3D Diffusion equation (e.g. heat equation)

$$Divergence\ \boldsymbol{\nabla}.\boldsymbol{u} = \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}$$

$$Heat\ flux\quad \boldsymbol{u} = -k\boldsymbol{\nabla}\phi$$

$$Heat\ equation\quad \boldsymbol{\nabla}.\boldsymbol{u} = 0\quad or\quad \boldsymbol{\nabla}.(-k\boldsymbol{\nabla}\phi) = 0$$

$$or\ (if\ homo\cancel{geneous) - k\boldsymbol{\nabla}.(\boldsymbol{\nabla}\phi) = -k}\nabla^2\phi = 0$$

Reaction-diffusion: Bidomain equations

intracellular domain

ϕ_i - electrical potential; σ_i – conductivity tensor

extracellular domain

ϕ_e - electrical potential; σ_e – conductivity tensor

V_m - voltage across cell membrane
A_m – surface to volume ratio of cell membrane
C_m – membrane capacitance

Conservation of current (given V_m solve for ϕ_e)

$$\nabla \cdot ((\sigma_i + \sigma_e)\, \nabla \phi_e) = -\nabla \cdot (\sigma_i \nabla V_m)$$

Current flow across cell membrane (solve for V_m)

$$\nabla \cdot (\sigma_i \nabla V_m) + \nabla \cdot (\sigma_i \nabla \phi_e) = A_m \left(C_m \frac{\partial V_m}{\partial t} + I_{ion} \right)$$

Large deformation elasticity

1. **Kinematics**
    - geometry
    - material coordinates
    - base vectors
    - metric tensors
    - displacement gradients
    - strain tensor, strain invariants (I_1, I_2, I_3)
    - volume constraints ($I_3 = 0$)

2. **Kinetics**
    - stress tensor
    - stress equilibrium relations (conservation of momentum)
    - stress-strain relations (material properties)

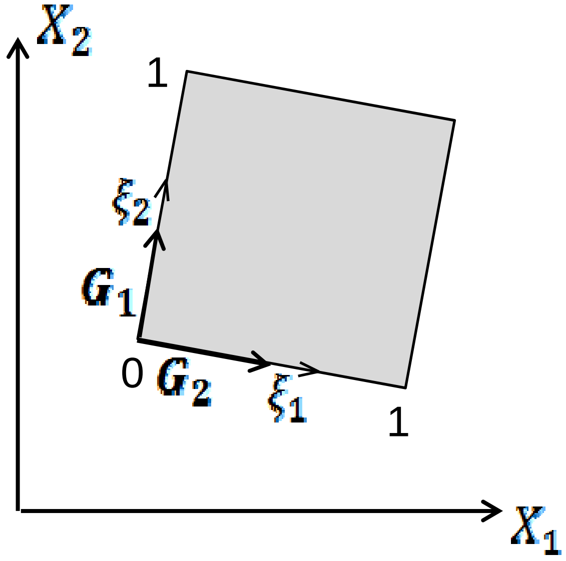
Nash and Hunter. *J. Elasticity.* 61(1-3):113-141, 2001

Consider material in undeformed state

Material coordinates

Base vectors in undeformed state

$$\boldsymbol{G}_1 = \frac{\partial \boldsymbol{X}}{\partial \xi_1} \qquad \boldsymbol{G}_2 = \frac{\partial \boldsymbol{X}}{\partial \xi_2}$$

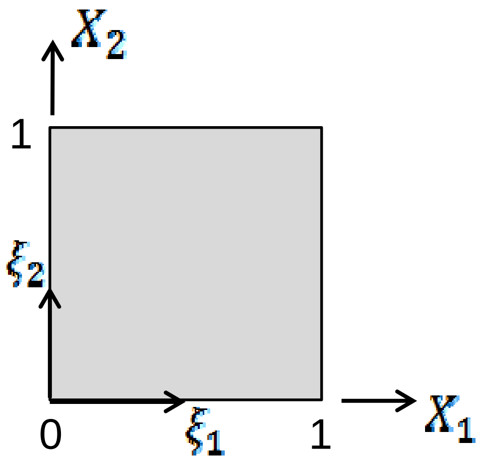


Metric tensor in undeformed state

$$G_{\alpha\beta} = \boldsymbol{G}_1 . \boldsymbol{G}_2 = \frac{\partial X_k}{\partial \xi_\alpha}\frac{\partial X_k}{\partial \xi_\beta}$$

For example

$$X_1 = \xi_1$$
$$X_2 = \xi_2$$



$$G_{11} = \frac{\partial X_1}{\partial \xi_1}\frac{\partial X_1}{\partial \xi_1} + \frac{\partial X_2}{\partial \xi_1}\frac{\partial X_2}{\partial \xi_1} = 1$$

$$G_{22} = \frac{\partial X_1}{\partial \xi_2}\frac{\partial X_1}{\partial \xi_2} + \frac{\partial X_2}{\partial \xi_2}\frac{\partial X_2}{\partial \xi_2} = 1$$

$$G_{12} = G_{21} = \frac{\partial X_1}{\partial \xi_1}\frac{\partial X_1}{\partial \xi_2} + \frac{\partial X_2}{\partial \xi_1}\frac{\partial X_2}{\partial \xi_2} = 0$$

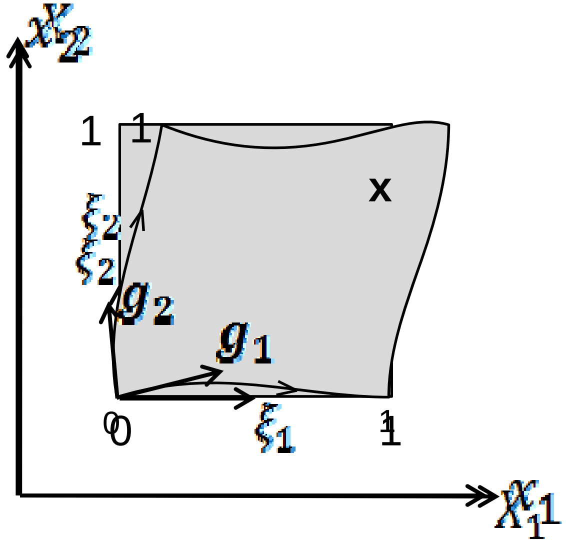
$$G_{\alpha\beta} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Material deforms under load ..

A point at (X_1,X_2) in undeformed state ...moves to (x_1,x_2) in deformed state

Base vectors tangent to material coordinates

$$\boldsymbol{g}_1 = \frac{\partial \boldsymbol{x}}{\partial \xi_1} \qquad \boldsymbol{g}_2 = \frac{\partial \boldsymbol{x}}{\partial \xi_2}$$



Metric tensor in deformed state

$$g_{\alpha\beta} = \boldsymbol{g}_1 \cdot \boldsymbol{g}_2 = \frac{\partial x_k}{\partial \xi_\alpha}\frac{\partial x_k}{\partial \xi_\beta}$$

Strain tensor

$$E_{\alpha\beta} = \frac{1}{2}\left(g_{\alpha\beta} - G_{\alpha\beta}\right)$$

Note on invariants

$g_{\alpha\beta}$ *has eigenvalues* $\lambda_1, \lambda_2, \lambda_3$

Invariants are:

$$I_1 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2$$

$$I_2 = \lambda_1^2\lambda_2^2 + \lambda_2^2\lambda_3^2 + \lambda_3^2\lambda_1^2$$

$$I_3 = \lambda_1^2\lambda_2^2\lambda_3^2$$

I_3 is the volume change

$I_3 = 1$ is used as a constraint on incompressible materials

Biaxial tension

$$x_1 = \lambda_1 \xi_1$$

$$x_2 = \lambda_2 \xi_2$$

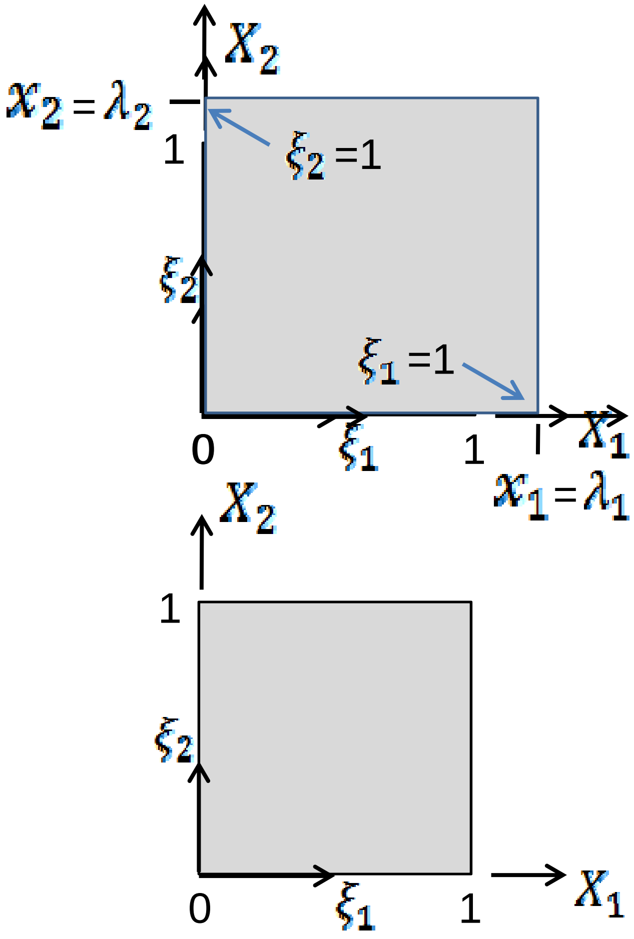
$$g_{11} = \frac{\partial x_1}{\partial \xi_1}\frac{\partial x_1}{\partial \xi_1} + \frac{\partial x_2}{\partial \xi_1}\frac{\partial x_2}{\partial \xi_1} = (\lambda_1)^2$$

$$g_{22} = \frac{\partial x_1}{\partial \xi_2}\frac{\partial x_1}{\partial \xi_2} + \frac{\partial x_2}{\partial \xi_2}\frac{\partial x_2}{\partial \xi_2} = (\lambda_2)^2$$

$$g_{12} = g_{21} = \frac{\partial x_1}{\partial \xi_1}\frac{\partial x_1}{\partial \xi_2} + \frac{\partial x_2}{\partial \xi_1}\frac{\partial x_2}{\partial \xi_2} = 0$$

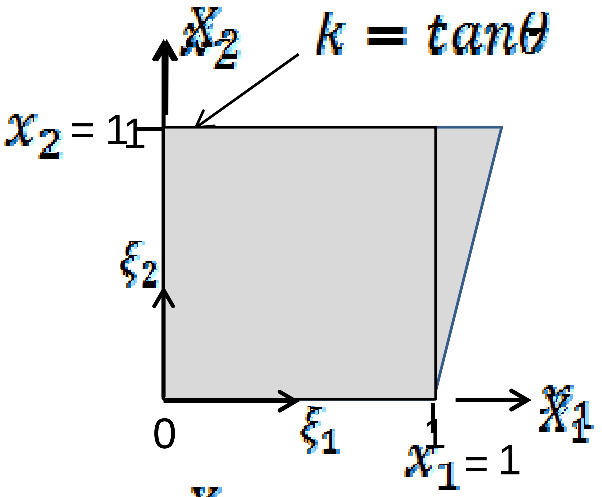
$$g_{\alpha\beta} = \begin{bmatrix} \lambda_1^2 & 0 \\ 0 & \lambda_2^2 \end{bmatrix}$$

$$E_{\alpha\beta} = \frac{1}{2}\left(g_{\alpha\beta} - G_{\alpha\beta}\right) = \begin{bmatrix} \frac{1}{2}(\lambda_1^2 - 1) & 0 \\ 0 & \frac{1}{2}(\lambda_2^2 - 1) \end{bmatrix}$$



Simple shear

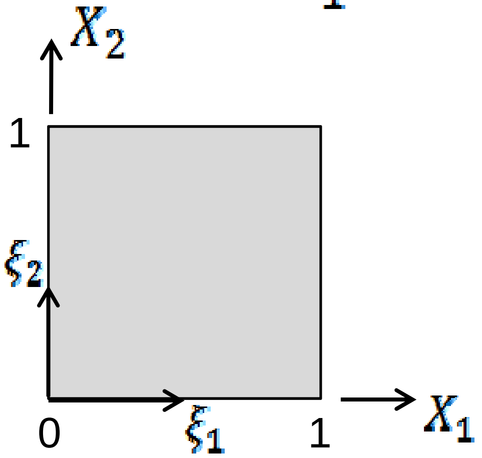
$$X_1 = \xi_1 + k\xi_2$$
$$X_2 = \xi_2$$



$$g_{11} = \frac{\partial x_1}{\partial \xi_1}\frac{\partial x_1}{\partial \xi_1} + \frac{\partial x_2}{\partial \xi_1}\frac{\partial x_2}{\partial \xi_1} = 1$$

$$g_{22} = \frac{\partial x_1}{\partial \xi_2}\frac{\partial x_1}{\partial \xi_2} + \frac{\partial x_2}{\partial \xi_2}\frac{\partial x_2}{\partial \xi_2} = 1$$

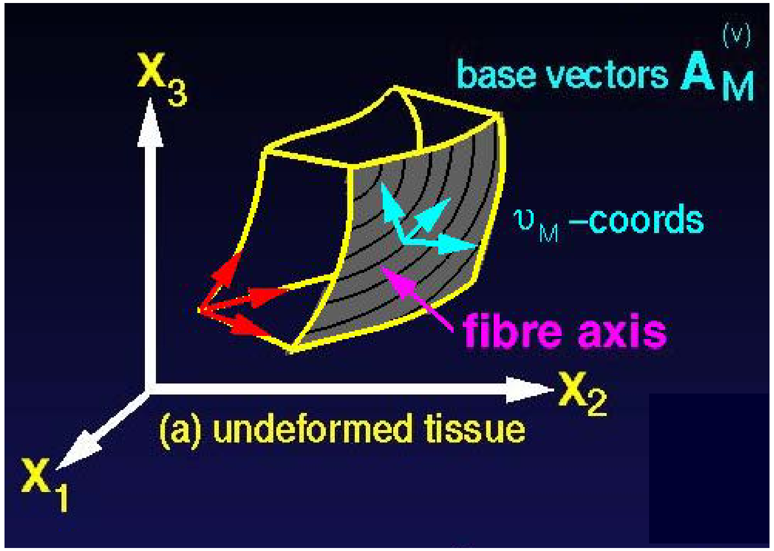
$$g_{12} = g_{21} = \frac{\partial x_1}{\partial \xi_1}\frac{\partial x_1}{\partial \xi_2} + \frac{\partial x_2}{\partial \xi_1}\frac{\partial x_2}{\partial \xi_2} = k$$

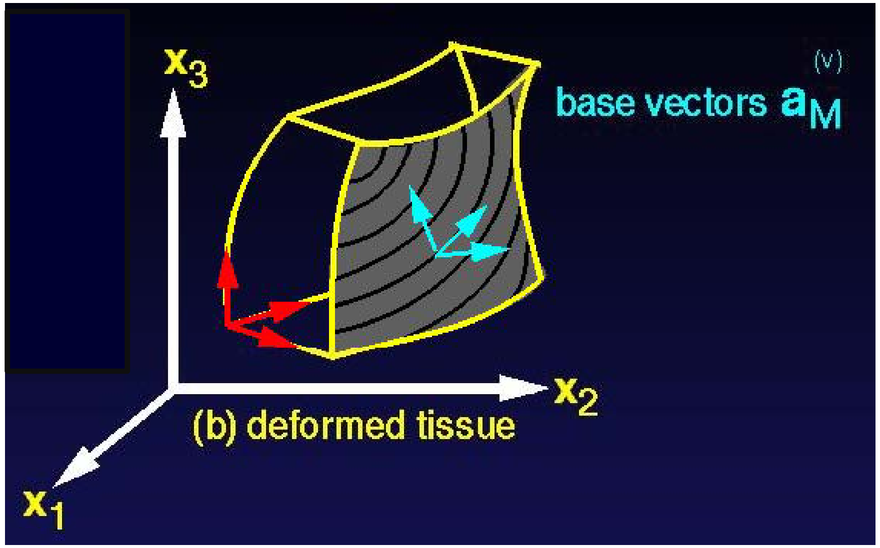


$$g_{\alpha\beta} = \begin{bmatrix} 1 & k \\ k & 1 \end{bmatrix}$$

$$E_{\alpha\beta} = \frac{1}{2}\left(g_{\alpha\beta} - G_{\alpha\beta}\right) = \begin{bmatrix} 0 & k \\ k & 0 \end{bmatrix}$$

Kinematics with fibre fields





$$\boldsymbol{A}_{\alpha}^{(\upsilon)} = \frac{\partial X_k}{\partial \upsilon_\alpha} \boldsymbol{g}_k^{(x)}$$

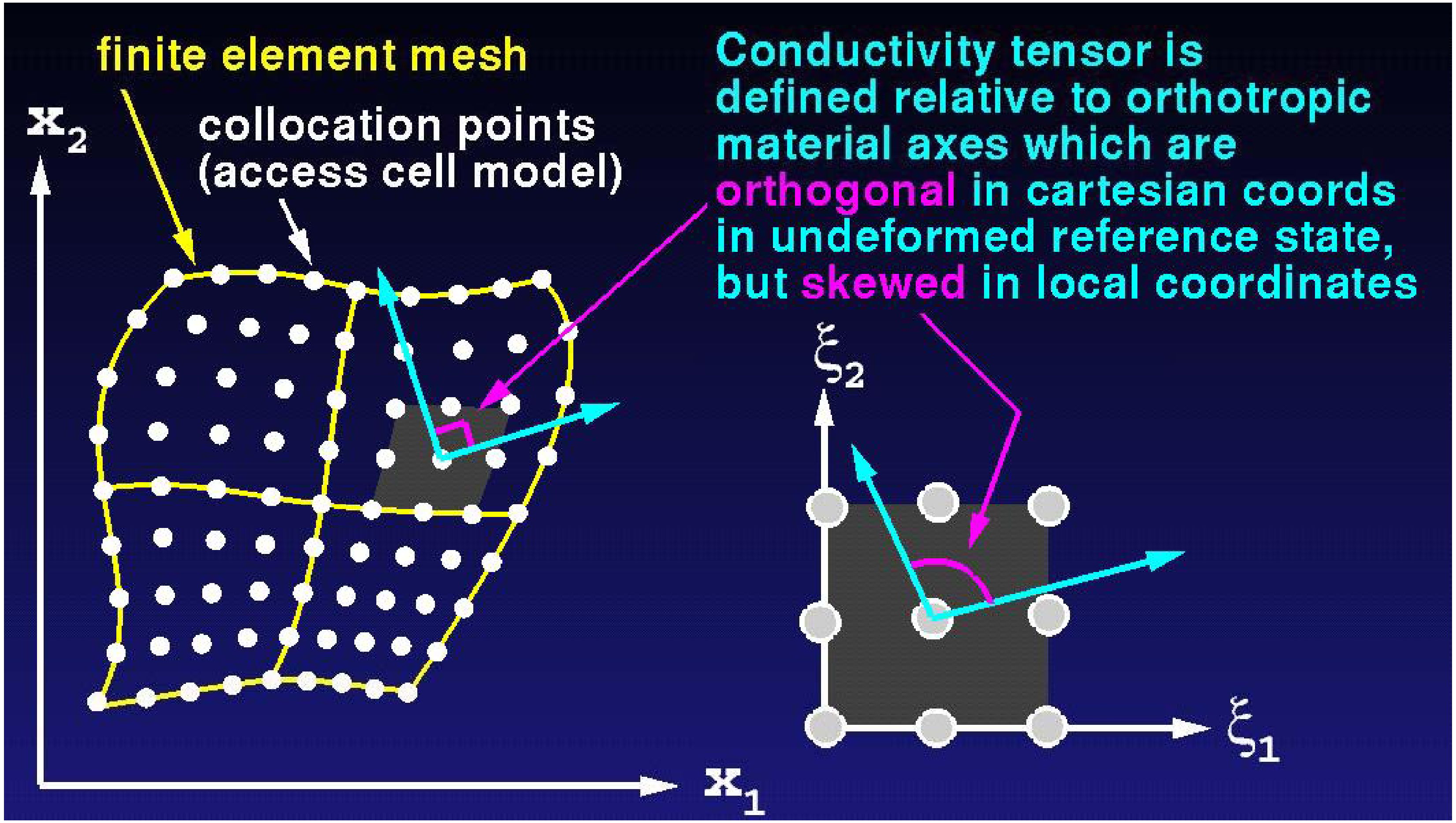
$$\boldsymbol{a}_{\alpha}^{(\upsilon)} = \frac{\partial X_k}{\partial \upsilon_\alpha} \boldsymbol{g}_k^{(x)}$$

$$A_{\alpha\beta}^{(\upsilon)} = \boldsymbol{A}_{\alpha}^{(\upsilon)} . \boldsymbol{A}_{\beta}^{(\upsilon)}$$

$$a_{\alpha\beta}^{(\upsilon)} = \boldsymbol{a}_{\alpha}^{(\upsilon)} . \boldsymbol{a}_{\beta}^{(\upsilon)}$$

$$E_{\alpha\beta} = \frac{1}{2}\left(a_{\alpha\beta}^{(\upsilon)} - A_{\alpha\beta}^{(\upsilon)}\right)$$

Note: Effect of deformation on conductivity tensor



Conductivity tensor is defined relative to orthotropic material axes which are orthogonal in cartesian coords in undeformed reference state, but skewed in local coordinates

Stress-strain properties

Passive tissue material properties

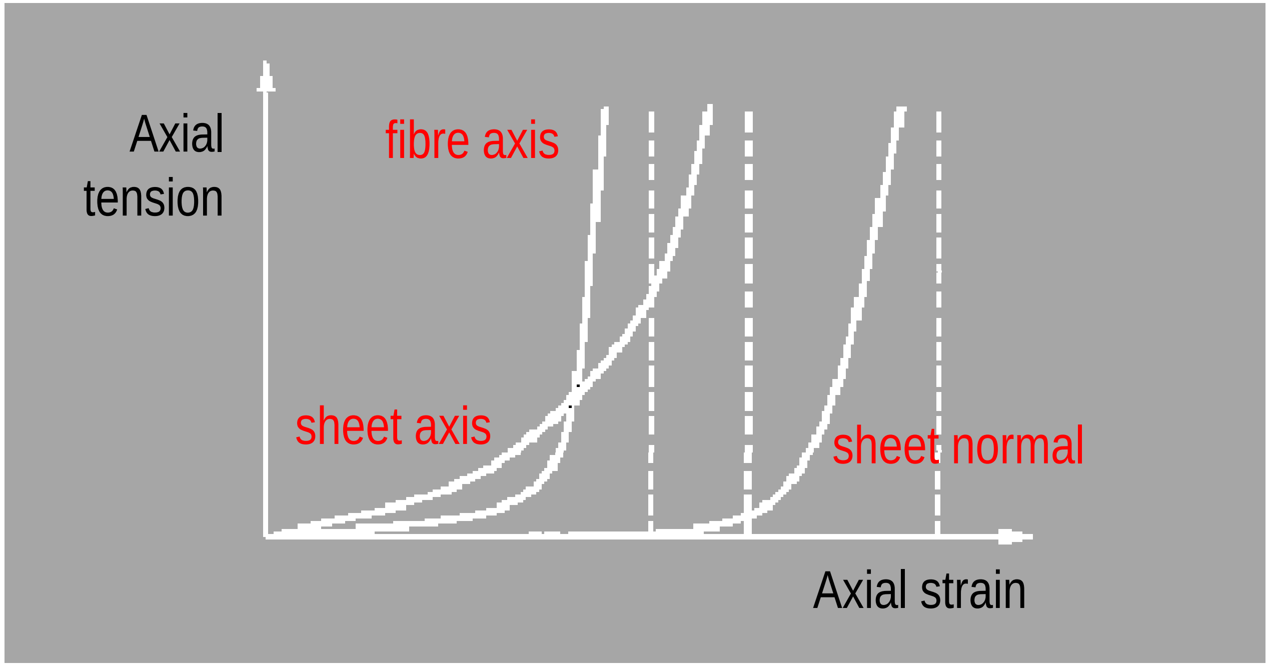
Orthotropic constitutive law

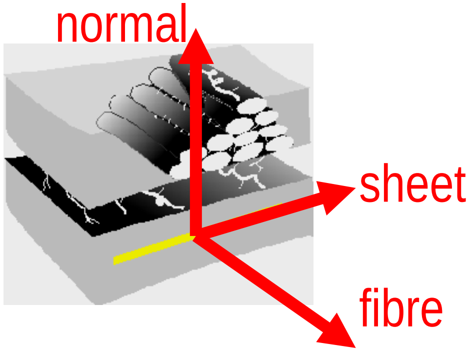
2nd Piola-Kirchhoff stress tensor:

$$T^{\alpha\beta} = \frac{1}{2}\left(\frac{\partial W}{\partial E_{\alpha\beta}} + \frac{\partial W}{\partial E_{\beta\alpha}}\right) - p a^{\alpha\beta}_{(\nu)}$$

Where strain energy function W for an isotropic material is
$W=W(I_1, I_2, I_3)$ with $I_3=1$ for incompressible material.

But for soft tissues …





$$
\begin{aligned}
W &= k_{11}\frac{E_{11}^2}{|a_{11}-E_{11}|^{b_{11}}} + k_{22}\frac{E_{22}^2}{|a_{22}-E_{22}|^{b_{22}}} + k_{33}\frac{E_{33}^2}{|a_{33}-E_{33}|^{b_{33}}} \\
&+ k_{12}\frac{E_{12}^2}{|a_{12}-E_{12}|^{b_{12}}} + k_{13}\frac{E_{13}^2}{|a_{13}-E_{13}|^{b_{13}}} + k_{23}\frac{E_{23}^2}{|a_{23}-E_{23}|^{b_{23}}}
\end{aligned}
$$

Governing equations for solid mechanics

Kinematics:	**finite strain theory, incompressible tissue**
Equilibrium eqtns:	**conservation of mass & momentum**
Constitutive eqtns:	**based on fibrous-sheet structure**
	nonlinearly elastic, viscoelastic, porous etc
Boundary conditions:	**displacement or force & contact mechanics**
Other factors:	**residual stress, growth & remodelling**

Galerkin finite element method

$$\int_{V_0} T^{\alpha\beta} F^j_\beta \, \delta v_j\big|_\alpha \; dV_0 = \int_{V_0} \rho_0 \left(b^j - f^j\right) \delta v_j \; dV_0 + \int_{S_2} p_{(appl)} \, \frac{g^{3M}_{(\xi)}}{\sqrt{g^{33}_{(\xi)}}} \, \frac{\partial x_j}{\partial \xi_M} \, \delta v_j \; dS$$

$$\iiint_{V_e} \left(\sqrt{I_3} - 1\right) \psi^p \, \sqrt{G^{(\xi)}} \; d\xi_3 d\xi_2 d\xi_1 = 0$$

Costa KD, Hunter PJ, Wayne JS, Waldman LK, Guccione JM & McCulloch AD. *ASME J. Biomech. Eng*. 118:464-472, 1996

Nash and Hunter. *J. Elasticity.* 61(1-3):113-141, 2001