \quad \text{(C3)}$$

Substituting Eq. C3 into Eq.3, we get

$$\sigma = \sigma^b + \sigma^f \ ,$$

$$\boldsymbol{\sigma}^{\boldsymbol{b}} = \kappa \ \mathrm{tr}(\boldsymbol{\varepsilon}) \boldsymbol{I} + 2\mu \ \mathrm{dev}(\boldsymbol{\varepsilon}), \quad \text{(C4)}$$

$$\boldsymbol{\sigma^f} = \sum_{a=1}^{3} \frac{\partial U(\varepsilon_a)}{\partial \varepsilon_a} \boldsymbol{n_a} \otimes \boldsymbol{n_a}$$

For linear bulk and fibrous response ($\lambda_c = 1$ and $m = 0$ in Eq. 4), Eq. C4 can be rewritten as,

$$\sigma = \sigma^b + \sigma^f$$

$$\boldsymbol{\sigma^b} = \frac{E_b}{3(1-2\nu)} \operatorname{tr}(\boldsymbol{\varepsilon})\boldsymbol{I} + \frac{E_b}{1+\nu} \operatorname{dev}(\boldsymbol{\varepsilon}) \tag{C5}$$

$$\boldsymbol{\sigma^f} = \sum_{a=1}^{3} E_f\, \boldsymbol{n_a} \otimes \boldsymbol{n_a}.$$

For infinitesimal strains, we have the geometric relations,

$$\varepsilon_r = \frac{du}{dr}, \qquad \varepsilon_\theta = \varepsilon_\varphi = \frac{u}{r}, \qquad J = 1, \tag{C6}$$

Here u is the radial displacement and the constitutive law Eq. C5 can be rewritten as,

$$\sigma_r = \frac{E_b}{(1-2\nu)(1+\nu)} \left[(1-\nu)\frac{du}{dr} + 2\nu\frac{u}{r}\right] + E_f\frac{du}{dr} \tag{C7}$$

$$\sigma_\theta = \sigma_\varphi = \frac{E_b}{(1-2\nu)(1+\nu)} \left(\frac{u}{r} + \nu\frac{du}{dr}\right)$$

The condition for mechanical equilibrium $\frac{d\sigma_r}{dr} + \frac{2}{r}(\sigma_r - \sigma_\theta) = 0$ can then be written as,

$$\left[1 + \frac{(1+\nu)(1-2\nu)}{(1-\nu)}\frac{E_f}{E_b}\right]\left(\frac{d^2u}{dr^2} + \frac{2}{r}\frac{du}{dr}\right) - 2\frac{u}{r^2} = 0 \tag{C8}$$

The boundary condition is

$$u(r_0) = u_0, u(\infty) = 0 \tag{C9}$$

The solution is

$$u(r)/u_0 = (r_0/r)^n \tag{C10}$$

$$\sigma_r(r)/\sigma_r(r_0) = (r_0/r)^{n+1}$$

Here $n = \frac{1}{2}\left(\sqrt{\frac{9+\chi}{1+\chi}} + 1\right)$ and $\chi = \frac{(1+\nu)(1-2\nu)}{(1-\nu)}\frac{E_f}{E_b}$

The strains and stresses can then be expressed as

$$\varepsilon_r = -n\frac{u_0}{r_0}\left(\frac{r_0}{r}\right)^{n+1} \tag{C11}$$

$$\varepsilon_\theta = \varepsilon_\varphi(r) = \frac{u_0}{r_0}\left(\frac{r_0}{r}\right)^{n+1}$$

$$\sigma_r = -\left\{\frac{E_b}{(1+\nu)(1-2\nu)}[(1-\nu)n-2\nu] + nE_f\right\}\frac{u_0}{r_0}\left(\frac{r_0}{r}\right)^{n+1}$$

$$\sigma_\theta = \sigma_\varphi = \frac{E_b}{(1+\nu)(1-2\nu)}[1-\nu n]\frac{u_0}{r_0}\left(\frac{r_0}{r}\right)^{n+1}$$

In the limit of strong fibrous response, $E_f/E_b \gg 1$, we find that the exponent $n \to 1$, whereas for an isotropic material for which $E_f/E_b \ll 1$, we find that $n \to 2$. Thus, stresses decay less precipitously, leading to an increased zone of influence in fibrous materials. This result is also consistent with theoretical estimates by Sander (11), who considered a less general case, $E_f/E_b \gg 1$, without including the effect of the Poisson's ratio, ν.

D: Strain energy function with the modified right Cauchy–Green tensor

Holzapfel et al. (9, 12) developed a constitutive law to describe the mechanical response of arterial tissue with a strain energy function

$$W_f = W_b(\bar{I}_1, J) + \overline{W_f}(\bar{\boldsymbol{C}}) = W_b(\bar{I}_1, J) + \sum_{i=4,6} f_i(\bar{I}_i) \tag{D1}$$

$$f = \begin{cases} 0, \bar{I}_i < 1 \\ \frac{k_1}{2k_2}\{\exp[k_2(\bar{I}_i - 1)^2] - 1\}, \bar{I}_i \geq 1, \end{cases}$$

where the first term W_b represents the isotropic bulk response of the matrix (same as our model) and the second term $\overline{W_f}$ represents anisotropic stiffening due to two families of reinforcing collagen fibers that evolve during loading. The modified right Cauchy–Green tensor is $\bar{\boldsymbol{C}} = \boldsymbol{C}/J^{2/3}$. $\bar{I}_1$, $\bar{I}_4$ and $\bar{I}_6$ are the modified invariants of $\bar{\boldsymbol{C}}$, which represent the squares of the stretches along the two families of fibers,

$$\bar{I}_1 = \mathrm{tr}(\bar{\boldsymbol{C}}) \qquad \bar{I}_4 = \boldsymbol{N_4}\bar{\boldsymbol{C}}\boldsymbol{N_4} \qquad \bar{I}_6 = \boldsymbol{N_6}\bar{\boldsymbol{C}}\boldsymbol{N_6} \tag{D2}$$

where $\boldsymbol{N_4}$ and $\boldsymbol{N_6}$ are the unit vectors along the fibers in the reference configuration. Then, the Cauchy stress has the form,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma^b} + \boldsymbol{\sigma^f} = \boldsymbol{\sigma^b} + \sum_{i=4,6} 2\frac{\partial f_i(\bar{I}_i)}{\partial \bar{I}_i}\mathrm{dev}(\boldsymbol{n_i} \otimes \boldsymbol{n_i}) \tag{D3}$$

where $\boldsymbol{n_4} = \boldsymbol{FN_4}$ and $\boldsymbol{n_6} = \boldsymbol{FN_6}$ are the fiber vectors in the current configuration:

$$\boldsymbol{n_4} = \boldsymbol{FN_4}, \qquad \boldsymbol{n_6} = \boldsymbol{FN_6} \tag{D4}$$

An iterative procedure starting with an arbitrary configuration of the fibers is implemented to find the fiber vectors in the reference and current configurations, $\boldsymbol{N_4}$ and $\boldsymbol{n_4}$. By considering this constitutive law for the case of spherically-symmetric contractile strain, we show in Appendix E that this constitutive law cannot show long-range transmission of forces.

To enable the long range formation in fibrous media, the above strain energy function for collagen fiber alignment can be modified by using a Cauchy-Green deformation tensor instead of a modified Cauchy-Green deformation tensor. Denoting the principal stretches by λ_a, we retain the functional form of the function, $f(\lambda_a)$, such that it vanishes when the principal stretches are negative to get

$$f(\lambda_a) = \begin{cases} 0, \lambda_a < 1 \\ \frac{C_{k1}}{2C_{k2}}[\exp(C_{k2}({\lambda_a}^2 - 1)^2) - 1], \lambda_a \geq 1 \end{cases} \quad \text{(D5)}$$

$$\frac{\partial f(\lambda_a)}{\partial \lambda_a} = \begin{cases} 0, \lambda_a < 1 \\ 2C_{k1}\exp(C_{k2}({\lambda_a}^2 - 1)^2)({\lambda_a}^2 - 1)\lambda_a, \lambda_a \geq 1 \end{cases} \quad \text{(D6)}$$

$$\frac{\partial^2 f(\lambda_i)}{\partial {\lambda_a}^2} = \begin{cases} 0, \lambda_a < 1 \\ 2C_{k1}\exp(C_{k2}({\lambda_a}^2 - 1)^2)[4C_{k2}{\lambda_a}^6 - 8C_{k2}{\lambda_a}^4 + (3 + 4C_{k2}){\lambda_a}^2 - 1], \lambda_a \geq 1 \end{cases} \quad \text{(D7)}$$

Here C_{k1} and C_{k1} are the parameters for initial stiffness and strain-hardening. Note that $\bar{I}_i$ in the original form is replaced with I_i. We set $\chi = (1 + \nu)(1 - 2\nu)C_{k1}/(1 - \nu)E_b = 0.2$ and $C_{k2} = 500$ in our numerical simulations (Fig. 7).

E: Analytical solution for the constitutive law with the modified right Cauchy–Green tensor

Consider the special case of a spherical cell with isotropic contraction embedded in a fibrous matrix. As in the case of linear analysis in Appendix B, the deviatoric constitutive law in Eq. D3 can be rewritten for infinitesimal strains,

$$\boldsymbol{\sigma} = \kappa\, \mathrm{tr}(\boldsymbol{\varepsilon})\, \boldsymbol{I} + 2\mu\mathbf{e} + \sum_{i=4,6} \frac{\partial U(e_i)}{\partial e_i} \mathrm{dev}(\boldsymbol{n_i} \otimes \boldsymbol{n_i}) \quad \text{(E1)}$$

Here the fiber energy function can be express as $f(\overline{I_i}) = U(e_i)$ with $\overline{I_i} = 1 + 2e_i$. For spherical symmetry, the deviatoric strain $e_r = \frac{2}{3}(\varepsilon_r - \varepsilon_\theta) \geq 0$ and $e_\theta = e_\varphi = \frac{1}{3}(\varepsilon_\theta - \varepsilon_r) \leq 0$, so Eq. E1 can be rewritten as,

$$\sigma_r = \frac{E_b}{3(1 - 2\nu)}(\varepsilon_r + 2\varepsilon_\theta) + \frac{2}{3}[\frac{E_b}{(1 + \nu)} + E_f](\varepsilon_r - \varepsilon_\theta) \quad \text{(E2)}$$

$$\sigma_\theta = \frac{E_b}{3(1 - 2\nu)}(\varepsilon_r + 2\varepsilon_\theta) - \frac{1}{3}[\frac{E_b}{(1 + \nu)} + E_f](\varepsilon_r - \varepsilon_\theta)$$

Using the relations $\varepsilon_r = \frac{du}{dr}, \varepsilon_\theta = \varepsilon_\varphi = \frac{u}{r}$ (E3) and the condition for mechanical equilibrium,

$$\frac{d\sigma_r}{dr} + \frac{2}{r}(\sigma_r - \sigma_\theta) = 0 \qquad \text{(E4)}$$

we get

$$\frac{d^2u}{dr^2} + \frac{2}{r}\frac{du}{dr} - 2\frac{u}{r^2} = 0 \qquad \text{(E5)}$$

From boundary conditions: $u(r_0) = u_0, u(\infty) = 0$, the solution of Eq. E5 is

$$u(r)/u_0 = (r_0/\,r)^2 \qquad \text{(E6)}$$

$$\sigma_r(r)/\,\sigma_r(r_0) = \ (r_0/\,r)^3$$

Comparing this with Eq. C 10, we find that the constitutive law of Holzapfel et al. (9, 12) does not show long range force transmission.

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