COMSOL used for simulating biological remodelling

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Joint work with

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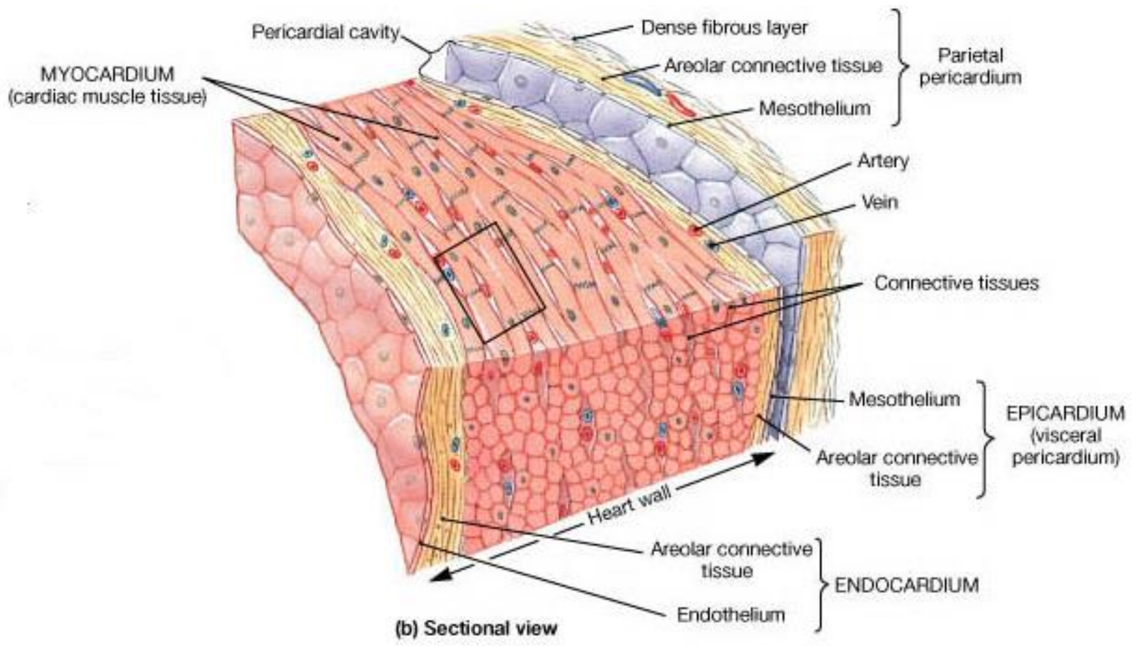
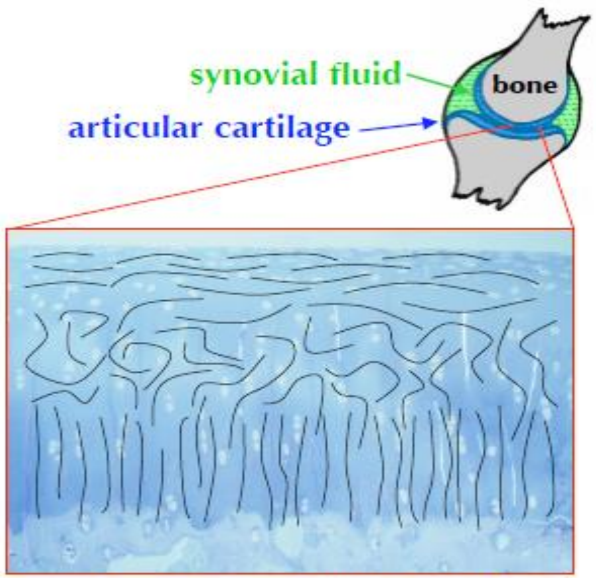
Biological tissues: an overview

- Highly complex physical systems
- Hydrated, fibre-reinforced, heterogeneous and anisotropic porous media.
- Description of mechanical interactions
- Anelastic distortions



Articular cartilage

In articular cartilage, the fibres are distributed in a non-uniform way and this influences, for example, the stiffness of the tissue and the flow of the interstitial fluid.

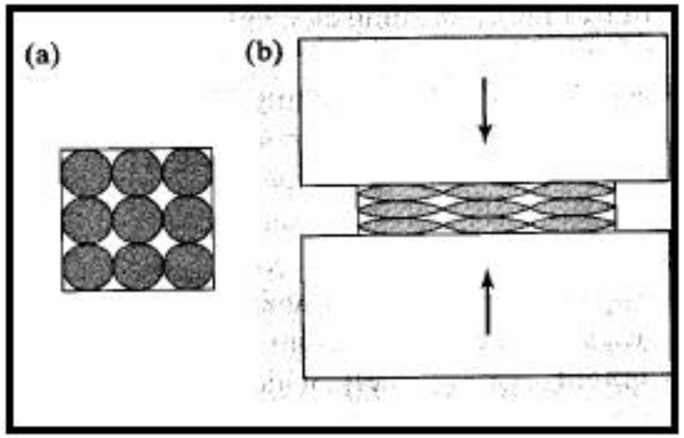


A sample of articular cartilage.

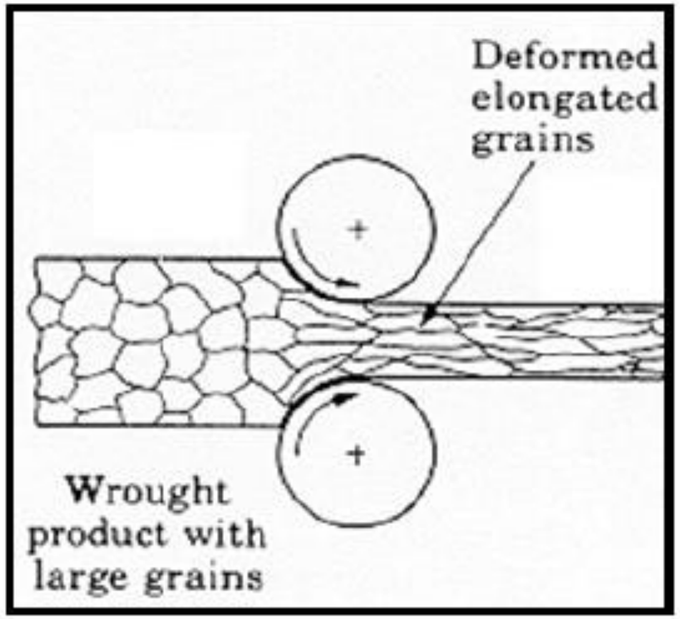
- <u>Deep zone</u> (oriented perpendicularly to the interface)
- <u>Middle zone</u> (random distributed)
- <u>Upper zone</u> (the fibres are parallel to the interface)
- *Transversely isotropic* behaviour

[Joint work with Salvatore Federico, Gaetano Giaquita, Walter Herzog, Guido La Rosa, (2004,2005)], [Mansour, J.M. (2003), Biomechanics of cartilage, Chapter 5, page 68]

Remodelling: change of internal structure



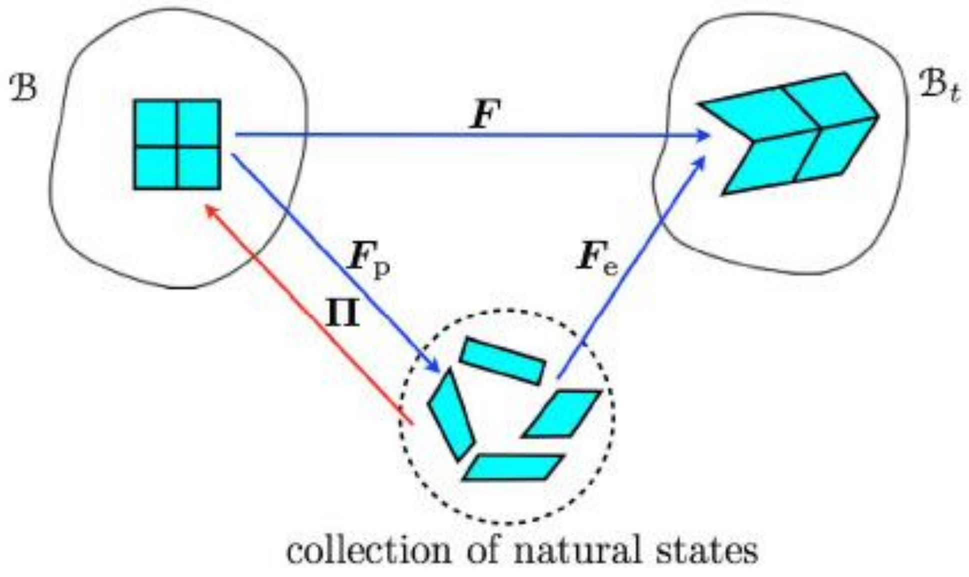
Unconfined compression



Cold rolling

The change of the body's shape (visible phenomenon) is accompanied by a reorganization of its internal structure (hidden phenomenon), which causes macroscopic variations of the mechanical properties of the material.

The implant tensor



- Reference configuration $\mathcal{B}$
- Actual configuration $\mathcal{B}_t$
- Deformation gradient $\boldsymbol{F}$
- BKL decomposition: $\boldsymbol{F} = \boldsymbol{F}_e\boldsymbol{F}_p$
- Epstein-Maugin decomposition: $\boldsymbol{F} = \boldsymbol{F}_e\boldsymbol{\Pi}^{-1}$
- $\boldsymbol{\Pi}$ is said to be the implant tensor

Fibre pattern

- Unit sphere: set of all unit vectors emanating from $X \in \mathcal{B}$

  $$\mathbb{S}^2_X\mathcal{B} = \{\mathfrak{m}_X \in T_X\mathcal{B} : \ \|\mathfrak{m}_X\| = 1\}$$

- Probability density that a fibre is aligned along $\mathfrak{m}_X$

  $$\wp_X : \mathbb{S}^2_X\mathcal{B} \to \mathbb{R}^+_0, \ \mathfrak{m}_X \to \wp_X(\mathfrak{m}_X)$$

- Directional average of a physical quantity associated with the fibres $\mathfrak{F}_X : \mathbb{S}^2_X\mathcal{B} \to \mathbb{R}$

  $$\langle\langle\mathfrak{F}_X\rangle\rangle = \int_{\mathbb{S}^2_X\mathcal{B}} \mathfrak{F}_X(\mathfrak{m}_X)\wp_X(\mathfrak{m}_X) = \int_0^{2\pi}\int_0^{\pi} \mathfrak{F}_X(\hat{\mathfrak{m}}_X(\Theta,\Phi))\wp_X(\hat{\mathfrak{m}}_X(\Theta,\Phi))\sin(\Theta)d\Theta d\Phi$$

  where

  $$\mathfrak{m}_X = \hat{\mathfrak{m}}_X(\Theta,\Phi) = \sin\Theta\cos\Phi\,\mathfrak{e}_1 + \sin\Theta\sin\Phi\,\mathfrak{e}_2 + \cos\Theta\,\mathfrak{e}_3$$

  with $(\Theta,\Phi) \in [0,\pi[\times[0,2\pi]$, and $\{\mathfrak{e}_\alpha\}_{\alpha=1}^3$ orthonormal basis in $T_X\mathcal{B}$.

- Transverse isotropy

  $\exists\ \mathfrak{m}_0$ such that, for $\boldsymbol{H}_0 :\ \boldsymbol{H}_0\mathfrak{m}_0 = \pm\mathfrak{m}_0$, $\wp_X(\boldsymbol{H}_0\mathfrak{m}_X) = \wp_X(\pm\mathfrak{m}_X)\ \forall\ X \in \mathcal{B}$

- Parity Symmetry

  $\wp_X(\mathfrak{m}_X) = \wp_X(-\mathfrak{m}_X)$, for all $X \in \mathcal{B}$

Constitutive framework: strain energy function

- Hyperelastic behaviour from the collection of natural states
- Strain energy function

$$W_{\mathrm{R}}(\boldsymbol{C}, X, t) = \frac{1}{J_{\Pi}(X,t)} \hat{W}_{\kappa}(\boldsymbol{C}_{\mathrm{e}}(X,t))$$
$$= \frac{1}{J_{\Pi}(X,t)} \left(\Phi_{\mathrm{s}\nu} \hat{U}(J_{\mathrm{e}}) + \Phi_{0\mathrm{s}\nu} \hat{W}_0(\boldsymbol{C}_{\mathrm{e}}) + \Phi_{1\mathrm{s}\nu} \hat{W}_{\mathrm{e}}(\boldsymbol{C}_{\mathrm{e}}) \right)$$

with

- $J_{\Pi}(X,t) = \det(\boldsymbol{\Pi}(X,t))$, $J_{\mathrm{e}}(X,t) = \det(\boldsymbol{F}_{\mathrm{e}}(X,t))$;
- $\Phi_{\mathrm{s}\nu}(X,t) = J_{\mathrm{e}}(X,t)\phi_{\mathrm{s}}(X)$, $\Phi_{0\mathrm{s}\nu}(X,t) = J_{\mathrm{e}}(X,t)\phi_{0\mathrm{s}\nu}(X)$, $\Phi_{1\mathrm{s}\nu}(X,t) = J_{\mathrm{e}}(X,t)\phi_{1\mathrm{s}\nu}(X)$ are, respectively, the volumetric fractions of the solid phase, the matrix and the fibres, such that $\phi_{0\mathrm{s}} + \phi_{1\mathrm{s}} = \phi_{\mathrm{s}}$;
- $\boldsymbol{C}_{\mathrm{e}} = \boldsymbol{F}_{\mathrm{e}}^T.\boldsymbol{F}_{\mathrm{e}} = \boldsymbol{\Pi}^T \boldsymbol{C} \boldsymbol{\Pi}$ is the elastic part of the right Cauchy-Green deformation tensor $\boldsymbol{C}$.

Strain energy of the matrix

$$\hat{W}_0(\boldsymbol{C}_\mathrm{e}) = \alpha_0 \frac{\exp\left(\alpha_1[I_1 - 3] + \alpha_2[I_2 - 3]\right)}{[I_3]^{\alpha_3}}$$

$$I_1 = \mathrm{tr}(\boldsymbol{C}_\mathrm{e})$$

$$I_2 = \tfrac{1}{2}[(\mathrm{tr}(\boldsymbol{C}_\mathrm{e})^2 - \mathrm{tr}(\boldsymbol{C}_\mathrm{e}^2)]$$

$$I_3 = \det(\boldsymbol{C}_\mathrm{e})$$

$$\alpha_1 + 2\alpha_2 = \alpha_3 = 1$$

Ensemble potential

$$\hat{W}_\mathrm{e}(\boldsymbol{C}_\mathrm{e}) = \hat{W}_{1\mathrm{i}}(\boldsymbol{C}_\mathrm{e}) + \langle\!\langle \hat{W}_{1\mathrm{a}}(\boldsymbol{C}_\mathrm{e}, \mathfrak{m}) \rangle\!\rangle$$

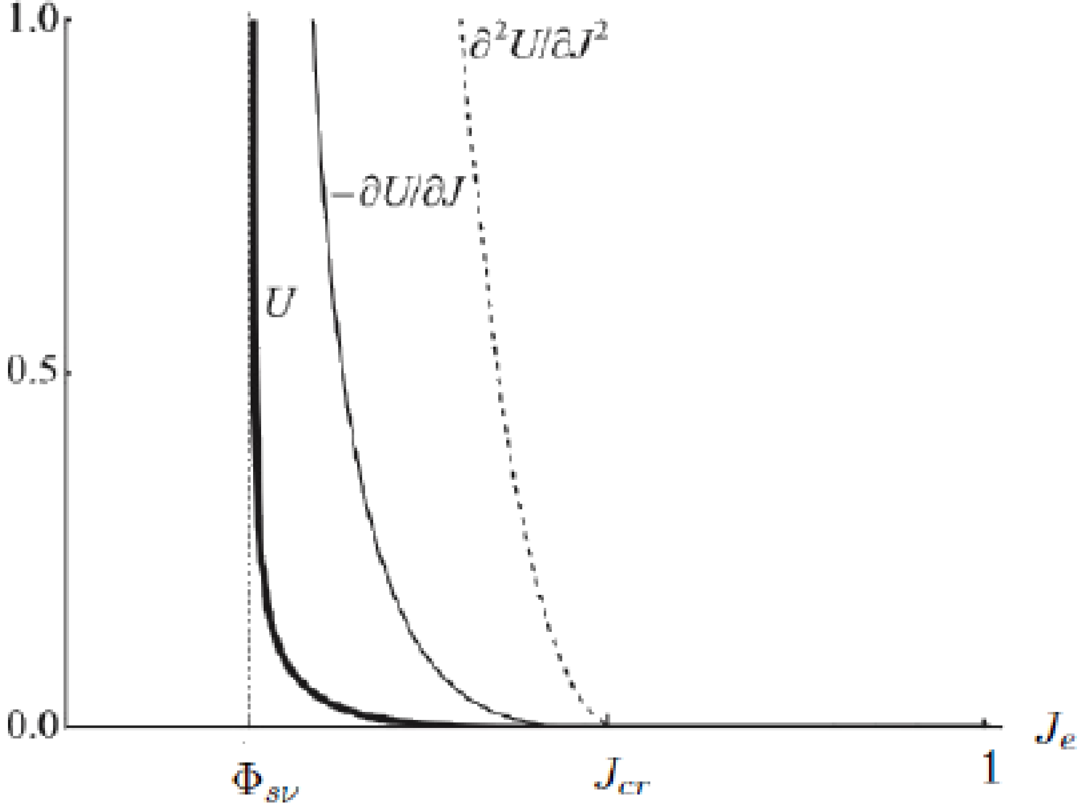
$$\hat{W}_{1\mathrm{i}} = \hat{W}_0(\boldsymbol{C}_\mathrm{e})$$

$$\hat{W}_{1\mathrm{a}}(\boldsymbol{C}_\mathrm{e}, \mathfrak{m}) = \mathcal{H}(I_{4\mathrm{e}} - 1)\tfrac{1}{2}c\,[I_{4\mathrm{e}} - 1]^2$$

$$I_{4\mathrm{e}} = \boldsymbol{C}_\mathrm{e} : \mathfrak{a}, \quad \mathfrak{a} = \mathfrak{m} \otimes \mathfrak{m}$$

Penalty term

$$\hat{U}(J_\mathrm{e}) = \mathcal{H}(J_\mathrm{cr} - J_\mathrm{e})(J_\mathrm{e} - J_\mathrm{cr})^{2q}(J - \Phi_{s\nu})^{-r}$$



$$J_\mathrm{crit} \in (\phi_{s\nu}, 1], q \geq 2 \in \mathbb{N}, r \in (0, 1]$$

Constitutive framework: Darcy's law

Linear relation between the filtration velocity and the gradient of pressure

- spatial formulation: $\boldsymbol{q} = \phi_{\mathrm{f}}(\boldsymbol{v}_{\mathrm{f}} - \boldsymbol{v}_{\mathrm{s}}) = \boldsymbol{k}\,\mathrm{grad}\,p$
- material formulation: $\boldsymbol{Q} = J\boldsymbol{F}^{-1}\boldsymbol{q} = \boldsymbol{K}\,\mathrm{Grad}\,p$

where

- $\boldsymbol{v}_{\mathrm{f}}$ is the velocity of the fluid phase and $\boldsymbol{v}_{\mathrm{s}}$ is the velocity of the solid phase;
- $\phi_{\mathrm{f}} = 1 - \phi_{\mathrm{s}}$ is the volumetric fraction of the fluid phase;
- $\boldsymbol{k}$ is the spatial permeability tensor and $\boldsymbol{K}$ is the material permeability tensor.

In particular

$$\boldsymbol{K} = \hat{\boldsymbol{K}}(\boldsymbol{F}, \boldsymbol{\Pi}, \zeta) = J\,\hat{k}_0(J, J_{\Pi}, \zeta)\,\boldsymbol{C}^{-1} + J^{-1}\,\hat{k}_0(J, J_{\Pi}, \zeta)\,\boldsymbol{\Pi}\left\langle\!\!\left\langle \frac{\mathfrak{a}}{I_{4\mathrm{e}}} \right\rangle\!\!\right\rangle \boldsymbol{\Pi}^T$$

where ζ is an axial coordinate and $k_0 = \hat{k}_0(J, J_{\Pi}, \zeta)$ is a Holmes-Mow type scalar permeability.

Problem setting (1/2)

The uknowns of the problem are the motion χ, the pore pressure p and the implant tensor $\mathbf{\Pi}$. The system of equations to solve is

$$\dot{J} - \mathrm{Div}[\boldsymbol{K}\,\mathrm{Grad}\,p] = 0,$$
$$\mathrm{Div}(-J\,p\mathbf{g}^{-1}\mathbf{F}^{-T} + \mathbf{P}_{\mathrm{sc}}) = \mathbf{0},$$
$$\mathrm{sym}(\boldsymbol{\Lambda}\boldsymbol{C}^{-1}) = \xi_p\left[\boldsymbol{S} - \frac{1}{3}\mathrm{tr}(\boldsymbol{C}\boldsymbol{S})\boldsymbol{C}^{-1}\right].$$

In addition, we suppose $J_\Pi = 1$ and $\xi_p = \lambda_0\phi_s^2 \frac{\left[||\mathrm{dev}(\sigma)|| - \sqrt{(2/3)}\sigma_y\right]_+}{||\mathrm{dev}(\sigma)||}$, with $\boldsymbol{\sigma}$ being the Cauchy stress tensor, σ_Y is a yield stress and $[\cdot]_+$ extacts the positive part of the function to which it is applied

Problem setting (2/2)

- The first equation is the balance of mass.
- The second equation is the moment balance equation, where $\boldsymbol{P}_{\mathrm{sc}} = \hat{\boldsymbol{P}}_{\mathrm{sc}}(\boldsymbol{F}, \boldsymbol{\Pi})$ is the constitutive part of the first Piola-Kirchoff stress tensor.
- The third equation is the law of evolution for the implant tensor $\boldsymbol{\Pi}$, where $\boldsymbol{\Lambda} = \dot{\boldsymbol{\Pi}}\boldsymbol{\Pi}^{-1}$ is the tensor of *inomogeneities velocity*.
- A pseudo-Gaussian probability distribution has been chosen

$$\wp(\Theta) = \hat{\wp}(\Theta, X, t) = \frac{\hat{\gamma}(\Theta, X, t)}{\int_0^{2\pi} \hat{\gamma}(\Theta', X, t)\sin(\Theta')d\Theta'}$$

$$\gamma(\Theta) = \hat{\gamma}(\Theta, X, t) = \exp\left(-\frac{[\Theta - Q(X)]^2}{2\omega(X)}\right),$$

where Q is the mean angle and ω is the variance.

Closing the system

Let us introduce the polar decomposition of the implant tensor

$$\Pi = \boldsymbol{H}.\boldsymbol{R} = \boldsymbol{HGR}$$

where

$\boldsymbol{H}$ is a symmetric positive definite tensor;

$\boldsymbol{R}$ is a rotation tensor;

By imposing $R^{\beta}_{\ \alpha} = \delta^{\beta}_{\ \alpha}$, we obtain

$$\Pi = \boldsymbol{HG}$$

and

$$\Lambda = \dot{\Pi}\Pi^{-1} = \dot{\boldsymbol{H}}\boldsymbol{H}^{-1}.$$

We can solve the flow rule for a symmetric tensor.

Simulations (1/2)

We simulated an unconfined compression test for a cylindrical specimen. In this case we imposed the following boundary conditions

$$\chi(X,t) = \chi(X,0) = X,$$
$$(\boldsymbol{K}\ \mathrm{Grad}\ p).\mathbf{N} = 0$$

on the lower boundary Γ_l,

$$(-J\,p\,\mathbf{g}^{-1}\mathbf{F}^{-T} + \mathbf{P}_{\mathrm{sc}}).\mathbf{N} = \mathbf{0},$$
$$p = 0$$

on the lateral boundary Γ_L and

$$\chi^z(X,t) = g(t),$$
$$\boldsymbol{K}\ (\mathrm{Grad}\ p).\mathbf{N} = 0$$

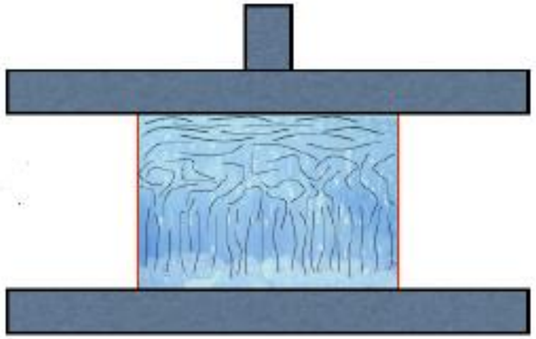
on the upper boundary Γ_u.

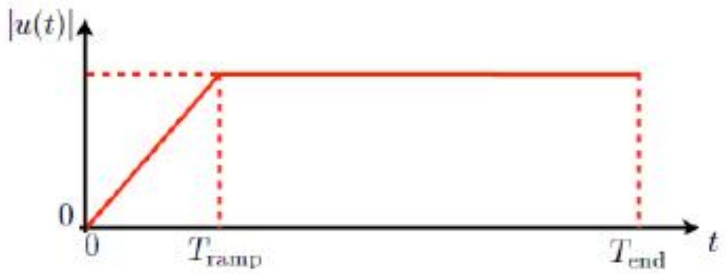
Simulations (2/2)

In the previous equations, g is an imposed displacement given by

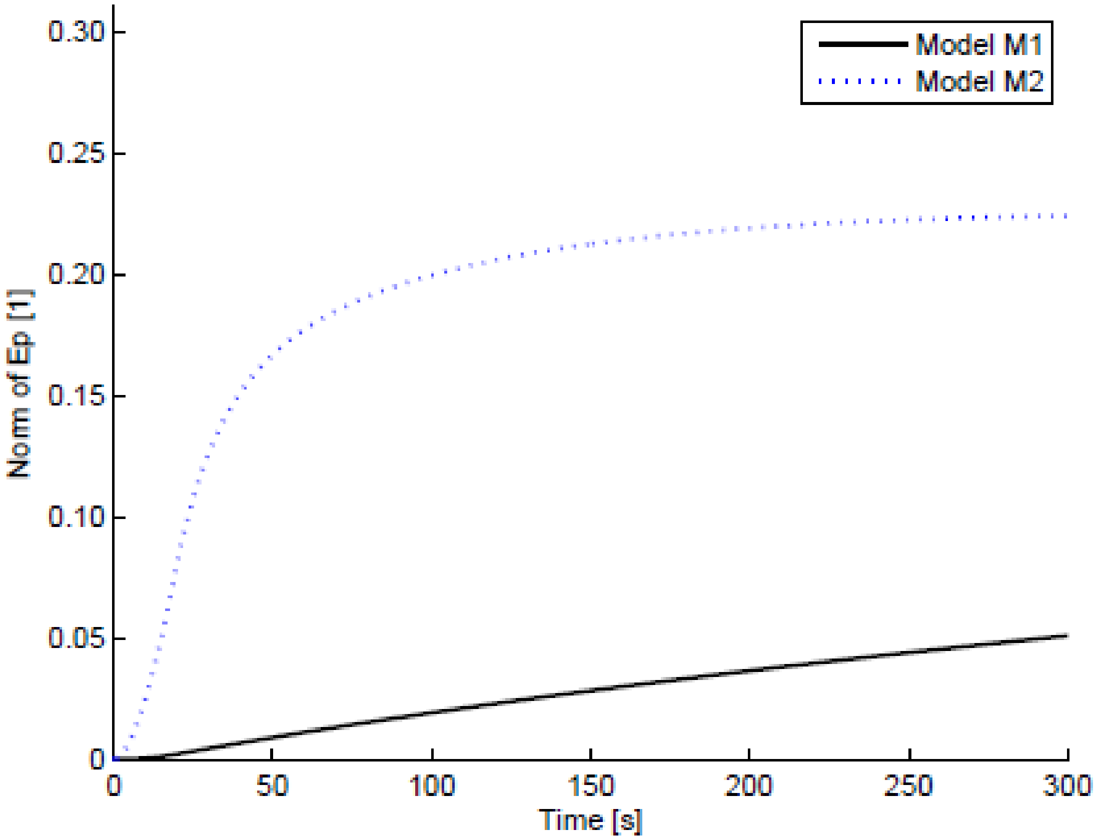
$$g = \begin{cases} L - \dfrac{t}{T_{\text{ramp}}} u_{\text{T}}, & t \in [0, T_{\text{ramp}}] \\ L - u_{\text{T}}, & t \in [T_{\text{ramp}}, T_{\text{end}}] \end{cases}$$

where T_{ramp} is the final instant of time of the loading ramp and u_T is a reference displacement.





Results: plastic strain behaviour



$\boldsymbol{E}_{\mathrm{p}} = \frac{1}{2}[\boldsymbol{\Pi}^{-1}.\boldsymbol{\Pi} - \boldsymbol{G}]$ is the Almansi-Euler like strain tensor associated to the anelastic distortions

Conclusions and future works

- Study of the mechanical properties of biological tissues
- Anelastic distortion
- Possibility to implement other flow rules: take into account correlation of the fibres
- Coupling anelatic distortions and evolution of the fibre pattern
- Introduction of the Forchemeier correction for the fluid flow

Thank you for your attention!