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

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Ninth U.S. National Congress on Computational Mechanics

July 24th, 2007 – San Francisco, CA
The motivating question

- What constitutes an ideal environment for tissue growth?

Engineered tendon constructs [Calve et al., 2004]
The motivating question

- What constitutes an ideal environment for tissue growth?

Engineered tendon constructs [Calve et al., 2004]

- Growth involves an addition or depletion of mass

Increasing collagen concentration with age
The narrow scope of this talk

Uniaxial tensile response

Response under cyclic load
The narrow scope of this talk

- **What causes the tissue to behave in this manner?**
The narrow scope of this talk

• 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 ⇒ Stiffness of tissue and fluid transport ⇒ Nutrient transport ⇒ Tissue growth
The governing equations—Lagrangian perspective

Reference quantities:
\( \rho_0^i \) – Species concentration
\( \Pi^i \) – Species production rate
\( M^i \) – Species relative flux
\( V^i \) – Species velocity
\( g \) – Body force
\( q^i \) – Interaction force
\( P^i \) – Partial First Piola Kirchhoff stress
The governing equations—Lagrangian perspective

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- Mass balance:
  \[
  \frac{\partial \rho_0^t}{\partial t} = \Pi^t - \nabla X \cdot M^t
  \]

- Momentum balance:
  \[
  \rho_0^t \frac{\partial V^t}{\partial t} = \rho_0^t (g + q^t) + \nabla X \cdot P^t - (\nabla X V^t)M^t
  \]

- Kinematics:
  \[
  F = F^{e^t} F^{g^t}; \text{ e.g. } F^{g^t} = \left( \frac{\rho^t}{\rho^t_{\text{ini}}} \right)^{\frac{1}{3}} 1
  \]
The governing equations—Eulerian perspective

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

- Mass balance:
  \[ \frac{\partial \rho^t}{\partial t} = \pi^t - \nabla_x \cdot m^t \]

- Momentum balance:
  \[ \rho^t \frac{\partial \mathbf{v}^t}{\partial t} = \rho^t (g^t + q^t) + \nabla_x \cdot \sigma^t - (\nabla_x \mathbf{v}^t) m^t \]

Current quantities:
- \( \rho^t \) – Species concentration
- \( \pi^t \) – Species production rate
- \( m^t \) – Species total flux
- \( v^t \) – Species velocity
- \( g \) – Body force
- \( q^t \) – Interaction force
- \( \sigma^t \) – Partial Cauchy stress
Solving these equations in practice—A first pass

• Close the equations with constitutive relationships
  ○ Solid: Hyperelastic material, \( P^s = \rho_0^s \frac{\partial e^s}{\partial F^{es}} \)
    Helmholtz free energy derived from entropic elasticity-based worm-like chain model
  ○ Fluid: Ideal, \( \det(F^f) - 1 P^f F^{eT} = h'(\rho^f) 1 \)
    \[
    h(\rho^f) = \frac{1}{2} \kappa_f \left( \frac{\rho_{0ini}^f}{\rho^f} - 1 \right)^2
    \]
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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 \( \mathbf{q}^\ell \), because \( \sum_\ell (\rho_\ell^0 \mathbf{q}^\ell + \Pi^\ell \mathbf{V}^\ell) = 0 \)
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• System-level motion determined, utilise a constitutive relationship to determine relative fluid flux
  \[ M^f = D^f \left( \rho_0^f F^T g + F^T \nabla X \cdot P^f - \nabla X (e^f - \theta \eta^f) \right) \]
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:

   Fluid-filled pore spaces see the overall deformation gradient

   $p^f = \frac{1}{3} \text{tr}[\sigma^s]$  

2. **Lower bound** model from stress homogenisation:

   Pore structure deforms with the solid phase ⇒ Fluid-filled pore spaces see the overall deformation gradient
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, $\rho^f$

  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

- Strength of coupling: \( C = \frac{\delta p^f}{\frac{1}{3} \delta \text{tr}[\sigma^s]} \)

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

- Lower bound: \( C = 1 \)
A closer look at the convergence

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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

\[ q^f = -D^f (v^f - v^s) - \nabla_x (e^f - \theta \eta^f) \]
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- Close the equations by specifying momentum transfer terms arising from dissipation inequality
  \[ q^f = -D^f (v^f - v^s) - \nabla_x (e^f - \theta \eta^f) \]
- Solve equations in a current volume defined by solid skeleton ⇒ No notion of any deformation gradient besides \( F^{is} \)
- 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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