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

H. Narayanan, K. Garikipati, K. Grosh & E. M. Arruda
University of Michigan

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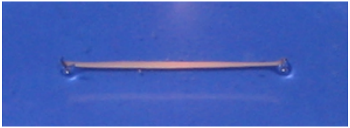
The motivating question

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



Engineered tendon constructs [Calve et al., 2004]

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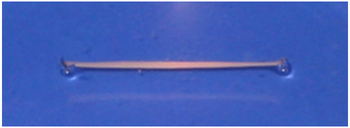

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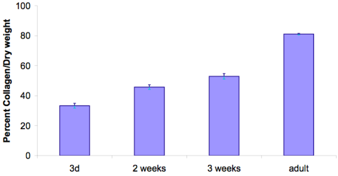
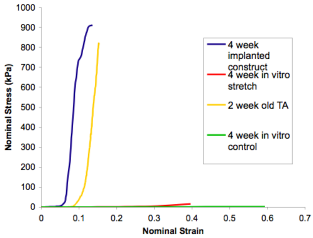


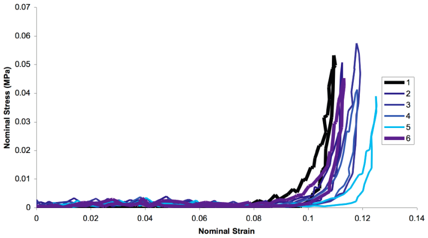
Increasing collagen concentration with age

- *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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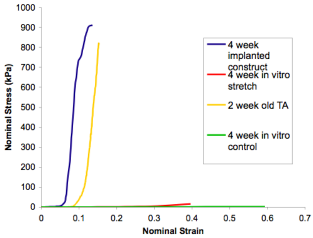

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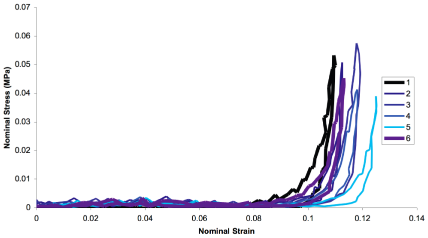

Response under cyclic load

- *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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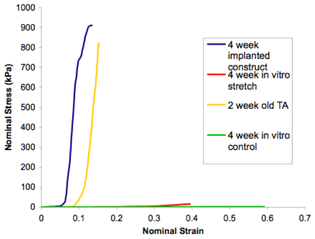

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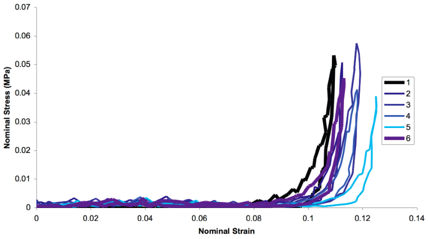

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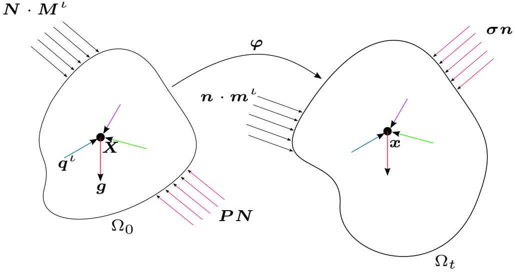
- Modelling of solid-fluid coupling ⇒ Stiffness of tissue and fluid transport ⇒ Nutrient transport ⇒ Tissue growth

The governing equations—Lagrangian perspective



Reference quantities:

ρ_0^ι – Species concentration
Π^ι – Species production rate
M^ι – Species relative flux
V^ι – Species velocity
g – Body force
q^ι – Interaction force
P^ι – Partial First Piola Kirchhoff stress

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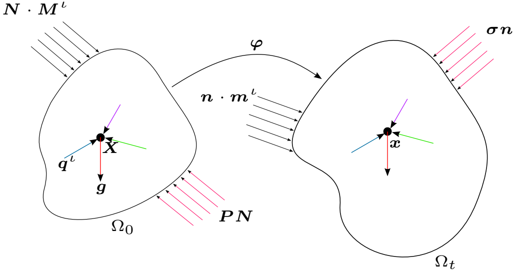

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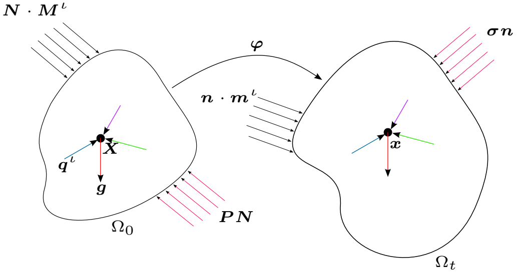
- Mass balance:
$$\frac{\partial \rho_0^\iota}{\partial t} = \Pi^\iota - \nabla_X \cdot M^\iota$$

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

- Kinematics:
$$F = F^{e^\iota} F^{g^\iota}; \text{ e.g. } F^{g^\iota} = \left(\frac{\rho^\iota}{\rho^\iota_{0_{\mathrm{ini}}}}\right)^{\frac{1}{3}} \mathbf{1}$$

The governing equations—Eulerian perspective



Current quantities:

ρ^{ι} – Species concentration
π^{ι} – Species production rate
$\boldsymbol{m}^{\iota}$ – Species total flux
$\boldsymbol{v}^{\iota}$ – Species velocity
$\boldsymbol{g}$ – Body force
$\boldsymbol{q}^{\iota}$ – Interaction force
$\boldsymbol{\sigma}^{\iota}$ – Partial Cauchy stress

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

- Mass balance:
  $$\frac{\partial \rho^{\iota}}{\partial t} = \pi^{\iota} - \boldsymbol{\nabla}_x \cdot \boldsymbol{m}^{\iota}$$

- Momentum balance:
  $$\rho^{\iota}\frac{\partial \boldsymbol{v}^{\iota}}{\partial t} = \rho^{\iota}\left(\boldsymbol{g}^{\iota} + \boldsymbol{q}^{\iota}\right) + \boldsymbol{\nabla}_x \cdot \boldsymbol{\sigma}^{\iota} - \left(\boldsymbol{\nabla}_x \boldsymbol{v}^{\iota}\right)\boldsymbol{m}^{\iota}$$

Solving these equations in practice—A first pass

- Close the equations with constitutive relationships
  - Solid: Hyperelastic material, $\boldsymbol{P}^s = \rho_0^s \frac{\partial e^s}{\partial \boldsymbol{F}^{\mathrm{e}^s}}$
    Helmholtz free energy derived from entropic elasticity-based worm-like chain model
  - Fluid: Ideal, $\det(\boldsymbol{F}^{\mathrm{e}^{\mathrm{f}}})^{-1} \boldsymbol{P}^{\mathrm{f}} \boldsymbol{F}^{\mathrm{e}^{\mathrm{f}\mathrm{T}}} = h'(\rho^{\mathrm{f}}) \mathbf{1}$

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

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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 $\boldsymbol{q}^\iota$, because $\sum\limits_\iota\left(\rho_0^\iota\boldsymbol{q}^\iota + \Pi^\iota\boldsymbol{V}^\iota\right) = 0$

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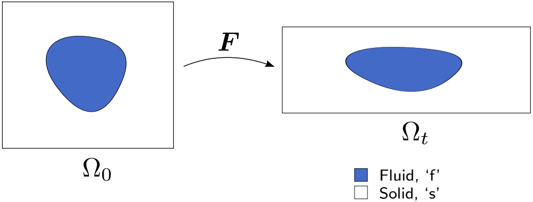
  - Avoid specification of $\boldsymbol{q}^\iota$, because $\sum_\iota \left(\rho_0^\iota \boldsymbol{q}^\iota + \Pi^\iota \boldsymbol{V}^\iota\right) = 0$
- System-level motion determined, utilise a constitutive relationship to determine relative fluid flux
  $$\boldsymbol{M}^f = \boldsymbol{D}^f \left(\rho_0^f \boldsymbol{F}^T \boldsymbol{g} + \boldsymbol{F}^T \boldsymbol{\nabla}_X \cdot \boldsymbol{P}^f - \boldsymbol{\nabla}_X (e^f - \theta \eta^f)\right)$$

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

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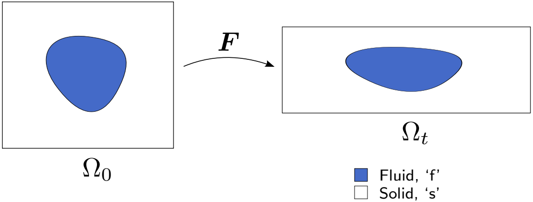

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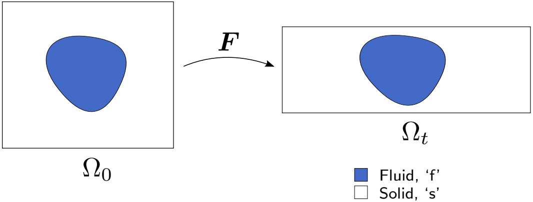
2. *Lower bound* model from stress homogenisation:



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

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

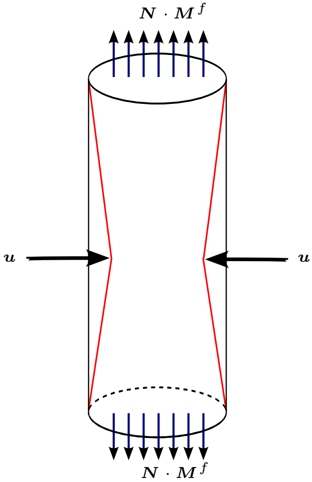
- Coupled implementation; staggered scheme

  `At each time step, repeat:`

  - `Fixing the concentration fields, solve the mechanics problem for displacements,` $\boldsymbol{u}$
  - `Fixing the displacement field, solve the mass transport problem for the concentration field,` ρ^f

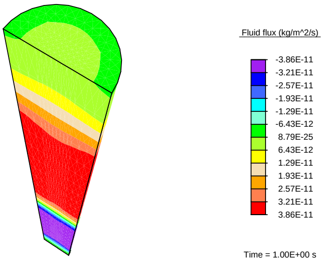
  `until both problems converge`

A demonstrative numerical experiment

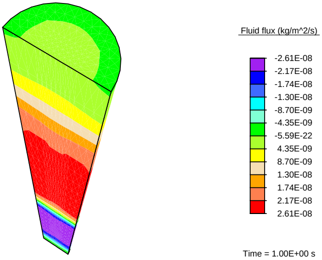


- Simulating a tendon immersed in a bath
- Constrict it radially to force fluid flow
- Biphasic model
  - Worm-like chain model for collagen
  - Ideal, nearly incompressible fluid
- Mobility from Han et al. (JMR 2000)

Implications of the assumptions



Lower bound vertical fluid flux



Upper bound vertical fluid flux

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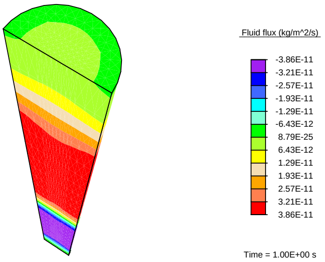
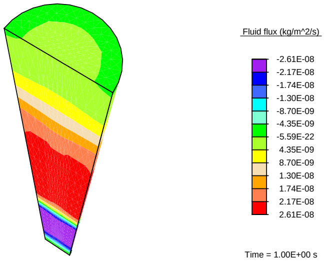


Lower bound vertical fluid flux



Upper bound vertical fluid flux

- Strength of coupling: $C = \frac{\delta p^{\mathrm{f}}}{\frac{1}{3}\delta \mathrm{tr}[\boldsymbol{\sigma}^s]}$

- Upper bound: $C \approx \frac{O(\kappa^{\mathrm{f}}\delta \boldsymbol{F}{:}\boldsymbol{F}^{-\mathrm{T}})}{O(\kappa^{\mathrm{s}}\delta \boldsymbol{F}{:}\boldsymbol{F}^{-\mathrm{T}})} = O(\frac{\kappa^{\mathrm{f}}}{\kappa^{\mathrm{s}}}) \gg 1$
- 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

$$\boldsymbol{q}^f = -\boldsymbol{D}^f \left(\boldsymbol{v}^f - \boldsymbol{v}^s\right) - \boldsymbol{\nabla}_x (e^f - \theta \eta^f)$$

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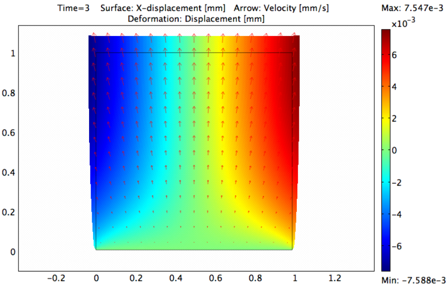
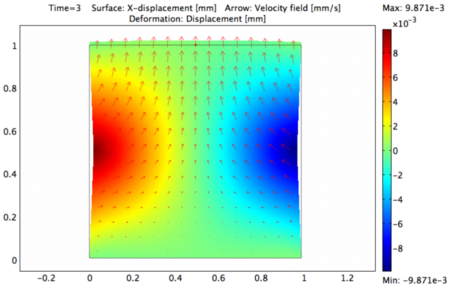
- Solve equations in a current volume defined by solid skeleton $\Rightarrow$ No notion of any deformation gradient besides $\boldsymbol{F}^s$
- Impose additional constraints such as intrinsic incompressibility and saturation

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
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