

The numerical implications of multi-phasic mechanics assumptions underlying growth models

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The motivating question

- *What constitutes an ideal environment for tissue growth?*



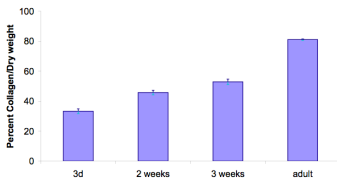
Engineered tendon constructs [Calve et al., 2004]

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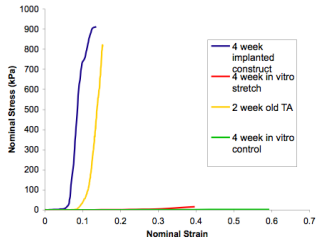
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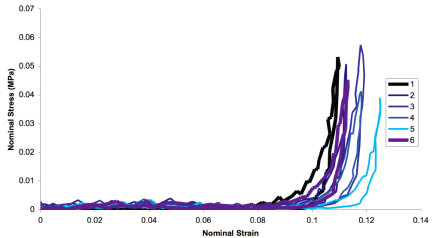
Increasing collagen concentration with age

- *Growth* involves an addition or depletion of mass

The narrow scope of this talk

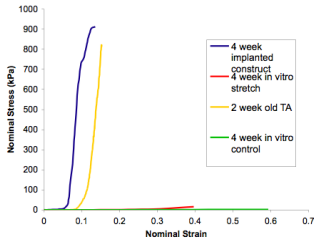


Uniaxial tensile response

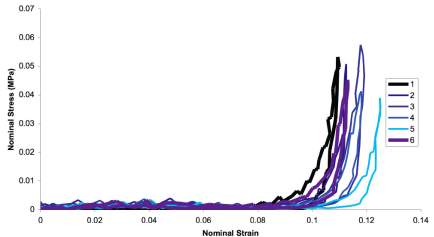


Response under cyclic load

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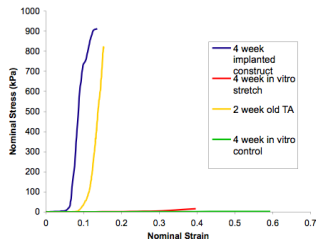
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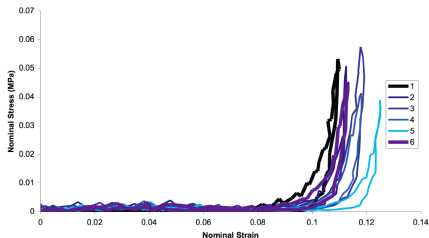
Response under cyclic load

- *What causes the tissue to behave in this manner?*
- Some recent modelling efforts based on mixture theory: Ateshian (BMMB 2007), Lemon et al. (Math. Bio. 2006), Loret and Simões (JMPS 2005)

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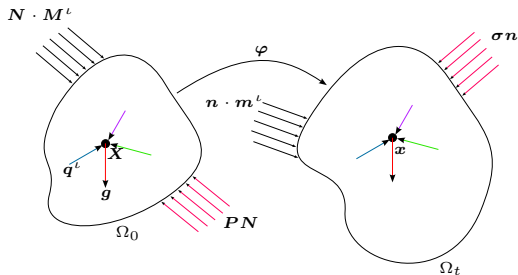
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Response under cyclic load

- *What causes the tissue to behave in this manner?*
- Some recent modelling efforts based on mixture theory: Ateshian (BMMB 2007), Lemon et al. (Math. Bio. 2006), Loret and Simões (JMPS 2005)
- Modelling of solid-fluid coupling $\Rightarrow$ Stiffness of tissue and fluid transport $\Rightarrow$ Nutrient transport $\Rightarrow$ Tissue growth

The governing equations—Lagrangian perspective



Reference quantities:

ρ_0^ℓ – Species concentration

Π^ℓ – Species production rate

M^ℓ – Species relative flux

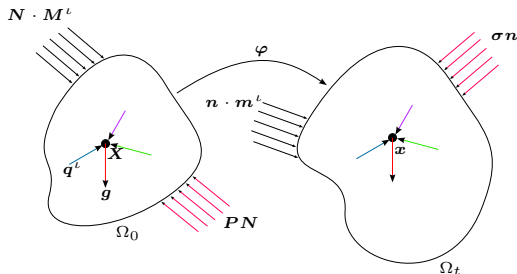
V^ℓ – Species velocity

g – Body force

q^ℓ – Interaction force

P^ℓ – Partial First Piola Kirchhoff stress

The governing equations—Lagrangian perspective



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- Mass balance:

$$\frac{\partial \rho_0^\ell}{\partial t} = \Pi^\ell - \nabla_X \cdot M^\ell$$

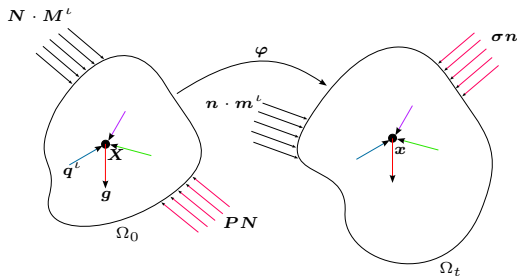
- Momentum balance:

$$\rho_0^\ell \frac{\partial V^\ell}{\partial t} = \rho_0^\ell (g + q^\ell) + \nabla_X \cdot P^\ell - (\nabla_X V^\ell) M^\ell$$

- Kinematics:

$$F = F^{e^\ell} F^{g^\ell}; \text{ e.g. } F^{g^\ell} = \left(\frac{\rho^\ell}{\rho_{0\text{ini}}^\ell} \right)^{\frac{1}{3}} \mathbf{1}$$

The governing equations—Eulerian perspective



Current quantities:

- ρ^ℓ – Species concentration
- π^ℓ – Species production rate
- m^ℓ – Species total flux
- v^ℓ – Species velocity
- g – Body force
- q^ℓ – Interaction force
- σ^ℓ – Partial Cauchy stress

- Imposition of relevant boundary conditions best represented and understood in the current configuration

- Mass balance:

$$\frac{\partial \rho^\ell}{\partial t} = \pi^\ell - \nabla_x \cdot m^\ell$$

- Momentum balance:

$$\rho^\ell \frac{\partial v^\ell}{\partial t} = \rho^\ell (g^\ell + q^\ell) + \nabla_x \cdot \sigma^\ell - (\nabla_x v^\ell) m^\ell$$

Solving these equations in practice—A first pass

- Close the equations with constitutive relationships
 - Solid: Hyperelastic material, $\mathbf{P}^s = \rho_0^s \frac{\partial e^s}{\partial \mathbf{F}^{es}}$
Helmholtz free energy derived from entropic elasticity-based worm-like chain model
 - Fluid: Ideal, $\det(\mathbf{F}^{ef})^{-1} \mathbf{P}^f \mathbf{F}^{efT} = h'(\rho^f) \mathbf{1}$

$$h(\rho^f) = \frac{1}{2} \kappa^f \left(\frac{\rho_{0ini}^f}{\rho^f} - 1 \right)^2$$

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- Sum species momentum balances to solve system-level balance law
 - Reduce number of partial differential equations by one
 - Avoid specification of $\mathbf{q}^l$, because $\sum_l (\rho_0^l \mathbf{q}^l + \Pi^l \mathbf{V}^l) = 0$

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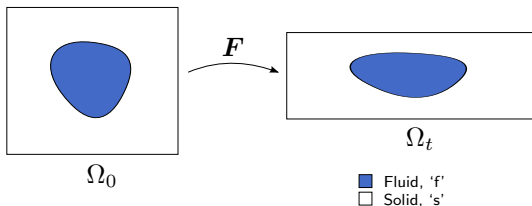
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- System-level motion determined, utilise a constitutive relationship to determine relative fluid flux

$$\mathbf{M}^f = \mathbf{D}^f \left(\rho_0^f \mathbf{F}^T \mathbf{g} + \mathbf{F}^T \nabla_X \cdot \mathbf{P}^f - \nabla_X (e^f - \theta \eta^f) \right)$$

Assumptions on the micromechanics

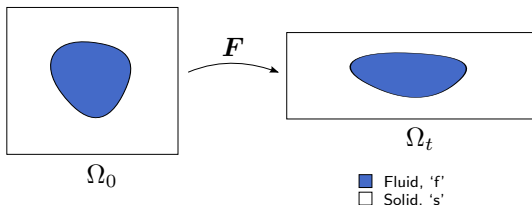
1. *Upper bound* model from strain homogenisation:



Pore structure deforms with the solid phase $\Rightarrow$ Fluid-filled pore spaces see the overall deformation gradient

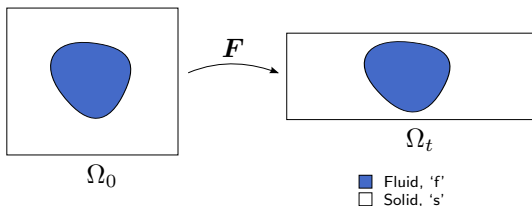
Assumptions on the micromechanics

1. *Upper bound* model from strain homogenisation:



Pore structure deforms with the solid phase $\Rightarrow$ Fluid-filled pore spaces see the overall deformation gradient

2. *Lower bound* model from stress homogenisation:



Fluid pressure in the current configuration is the same as hydrostatic stress of the solid, $p^f = \frac{1}{3} \text{tr}[\boldsymbol{\sigma}^s]$

An operator-splitting solution scheme

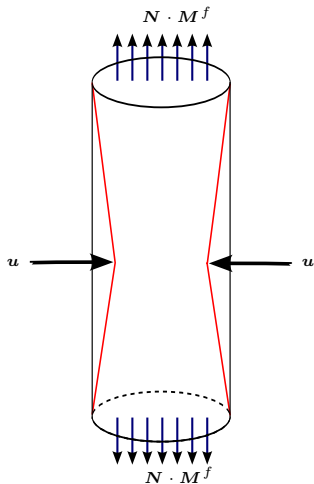
- Nonlinear projection methods to treat incompressibility
- Backward Euler for time-dependent mass balance
- Mixed method for stress/strain gradient-driven fluxes
- Large advective terms stabilised using SUPG
- Coupled implementation; staggered scheme

At each time step, repeat:

- Fixing the concentration fields, solve the mechanics problem for displacements, u
- Fixing the displacement field, solve the mass transport problem for the concentration field, ρ^f

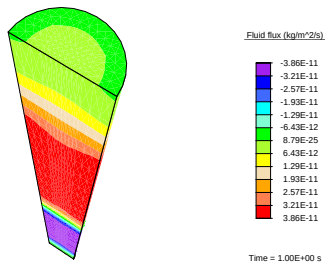
until both problems converge

A demonstrative numerical experiment

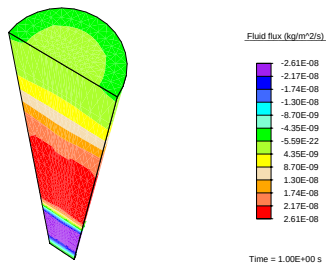


- Simulating a tendon immersed in a bath
- Constrict it radially to force fluid flow
- Biphasic model
 - Worm-like chain model for collagen
 - Ideal, nearly incompressible fluid
- Mobility from Han et al. (JMR 2000)

Implications of the assumptions

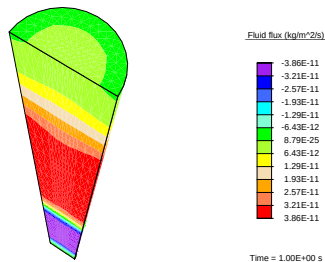


Lower bound vertical fluid flux

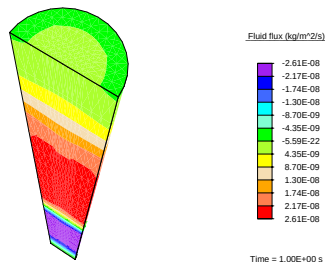


Upper bound vertical fluid flux

Implications of the assumptions



Lower bound vertical fluid flux



Upper bound vertical fluid flux

- Strength of coupling: $C = \frac{\delta p^f}{\frac{1}{3} \delta \text{tr}[\boldsymbol{\sigma}^s]}$
- Upper bound: $C \approx \frac{O(\kappa^f \delta \mathbf{F} : \mathbf{F}^{-T})}{O(\kappa^s \delta \mathbf{F} : \mathbf{F}^{-T})} = O\left(\frac{\kappa^f}{\kappa^s}\right) \gg 1$
- Lower bound: $C = 1$

A closer look at the convergence

Pass	Strongly coupled		Weakly coupled	
	Mechanics Residual	CPU (s)	Mechanics Residual	CPU (s)
1	2.138×10^{-02}	29.16	6.761×10^{-04}	28.5
	3.093×10^{-04}	55.85	1.075×10^{-04}	55.1
	2.443×10^{-06}	82.37	4.984×10^{-06}	81.8
	2.456×10^{-08}	109.61	1.698×10^{-08}	107.9
	4.697×10^{-14}	135.83	3.401×10^{-13}	134.1
	1.750×10^{-16}	163.18	1.1523×10^{-17}	161.1
2	5.308×10^{-06}	166.79	5.971×10^{-08}	192.5
	4.038×10^{-10}	193.36	4.285×10^{-11}	218.6
	1.440×10^{-14}	220.45	2.673×10^{-15}	246.1
	4.221×10^{-17}	247.04		
3	5.186×10^{-06}	250.62	2.194×10^{-09}	277.3
	3.852×10^{-10}	277.44	2.196×10^{-13}	304.2
	1.369×10^{-14}	304.16	1.096×10^{-17}	331.6
	4.120×10^{-17}	331.47		
4	5.065×10^{-06}	335.16	8.160×10^{-11}	363.2
	3.674×10^{-10}	362.24	7.923×10^{-15}	390.2
	1.300×10^{-14}	388.79		
	4.021×10^{-17}	416.08		
5	4.948×10^{-06}	419.59	3.078×10^{-12}	421.4
	3.503×10^{-10}	446.24	3.042×10^{-16}	448.6
	1.236×10^{-14}	473.20		
	3.924×10^{-17}	500.85		
6	4.832×10^{-06}	504.65	1.179×10^{-13}	479.9
	3.340×10^{-10}	531.28	1.291×10^{-17}	507.0
	1.174×10^{-14}	558.17		
	3.829×10^{-17}	585.27		

Solving these equations in practice—Reprise

- Better bounds exist, e.g. Lopez-Pamies and Castañeda (J. Elasticity 2005)
- *What if we were to solve the “detailed” problem instead?*
- Close the equations by specifying momentum transfer terms arising from dissipation inequality

$$\mathbf{q}^f = -\mathbf{D}^f (\mathbf{v}^f - \mathbf{v}^s) - \nabla_x (e^f - \theta \eta^f)$$

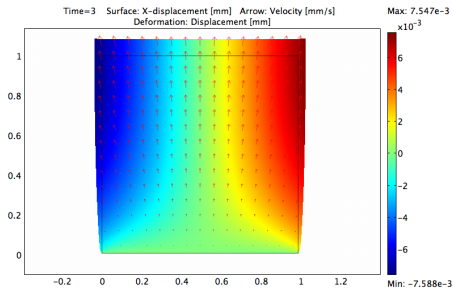
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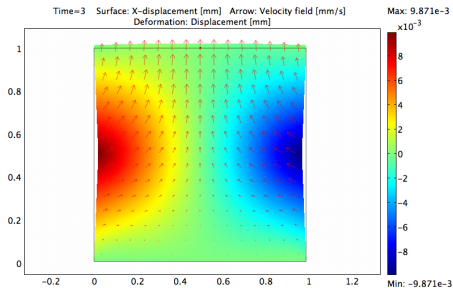
$$\mathbf{q}^f = -\mathbf{D}^f (\mathbf{v}^f - \mathbf{v}^s) - \nabla_x (e^f - \theta \eta^f)$$

- Solve equations in a current volume defined by solid skeleton
 $\Rightarrow$ No notion of any deformation gradient besides $\mathbf{F}^s$
- Impose additional constraints such as intrinsic incompressibility and saturation

Illustrative numerical experiments



Swelling of a balloon



Constriction of the edges

Conclusions, ongoing and future work

- Pointed out that solving system-level balance laws require judicious assumptions on the micromechanics
- Looked at some of the implications of assumptions on solid-fluid interactions—physics and numerics
- Using the mixture theory to determine the origin of rate-dependent response in engineered tendons
- Reinstated growth terms and associated kinematics—applying the formulation to growth-dominated problems like cancer
- Careful examination of the influence of different forms of momentum interaction terms
- For selected forms, determine the consequent degree of coupling between equations, and thus, the convergence of operator-splitting schemes

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