

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

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○ 40th Annual Technical Meeting of the Society of Engineering Science ○

Ann Arbor, October 12-15, 2003

## 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*

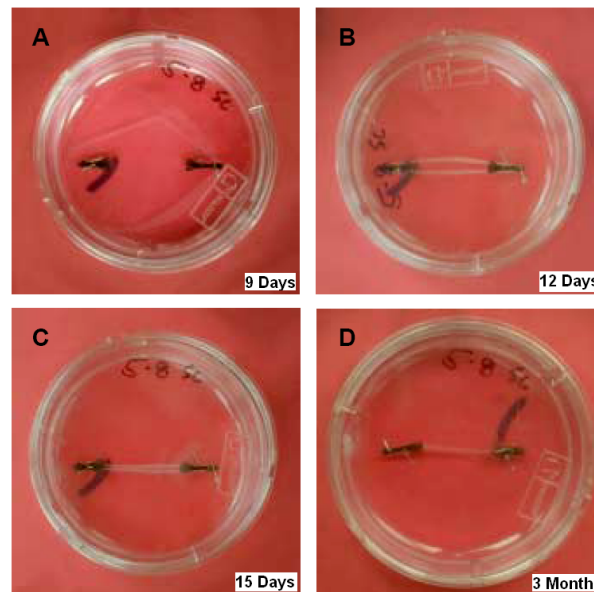
## physics of growth

- 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]



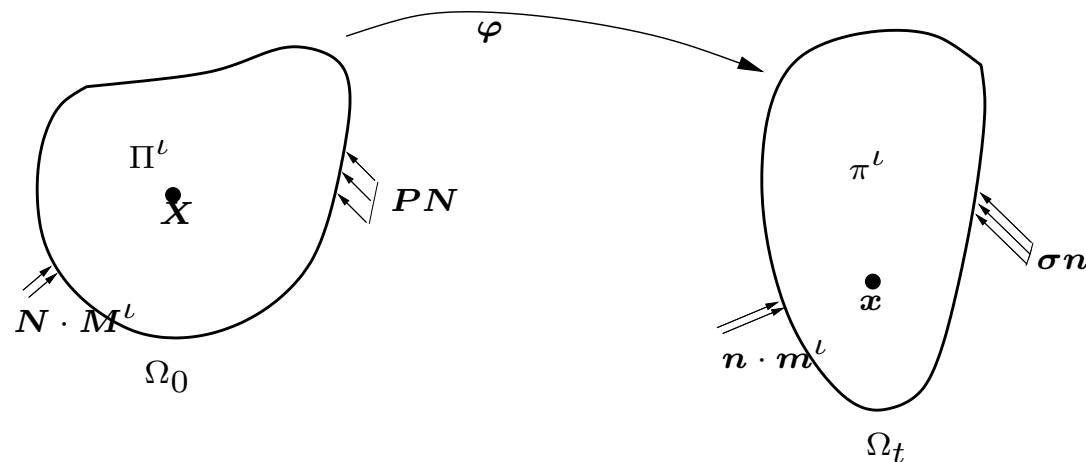
## modelling background

- 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  $\iota$ , in local form, in  $\Omega_0$

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

the sources/sinks satisfy

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

## balance of mass - equations

for a species  $\iota$ , in local form, in  $\Omega_0$

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

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  $\iota$ , in local form, in  $\Omega_0$

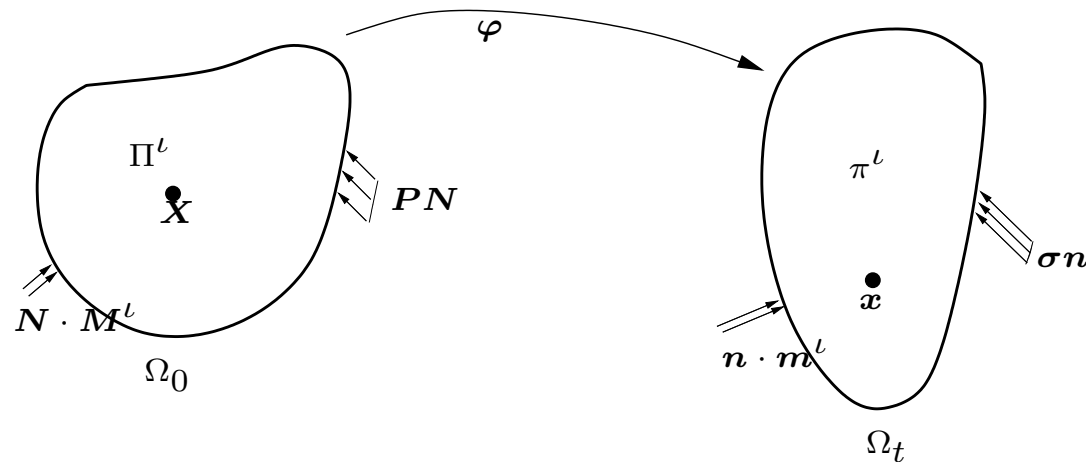
$$\frac{\partial \rho_0^\iota}{\partial t} = \Pi^\iota - \nabla_X \cdot \mathbf{M}^\iota, \quad \forall \iota = \alpha, \dots, \omega$$

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  $\iota$ , in local form, in  $\Omega_0$

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

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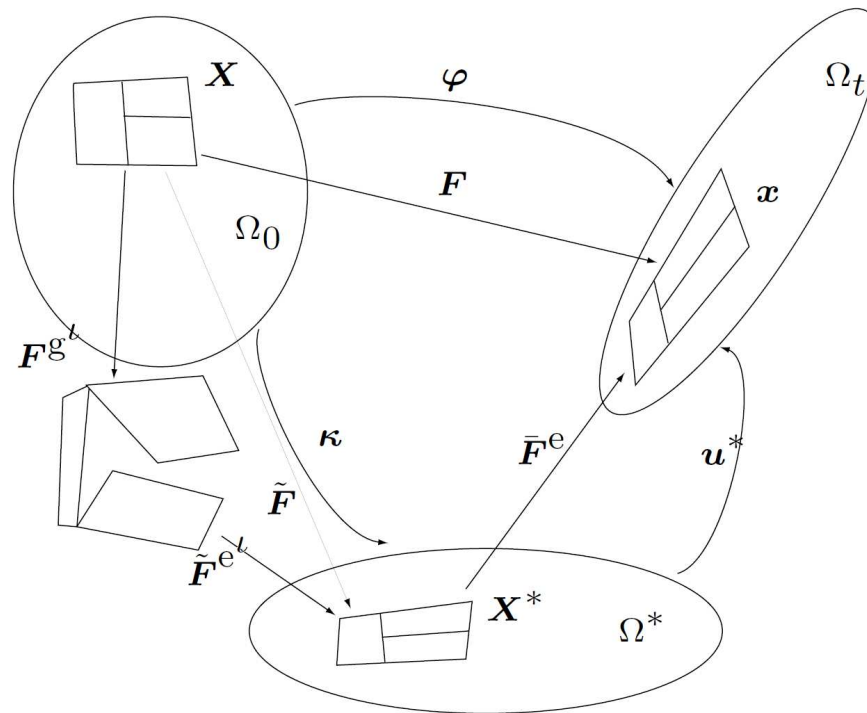
$$\rho_0^\iota \frac{\partial}{\partial t} (\mathbf{V} + \mathbf{V}^\iota) = \rho_0^\iota (\mathbf{g} + \mathbf{q}^\iota) + \nabla_X \cdot \mathbf{P}^\iota - (\nabla_X (\mathbf{V} + \mathbf{V}^\iota)) \mathbf{M}^\iota, \quad \forall \iota = \alpha, \dots, \omega$$

relation between mass sources  $\Pi^\iota$ 's and interaction forces  $\mathbf{q}^\iota$ 's,

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



# kinematics of growth



## kinematics of growth

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

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

## energy, first law

balance of energy for a species  $\iota$ , in local form, in  $\Omega_0$

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

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balance of energy for a species  $\iota$ , in local form, in  $\Omega_0$

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

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

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

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:

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

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

- $\mathbf{D}^\iota$  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:

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

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

## constitutive relations

constitutive relation for flux of each transported species:

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

- 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  $D^\iota$  from swartz et al. [1999]

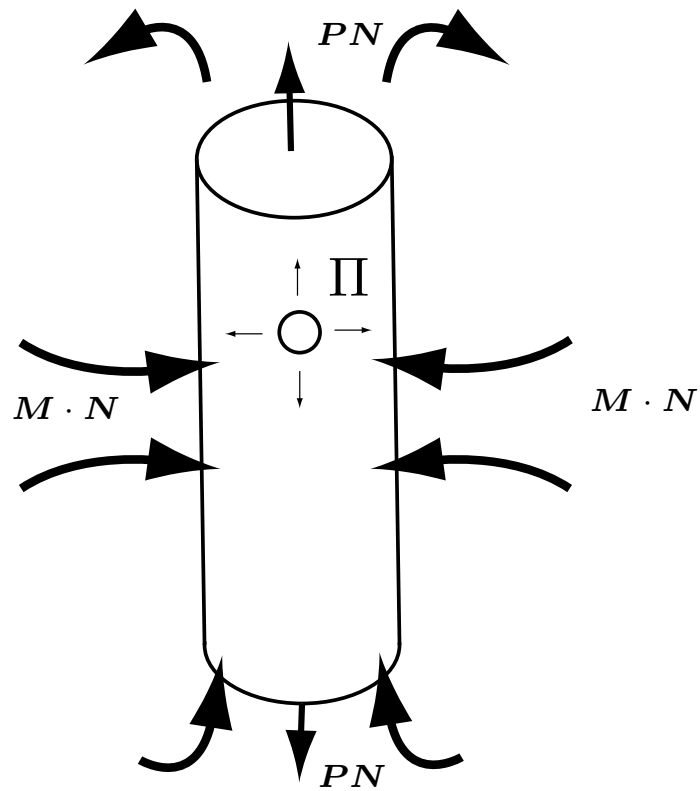
- “artificial” sources:

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

- entropy of mixing:

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

## 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

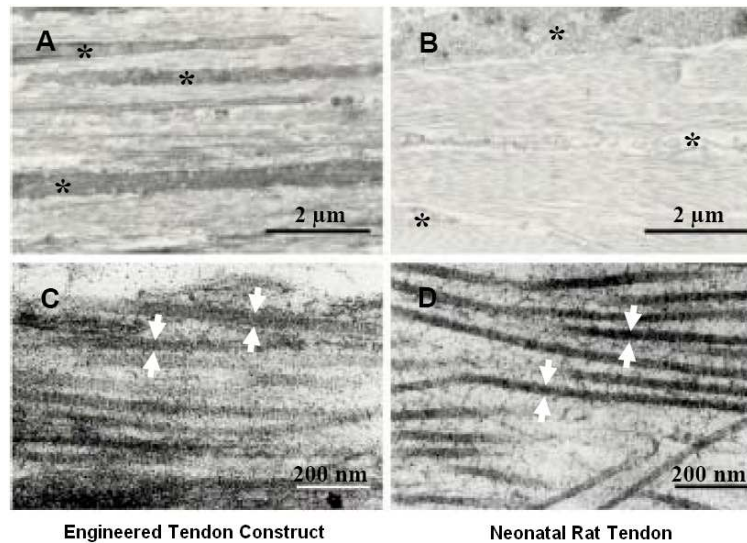
a continuum treatment of growth in tissue

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## biological model - morphological comparison

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

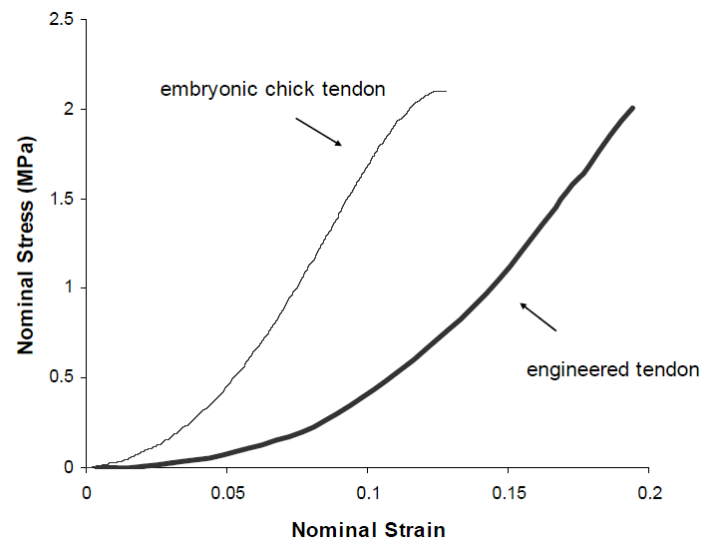
[calve et al., 2003]



## biological model - mechanical comparison

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

[calve et al., 2003]

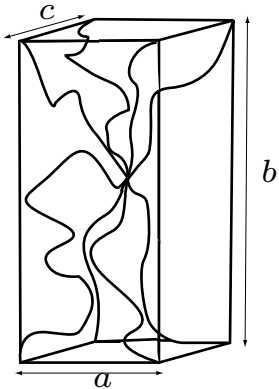


## cauchy stress

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



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

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

## Mass Balance - Equations

For a species, in the integral form

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

$\rho_0^\iota$  being the mass concentration of species  $\iota$  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  $\iota$ , in the integral form written in  $\Omega_0$  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

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

Relation between  $\Pi^{\iota}$ 's and  $\mathbf{q}^{\iota}$ '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  $\iota$ , in integral form in  $\Omega_0$ ,

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

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  $\iota$ ,

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

Where  $\tilde{e}^{\iota}$  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  $\Omega_0$ ,

$\Pi^\iota$  is the source/sink term for species  $\iota$

$\mathbf{M}^\iota$  is the mass flux term for species  $\iota$

$\mathbf{S}^\iota$  is the partial first Piola-Kirchhoff stress on species  $\iota$

$\mathbf{N}$  is the outward normal at the surface

$\mathbf{g}$  is the body force acting on the entire system

## The different terms - Mechanics

In the current configuration  $\Omega_t$ ,

$\pi^\iota$  is the source/sink term for species  $\iota$

$m^\iota$  is the mass flux term for species  $\iota$

$\sigma^\iota$  is the partial Cauchy stress on species  $\iota$

$n$  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

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

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

## The different terms - Energy

$e^\iota$  is the internal energy of each species  $\iota$

$\mathbf{F}$  is the deformation gradient

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

$r_0^\iota$  is the heat supplied to species  $\iota$  per unit reference volume

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