

A Continuum Treatment of Growth in Tissue – Mass Transport Coupled with Mechanics

H. Narayanan, K. Garikipati, E. M. Arruda, K. Gosh, S. Calve
University of Michigan, Ann Arbor

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broad goals

- mathematical and computational models of the processes of tissue development
 - models that are physiologically appropriate and thermodynamically valid
 - quantitative model motivated and validated by experiment
- experiments on and characterization of *in vitro* engineered tissue
 - model drives the controlled experiments

development of biological tissue

distinct processes of tissue development: [taber - 1995]

- **growth** – addition/loss of mass
 - *densification of bone*
- **remodelling** – change in microstructure
 - *alignment of trabeculae of bones to axis of external loading*
- **morphogenesis** – change in macroscopic form
 - *development of an embryo from a fertilized egg*

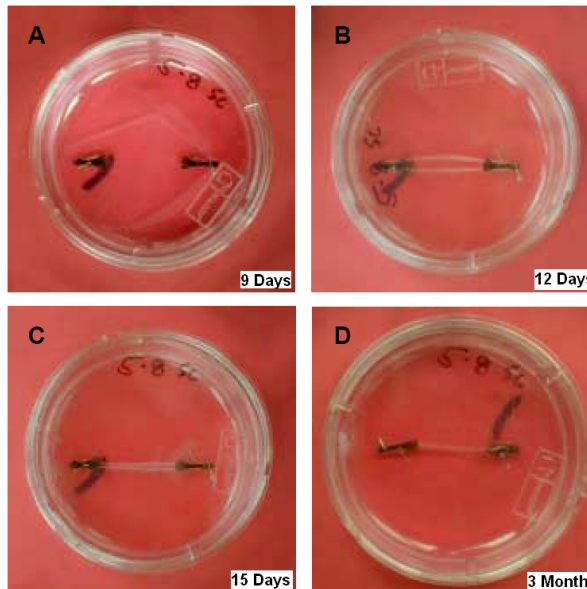
physics of growth

- open system with respect to mass
- interacting and interconverting species
- species diffusing with respect to a solid phase
 - *fluid, precursors, byproducts*
- mixture physics

our treatment involves the introduction of sources, sinks and fluxes of mass

biological model

engineered tissue *in vitro* that is morphologically and functionally similar to neonatal tissue:
[calve et al., 2003]



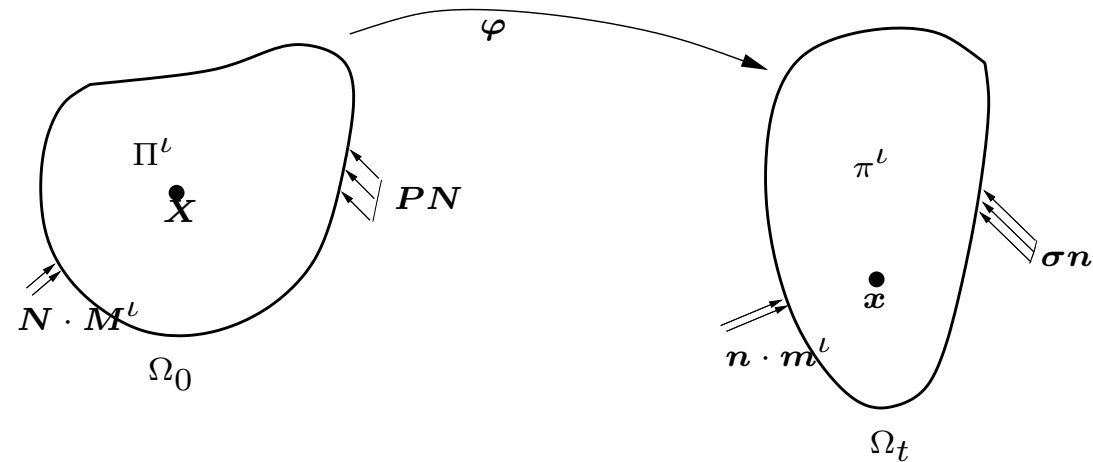
modelling background

- cowin and hegedus [1976]: solid tissue; mass source; irreversible sources of momentum and energy from perfusing fluid
- epstein and maugin [2000]: mass flux; irreversible fluxes of momentum and entropy
- kuhl and steinmann [2002]: configurational forces motivate mass flux

modelling of biological growth - this work

- multiple species undergoing transport, interconversion, mechanical and thermodynamic interactions
- other species deform with solid phase and diffuse with respect to it
- fully compatible with mixture theory
- detailed coupling of mechanics and mass balance
- thermodynamic consistency
- preliminary coupled computations

balance of mass



- tissue formed by reacting species – sources and sinks for species
- transport of precursors, fluid and byproducts – fluxes for species

balance of mass - equations

for a species ι , in local form, in Ω_0

$$\frac{\partial \rho_0^\iota}{\partial t} = \Pi^\iota - \nabla_X \cdot \mathbf{M}^\iota, \quad \forall \iota = \alpha, \dots, \omega$$

the sources/sinks satisfy

$$\sum_{\iota=\alpha}^{\omega} \Pi^\iota = 0.$$

balance of mass - equations

for a species ι , in local form, in Ω_0

$$\frac{\partial \rho_0^\iota}{\partial t} = \Pi^\iota - \nabla_X \cdot \mathbf{M}^\iota, \quad \forall \iota = \alpha, \dots, \omega$$

for the solid phase

$$\frac{\partial \rho_0^s}{\partial t} = \Pi^s$$

ignoring short range motion of cells; e.g., during initial stages of wound healing

balance of mass - equations

for a species ι , in local form, in Ω_0

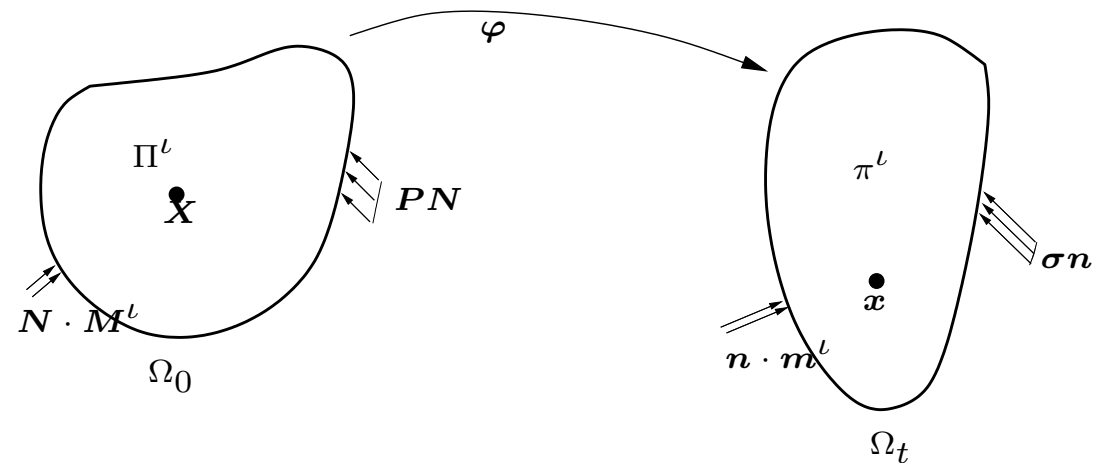
$$\frac{\partial \rho_0^\iota}{\partial t} = \Pi^\iota - \nabla_X \cdot \mathbf{M}^\iota, \quad \forall \iota = \alpha, \dots, \omega$$

for the fluid phase

$$\frac{\partial \rho_0^f}{\partial t} = -\nabla_X \cdot \mathbf{M}^f$$

if sources for interstitial fluids are absent; e.g., no lymph glands

balance of linear momentum



- linear momentum balance coupled with mass transport – sources/sinks and fluxes contribute to the momenta
- material velocity relative to the solid $\mathbf{V}^\ell = (1/\rho_0^\ell)\mathbf{F}\mathbf{M}^\ell$

balance of linear momentum - equations

for a species ι , in local form, in Ω_0

$$\rho_0^\iota \frac{\partial}{\partial t} (\mathbf{V} + \mathbf{V}^\iota) = \rho_0^\iota (\mathbf{g} + \mathbf{q}^\iota) + \nabla_X \cdot \mathbf{P}^\iota - (\nabla_X (\mathbf{V} + \mathbf{V}^\iota)) \mathbf{M}^\iota, \quad \forall \iota = \alpha, \dots, \omega$$

balance of linear momentum - equations

for a species ι , in local form, in Ω_0

$$\rho_0^\iota \frac{\partial}{\partial t} (\mathbf{V} + \mathbf{V}^\iota) = \rho_0^\iota (\mathbf{g} + \mathbf{q}^\iota) + \nabla_X \cdot \mathbf{P}^\iota - (\nabla_X (\mathbf{V} + \mathbf{V}^\iota)) \mathbf{M}^\iota, \quad \forall \iota = \alpha, \dots, \omega$$

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balance of linear momentum - equations

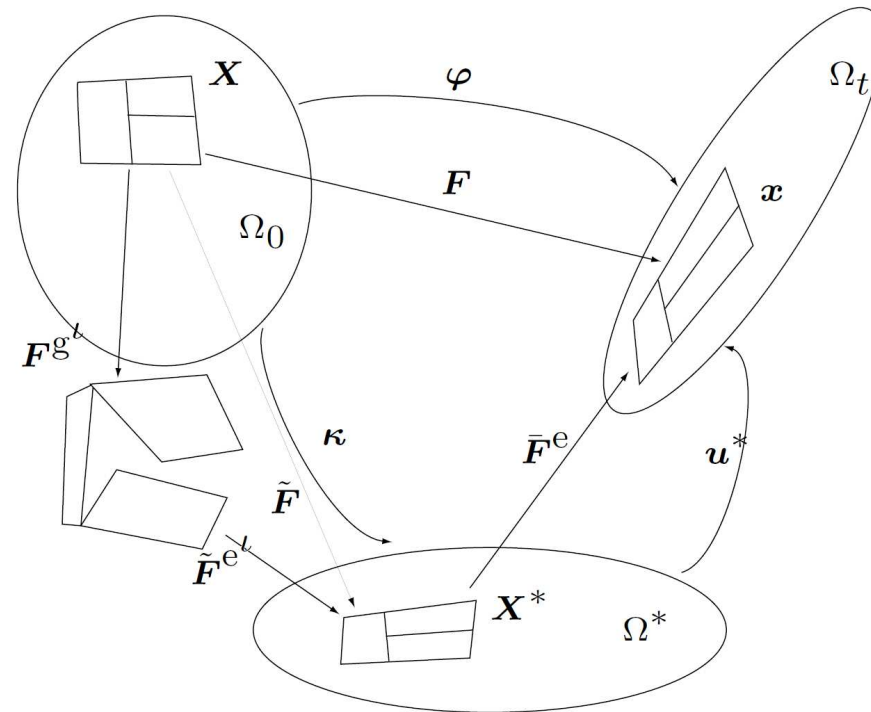
for a species ι , in local form, in Ω_0

$$\rho_0^\iota \frac{\partial}{\partial t} (\mathbf{V} + \mathbf{V}^\iota) = \rho_0^\iota (\mathbf{g} + \mathbf{q}^\iota) + \nabla_X \cdot \mathbf{P}^\iota - (\nabla_X (\mathbf{V} + \mathbf{V}^\iota)) \mathbf{M}^\iota, \quad \forall \iota = \alpha, \dots, \omega$$

relation between mass sources Π^ι 's and interaction forces \mathbf{q}^ι 's,

$$\sum_{\iota=\alpha}^{\omega} (\rho_0^\iota \mathbf{q}^\iota + \Pi^\iota \mathbf{V}^\iota) = 0$$

kinematics of growth



kinematics of growth

$$\mathbf{F} = \bar{\mathbf{F}}^e \tilde{\mathbf{F}}^{e^l} \mathbf{F}^{g^l}$$

- \mathbf{F}^{g^l} is a kinematic “growth” tensor , $\mathbf{F}^{e^l} = \bar{\mathbf{F}}^e \tilde{\mathbf{F}}^{e^l}$ is the elastic deformation gradient
- residual stress due to $\tilde{\mathbf{F}}^{e^l}$

energy, first law

balance of energy for a species ι , in local form, in Ω_0

$$\rho_0^\iota \frac{\partial e^\iota}{\partial t} = \mathbf{P}^\iota : \dot{\mathbf{F}} + \mathbf{P}^\iota : \nabla_X \mathbf{V}^\iota - \nabla_X \cdot \mathbf{Q}^\iota + r_0^\iota + \rho_0^\iota \tilde{e}^\iota - \nabla_X e^\iota \cdot (\mathbf{M}^\iota)$$

energy, first law

balance of energy for a species ι , in local form, in Ω_0

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energy, first law

balance of energy for a species ι , in local form, in Ω_0

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where the interaction terms satisfy the relation,

$$\sum_{\iota=\alpha}^{\omega} \left(\rho_0^\iota \mathbf{q}^\iota \cdot (\mathbf{V} + \mathbf{V}^\iota) + \Pi^\iota \left(e^\iota + \frac{1}{2} \|\mathbf{V} + \mathbf{V}^\iota\|^2 \right) + \rho_0^\iota \tilde{e}^\iota \right) = 0$$

entropy, second law

$$\sum_{\iota=\alpha}^{\omega} \rho_0^{\iota} \frac{\partial \eta^{\iota}}{\partial t} \geq \sum_{\iota=\alpha}^{\omega} \left(\frac{r^{\iota}}{\theta} - \nabla_X \eta^{\iota} \cdot M^{\iota} - \frac{\nabla_X \cdot Q^{\iota}}{\theta} + \frac{\nabla_X \theta \cdot Q^{\iota}}{\theta^2} \right)$$

combine first and second laws to get the dissipation inequality

constitutive relations

constitutive hypothesis: $e^\iota = \hat{e}^\iota(\mathbf{F}^{e^\iota}, \rho_0^\iota, \eta^\iota)$

constitutive relations consistent with the dissipation inequality:

$$\mathbf{P}^\iota = \rho_0^\iota \frac{\partial e^\iota}{\partial \mathbf{F}^{e^\iota}}, \forall \iota \quad \circ \text{ hyperelastic material}$$

$$\theta = \frac{\partial e^\iota}{\partial \eta^\iota}, \forall \iota \quad \circ \text{ thermal physics}$$

$$\mathbf{Q}^\iota = -\mathbf{K}^\iota \nabla_X \theta, \forall \iota \quad \circ \text{ fourier law}$$

$$\mathbf{u} \cdot \mathbf{K}^\iota \mathbf{u} \geq 0 \forall \mathbf{u} \in \mathbb{R}^3 \quad (\text{semi-positive definite conductivity})$$

constitutive relations

constitutive relation for flux of each transported species:

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

$$\mathbf{u} \cdot \mathbf{D}^\ell \mathbf{u} \geq 0 \forall \mathbf{u} \in \mathbb{R}^3$$

- \mathbf{D}^ℓ is the mobility

constitutive relations

constitutive relation for flux of each transported species:

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

- driving force due to inertia

constitutive relations

constitutive relation for flux of each transported species:

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

- driving force due to gravity

constitutive relations

constitutive relation for flux of each transported species:

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

- driving force due to stress gradient – darcy's law

constitutive relations

constitutive relation for flux of each transported species:

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

- driving force due to a chemical potential gradient

reduced dissipation inequality

with the constitutive relations ensuring the non-positiveness of certain terms the entropy inequality is reduced to

$$\begin{aligned} \mathcal{D} = & \sum_{\iota=\alpha}^{\omega} \left(\rho_0^{\iota} \frac{\partial e^{\iota}}{\partial \rho_0^{\iota}} \frac{\partial \rho_0^{\iota}}{\partial t} - \mathbf{P}^{\iota} : \nabla_X \mathbf{V}^{\iota} + \rho_0^{\iota} \mathbf{V}^{\iota} \cdot \left(\frac{\partial \mathbf{V}^{\iota}}{\partial t} + (\nabla_X \mathbf{V}^{\iota}) \mathbf{F}^{-1} \mathbf{V}^{\iota} \right) \right) \\ & + \sum_{\iota=\alpha}^{\omega} \Pi^{\iota} \left(e^{\iota} + \frac{1}{2} \|\mathbf{V} + \mathbf{V}^{\iota}\|^2 \right) \\ + & \sum_{\iota=\alpha}^{\omega} \left(\rho_0^{\iota} \frac{\partial}{\partial t} (\mathbf{V} + \mathbf{V}^{\iota}) - \rho_0^{\iota} \mathbf{g} - \nabla_X \cdot \mathbf{P}^{\iota} + \nabla_X (\mathbf{V} + \mathbf{V}^{\iota}) (\rho_0^{\iota} \mathbf{F}^{-1} \mathbf{V}^{\iota}) \right) \cdot \mathbf{V} \leq 0 \end{aligned}$$

preliminary coupled computations

- biphasic model
 - worm-like chain model for collagen
 - nearly incompressible interstitial fluid with bulk compressibility of water, $\kappa^f = 2.25$ GPa
- fluid mobility D^ν from swartz et al. [1999]

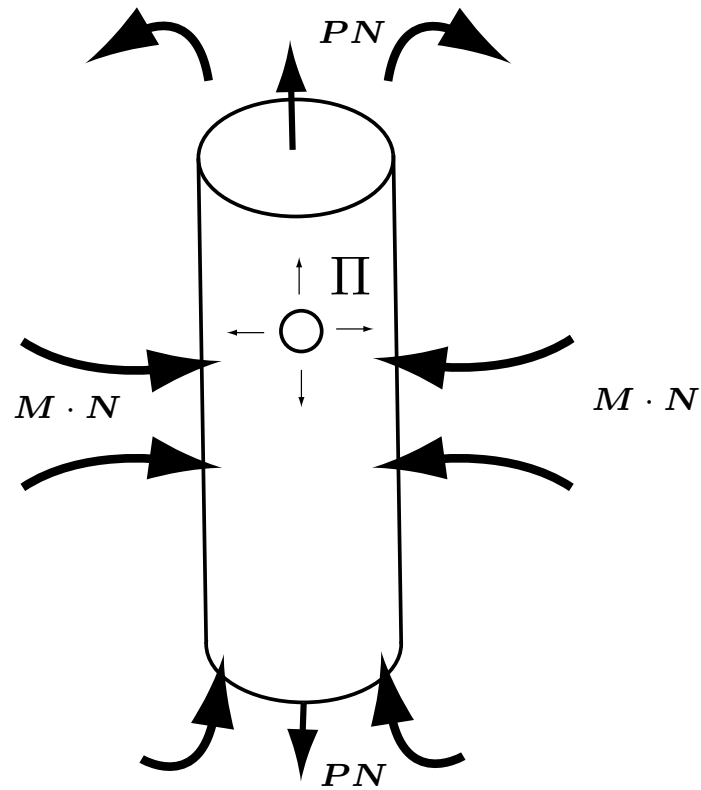
- “artificial” sources:

$$\Pi^f = k^f(\rho_0^f - \rho_{0\text{ini}}^f), \quad \Pi^s = -\Pi^f$$

- entropy of mixing:

$$\eta_{\text{mix}}^\nu = -\frac{k}{\mathcal{M}^\nu} \log \frac{\rho_0^\nu}{\rho_0}$$

preliminary coupled computations



preliminary coupled computations - evolution of fields

view stress gradient-driven flux

view gravity-driven flux. view inertia-driven flux

view concentration gradient-driven flux

view total flux

view stress

view fluid source

summary and further work

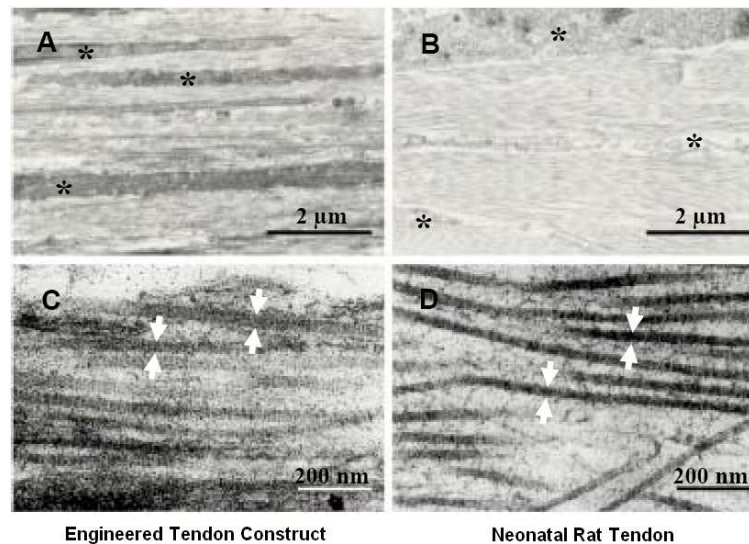
- physiologically consistent continuum formulation describing growth in an open system
- relevant driving forces arise from thermodynamics – coupling with mechanics
- consistent with mixture theory
- formulated a theoretical framework for the remodelling problem
- engineering and characterization of growing, functional biological tissue

a continuum treatment of growth in tissue

biological model - morphological comparison

morphological comparison of the engineered constructs to 2 day old neonatal rat tendon:

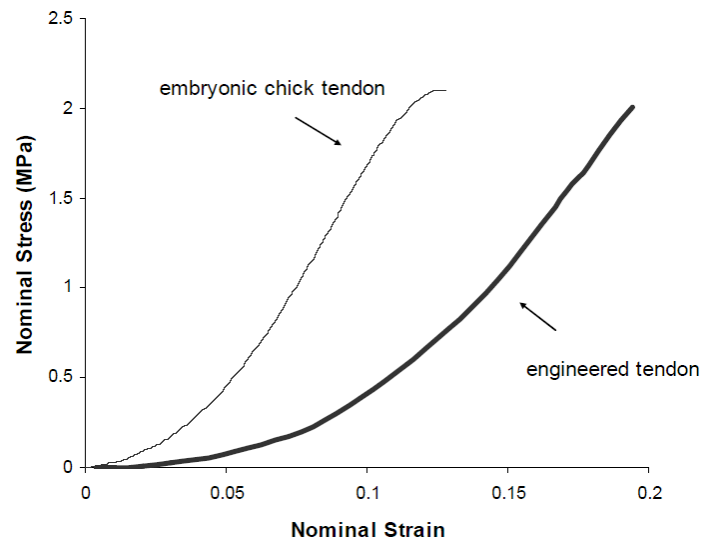
[calve et al., 2003]



biological model - mechanical comparison

comparison of the stress-strain response of the engineered construct to embryonic chicken tendon:

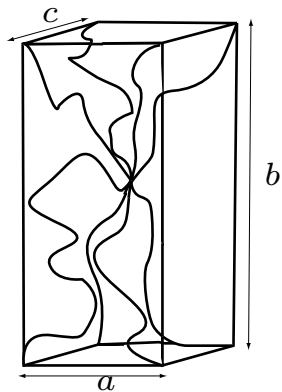
[calve et al., 2003]



cauchy stress

cauchy stress, $J^{e^\iota} \boldsymbol{\sigma}^\iota = \mathbf{P}^\iota \mathbf{F}^{e^\iota T}$, is symmetric

Worm-like chain model for solid collagen



$$\begin{aligned}
 \tilde{\rho}_0^s \hat{e}^s(\mathbf{F}^{e^s}, \rho_0^s) &= \frac{Nk\theta}{4A} \left(\frac{r^2}{2L} + \frac{L}{4(1-r/L)} - \frac{r}{4} \right) \\
 &- \frac{Nk\theta}{4\sqrt{2L/A}} \left(\sqrt{\frac{2A}{L}} + \frac{1}{4(1-\sqrt{2A/L})} - \frac{1}{4} \right) \log(\lambda_1^{a^2} \lambda_2^{b^2} \lambda_3^{c^2}) \\
 &+ \frac{\gamma}{\beta} (J^{e^t-2\beta} - 1) + 2\gamma \mathbf{1} : \mathbf{E}^{e^s}
 \end{aligned}$$

$$r = \frac{1}{2} \sqrt{a^2 \lambda_1^{e^2} + b^2 \lambda_2^{e^2} + c^2 \lambda_3^{e^2}}, \quad \lambda_I^e = \sqrt{\mathbf{N}_I \cdot \mathbf{C}^e \mathbf{N}_I}$$

Mass Balance - Equations

For a species, in the integral form

$$\frac{d}{dt} \int_{\Omega_0} \rho_0^\iota(\mathbf{X}, t) dV = \int_{\Omega_0} \Pi^\iota(\mathbf{X}, t) dV - \int_{\partial\Omega_0} \mathbf{M}^\iota(\mathbf{X}, t) \cdot \mathbf{N} dA, \quad \forall \iota = \alpha, \dots, \omega \quad (1)$$

ρ_0^ι being the mass concentration of species ι and $\sum_{\iota=\alpha}^{\omega} \rho_0^\iota = \rho_0$

The sources/sinks satisfy

$$\sum_{\iota=\alpha}^{\omega} \Pi^\iota = 0. \quad (2)$$

Balance of Linear Momentum - Equations

For a species ι , in the integral form written in Ω_0 is

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_0} \rho_0^\iota (\mathbf{V} + \mathbf{V}^\iota) dV &= \int_{\Omega_0} \rho_0^\iota \mathbf{g} dV + \int_{\Omega_0} \rho_0^\iota \mathbf{q}^\iota dV + \int_{\Omega_0} \Pi^\iota (\mathbf{V} + \mathbf{V}^\iota) dV \\ &+ \int_{\partial\Omega_0} \mathbf{S}^\iota \mathbf{N} dA - \int_{\partial\Omega_0} (\mathbf{V} + \mathbf{V}^\iota) \mathbf{M}^\iota \cdot \mathbf{N} dA \end{aligned} \quad (3)$$

$$\mathbf{q}^\iota = \sum_{\vartheta=\alpha, \vartheta \neq \iota}^{\omega} \mathbf{q}^{\iota\vartheta} \quad (4)$$

On application of balance of mass, in local form, for the entire system

$$\sum_{\iota=\alpha}^{\omega} \rho_0^{\iota} \frac{\partial}{\partial t} (\mathbf{V} + \mathbf{V}^{\iota}) = \sum_{\iota=\alpha}^{\omega} \rho_0^{\iota} (\mathbf{g} + \mathbf{q}^{\iota}) + \sum_{\iota=\alpha}^{\omega} \nabla_X \cdot \mathbf{S}^{\iota} - \sum_{\iota=\alpha}^{\omega} (\nabla_X (\mathbf{V} + \mathbf{V}^{\iota})) M^{\iota} \quad (5)$$

Relation between Π^{ι} 's and \mathbf{q}^{ι} 's,

$$\sum_{\iota=\alpha}^{\omega} (\rho_0^{\iota} \mathbf{q}^{\iota} + \Pi^{\iota} \mathbf{V}^{\iota}) = 0 \quad (6)$$

Balance of Angular Momentum - Equations

- In a purely mechanical theory, balance of angular momentum implies $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$.
- For a single species ι , in integral form in Ω_0 ,

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_0} \boldsymbol{\varphi} \times \rho_0^\iota (\mathbf{V} + \mathbf{V}^\iota) dV &= \int_{\Omega_0} \boldsymbol{\varphi} \times [\rho_0^\iota (\mathbf{g} + \mathbf{q}^\iota) + \Pi^\iota (\mathbf{V} + \mathbf{V}^\iota)] dV \\ &+ \int_{\partial\Omega_0} \boldsymbol{\varphi} \times (\mathbf{S}^\iota - (\mathbf{V} + \mathbf{V}^\iota) \otimes \mathbf{M}^\iota) \mathbf{N} dA \end{aligned} \quad (7)$$

On simplification,

$$\int_{\Omega_0} \mathbf{V} \times \rho_0^\iota \mathbf{V}^\iota dV = - \int_{\Omega_0} \boldsymbol{\epsilon} : \left(\left(\mathbf{S}^\iota - (\mathbf{V} + \mathbf{V}^\iota) \otimes \underbrace{\mathbf{M}^\iota}_{\rho_0^\iota \mathbf{F}^{-1} \mathbf{V}^\iota} \right) \mathbf{F}^T \right) dV \quad (8)$$

On localizing,

$$(\mathbf{S}^\iota - \mathbf{V}^\iota \otimes \rho_0^\iota \mathbf{F}^{-1} \mathbf{V}^\iota) \mathbf{F}^T = \mathbf{F} (\mathbf{S}^\iota - \mathbf{V}^\iota \otimes \rho_0^\iota \mathbf{F}^{-1} \mathbf{V}^\iota)^T \quad (9)$$

But, $(\mathbf{V}^\iota \otimes \mathbf{F}^{-1} \mathbf{V}^\iota) \mathbf{F}^T = \mathbf{V}^\iota \otimes \mathbf{V}^\iota$, which implies the symmetry: $\mathbf{S}^\iota \mathbf{F}^T = \mathbf{F} (\mathbf{S}^\iota)^T$

This implies the partial Cauchy stresses are symmetric: $\boldsymbol{\sigma}^\iota = (\boldsymbol{\sigma}^\iota)^T$

Balance of Energy - Equations

$$\begin{aligned}
 \frac{d}{dt} \int_{\Omega_0} \rho_0^\iota \left(e^\iota + \frac{1}{2} \|\mathbf{V} + \mathbf{V}^\iota\|^2 \right) dV &= \int_{\Omega_0} (\rho_0^\iota \mathbf{g} \cdot (\mathbf{V} + \mathbf{V}^\iota) + r_0^\iota) dV \\
 &\quad + \int_{\Omega_0} \rho_0^\iota \mathbf{q}^\iota \cdot (\mathbf{V} + \mathbf{V}^\iota) dV \\
 &\quad + \int_{\Omega_0} \left(\Pi^\iota \left(e^\iota + \frac{1}{2} \|\mathbf{V} + \mathbf{V}^\iota\|^2 \right) + \rho_0^\iota \tilde{e}^\iota \right) dV \\
 + \int_{\partial\Omega_0} \left((\mathbf{V} + \mathbf{V}^\iota) \cdot \mathbf{S}^\iota - \mathbf{M}^\iota \left(e^\iota + \frac{1}{2} \|\mathbf{V} + \mathbf{V}^\iota\|^2 \right) - \mathbf{Q}^\iota \right) \cdot \mathbf{N} dA. &\quad (10)
 \end{aligned}$$

On simplification localizing, and summing over all ι ,

$$\begin{aligned} \sum_{\iota=\alpha}^{\omega} \rho_0^{\iota} \frac{\partial e^{\iota}}{\partial t} &= \sum_{\iota=\alpha}^{\omega} \left(\mathbf{S}^{\iota} : \dot{\mathbf{F}} + \mathbf{S}^{\iota} : \nabla_X \mathbf{V}^{\iota} - \nabla_X \cdot \mathbf{Q}^{\iota} + r_0^{\iota} + \rho_0^{\iota} \tilde{e}^{\iota} \right) \\ &\quad - \sum_{\iota=\alpha}^{\omega} \nabla_X e^{\iota} \cdot (\mathbf{M}^{\iota}) \end{aligned} \quad (11)$$

Where \tilde{e}^{ι} satisfies the relation,

$$\sum_{\iota=\alpha}^{\omega} \left(\rho_0^{\iota} \mathbf{q}^{\iota} \cdot (\mathbf{V} + \mathbf{V}^{\iota}) + \Pi^{\iota} \left(e^{\iota} + \frac{1}{2} \|\mathbf{V} + \mathbf{V}^{\iota}\|^2 \right) + \rho_0^{\iota} \tilde{e}^{\iota} \right) = 0 \quad (12)$$

The different terms - Mechanics

In the reference configuration Ω_0 ,

Π^ι is the source/sink term for species ι

M^ι is the mass flux term for species ι

S^ι is the partial first Piola-Kirchhoff stress on species ι

N is the outward normal at the surface

g is the body force acting on the entire system

The different terms - Mechanics

In the current configuration Ω_t ,

π^ι is the source/sink term for species ι

m^ι is the mass flux term for species ι

σ^ι is the partial Cauchy stress on species ι

n is the outward normal at the surface

g is the body force acting on the entire system

The different terms - Mechanics

\mathbf{V} is the velocity of the solid phase

\mathbf{V}^ι is the material velocity relative to the solid phase defined as $\mathbf{V}^\iota = (1/\rho_0^\iota) \mathbf{F} \mathbf{M}^\iota$

\mathbf{q}^ι is the net force exerted on species ι by all other species in the system

The different terms - Energy

e^ι is the internal energy of each species ι

\mathbf{F} is the deformation gradient

\mathbf{Q}^ι is the heat flux term for species ι

r_0^ι is the heat supplied to species ι per unit reference volume

\tilde{e} is the internal energy transferred to species ι from all other species