REVIEW
MECHANICAL MODELING OF BIOLOGICAL/BIOINSPIRED MATERIALS

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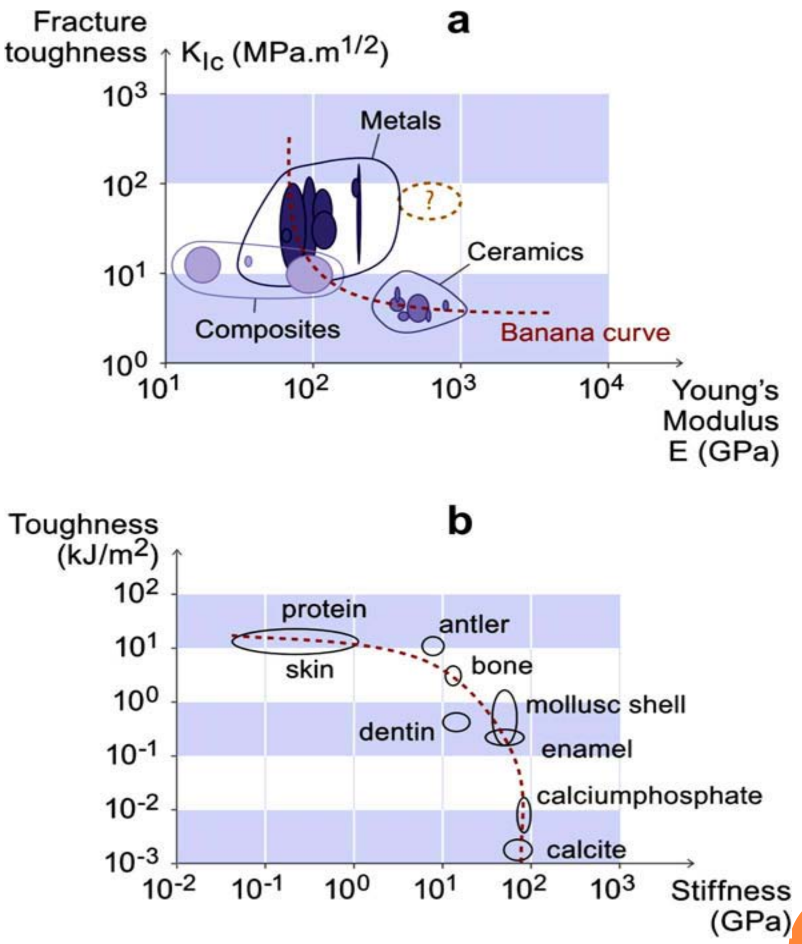
OUTSTANDING PROPERTIES AND FUNCTIONS

- Mutually inclusive properties,
  e.g., high toughness, high stiffnes

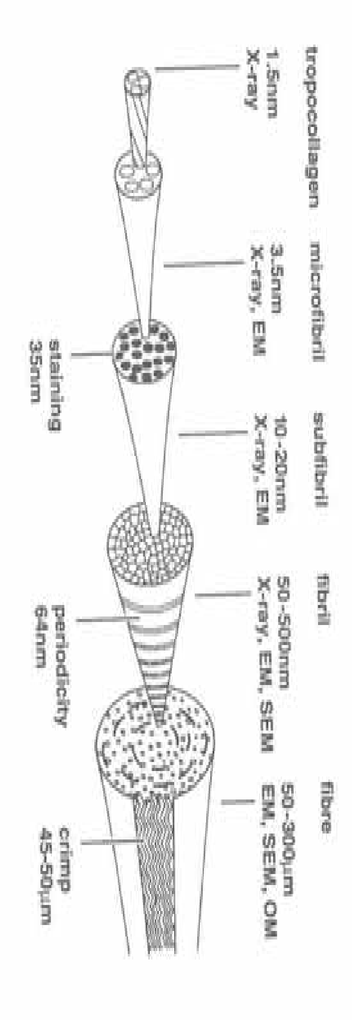


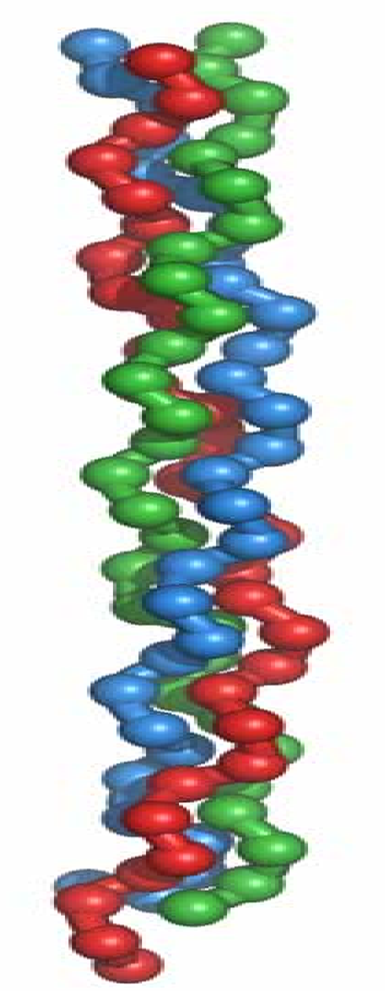
Espinosa et al. (2009), *Prog. Mater. Sci.* 54 ,1059.

MODELING CHALLEN

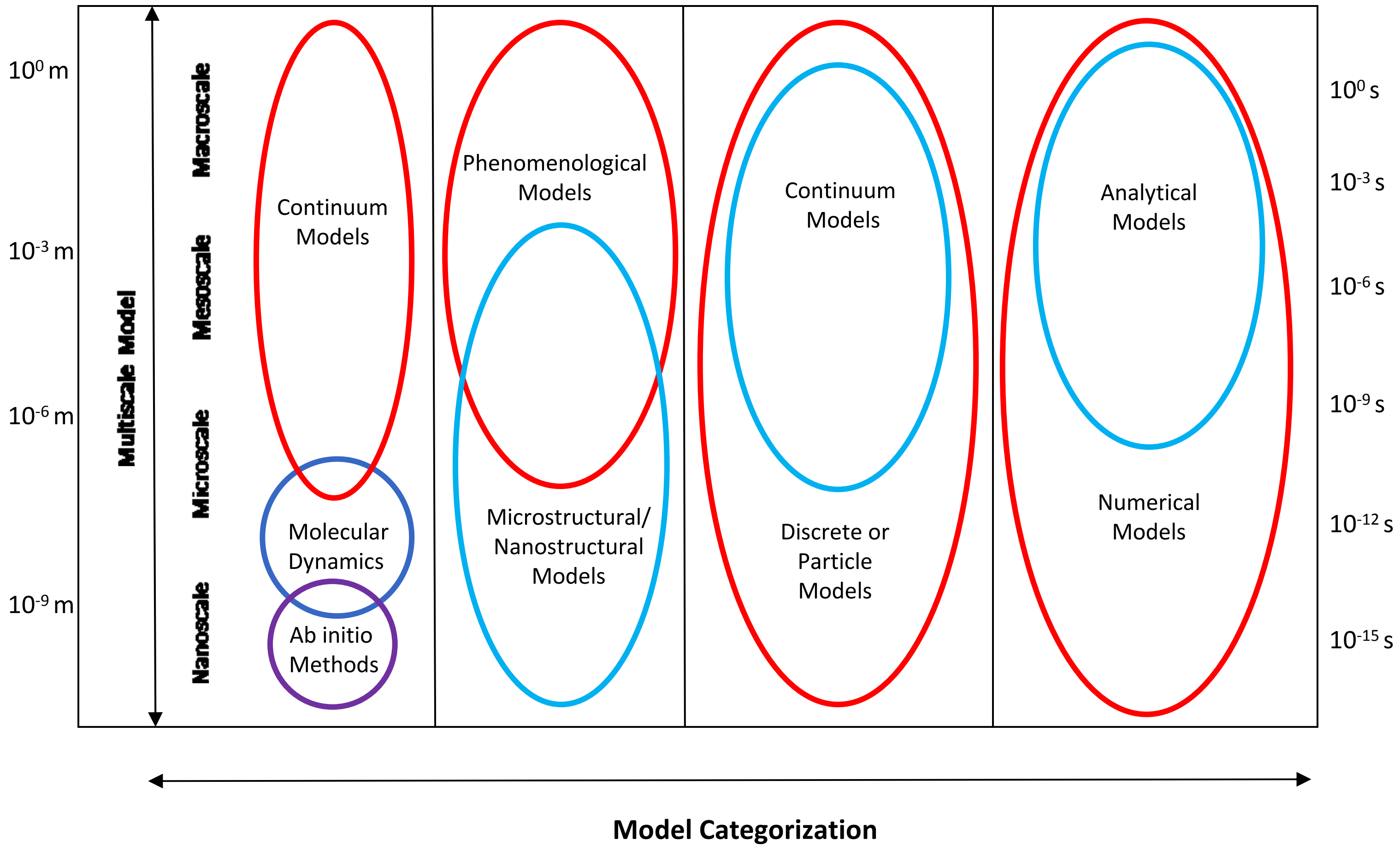
- Hierarchical architecture
- Complex microstructures
- Complex material properties: soft/hard composite, anisotropy, inhomogeneity,

  time-dependence
- Multi-physics



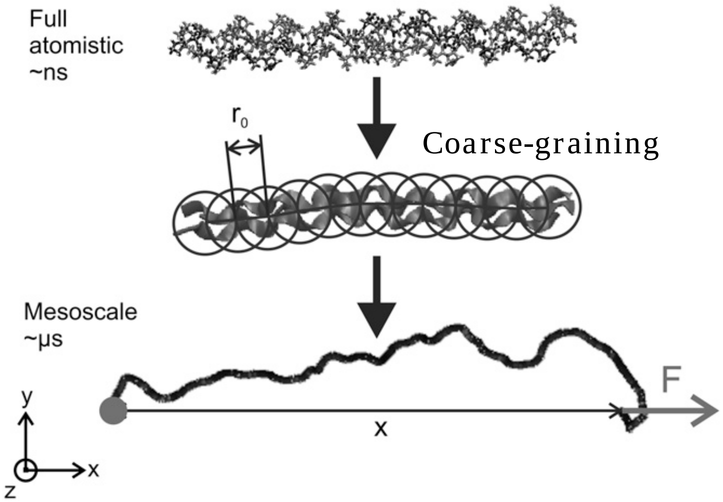


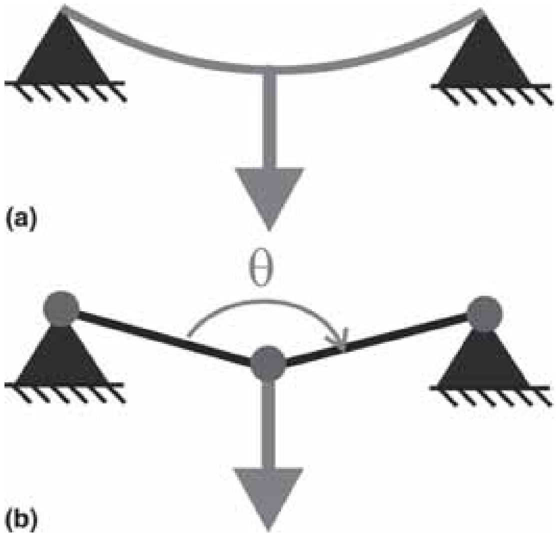
MODELING STRATEGIES



MULTISCALE MODEL (SEQUENTIAL)

TROPOCOLLAGEN MOLECULE





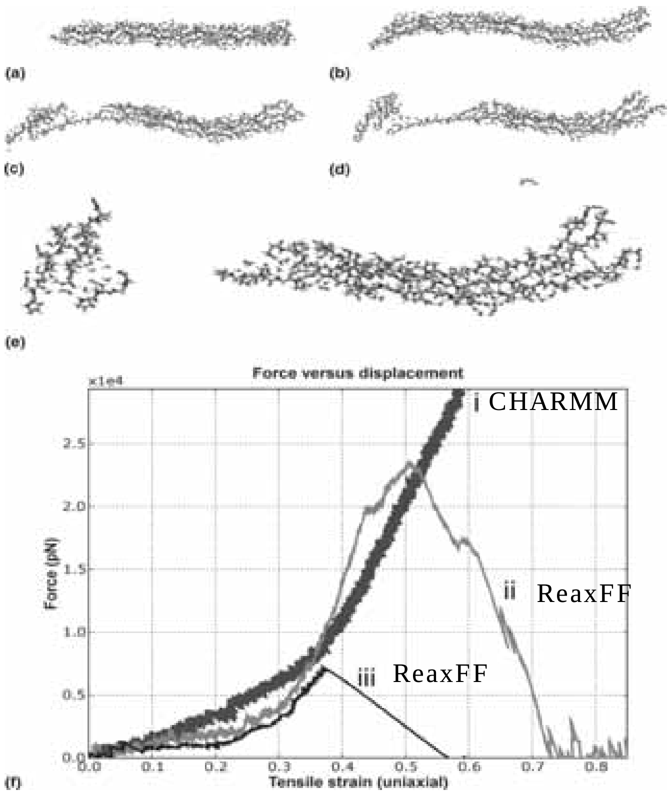
Scale bridging:
L = 8.4 nm to L = 280 nm

Scale bridging:
parameter passing via
energy equivalence

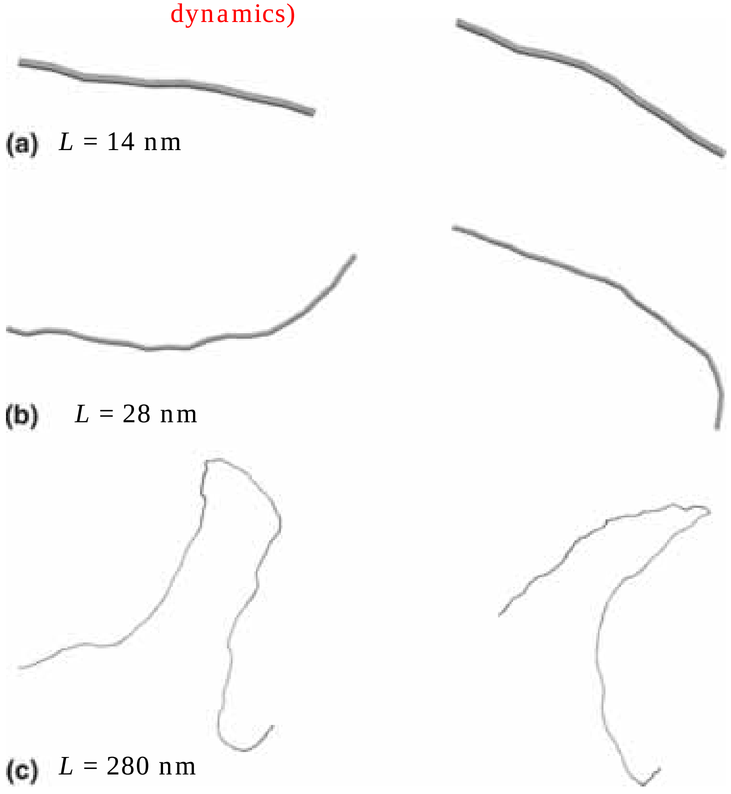
Buehler, M.J. (2006), *J. Mater. Res.*, 21, 1947.

MULTISCALE MODEL
TROPOCOLLAGEN MOLECULE

Nanoscale (molecular dynamics)



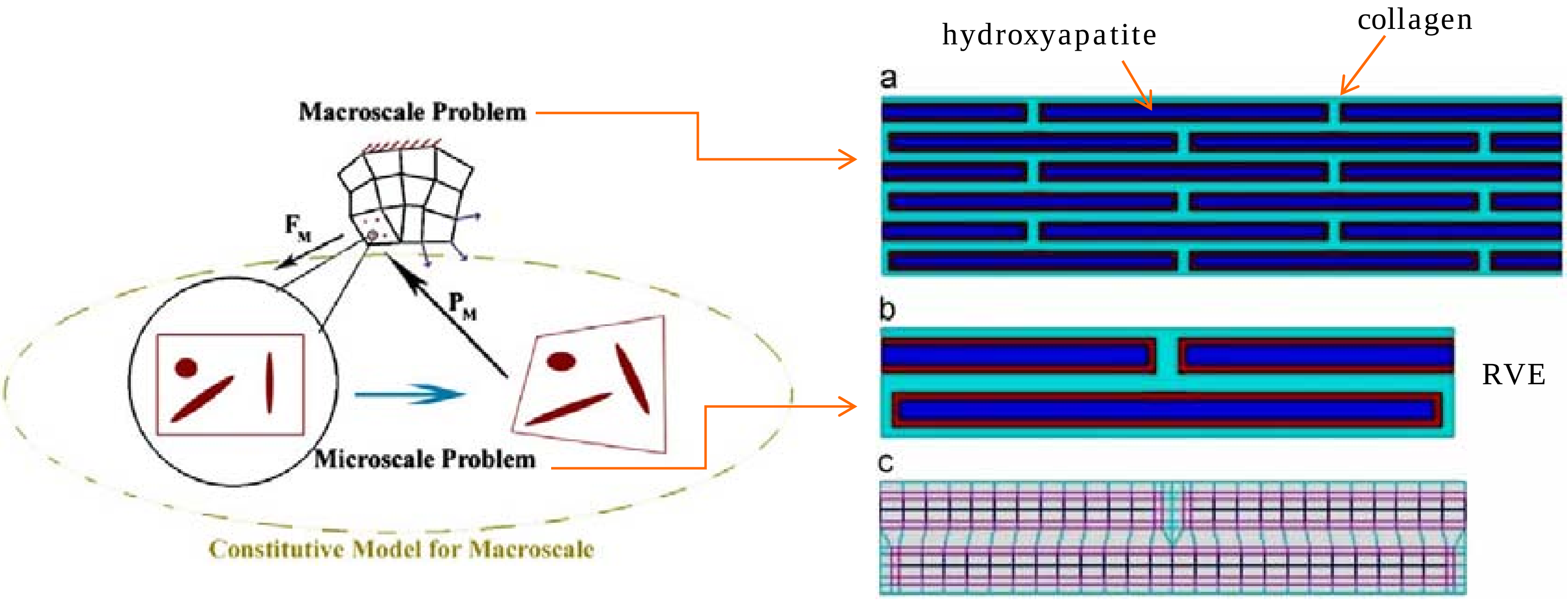
Mesoscale (molecular dynamics)



Buehler, M.J. (2006), *J. Mater. Res.*, 21, 1947.

MULTISCALE MODEL (SEQUENTIAL)

CORTICAL BONE



Scale bridging:
passing of field variables via homogenization

finite element meshing of RVE

Ghanbari, J., Naghdabadi, R. (2009), *J. Biomech.* 42, 1560.

MULTISCALE MODEL
ISSUES AND CHALLENGES

(1) Scale bridging across several spatial orders

--- Treatment of hierarchy across scales ?

--- Inadequate modeling of cross-scale interactions ?

--- Loss of accuracy (propagation of errors), robustness, stability, convergence?

--- Lack of a rigorous mathematical foundation ?

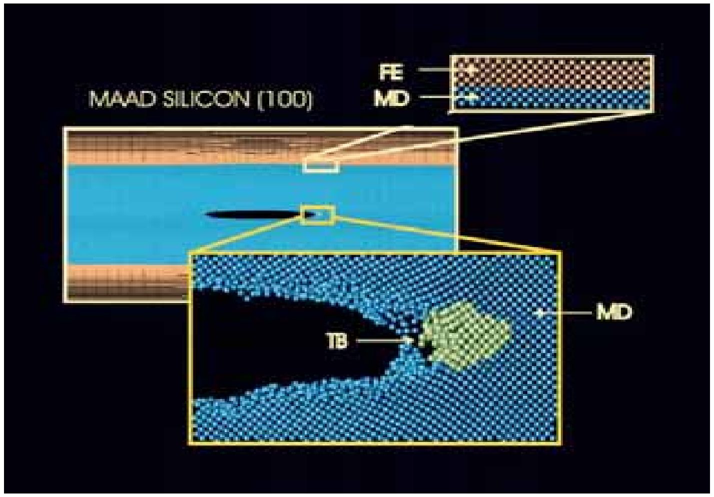
--- Multi-physics problems?

MULTISCALE MODEL

ISSUES AND CHALLENGES

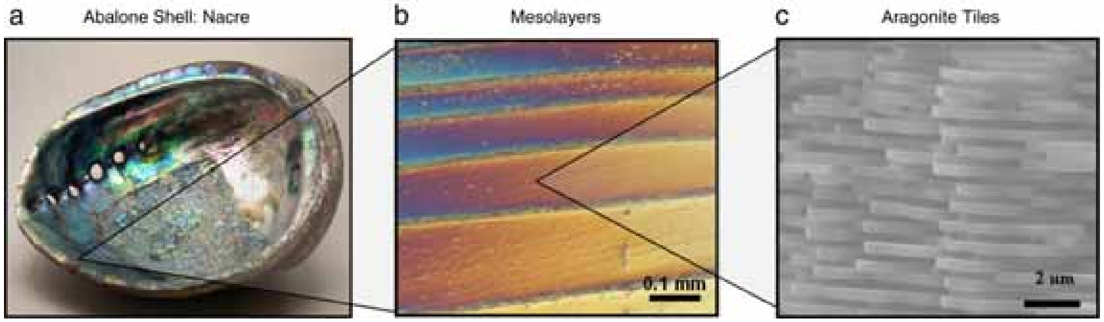
(2) Concurrent multiscale model

- Solving all degrees of freedom in one step
- No assumptions of the type adopted in coarse-graining



J. Broughton, F. Abraham, N. Bernstein, and E. Kaxiras (1999),
Phys. Rev. B 60, 2391.

- Handling of points-within-point in hierarchical structure?

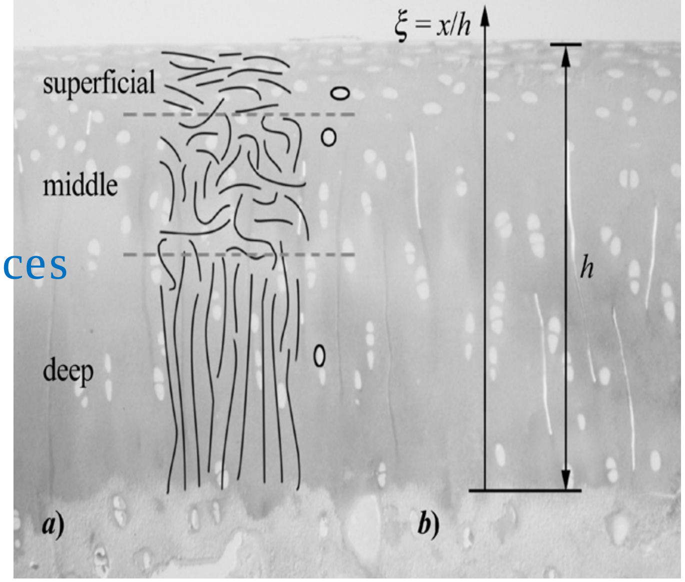


Chen et al. (2008), *J. Mech. Behav. Biomed. Mater.* 1, 208.

MICROSTRUCTURAL MODELS

- Spatial and orientational inhomogeneities
- Hierarchical architecture
- Material anisotropy
- Composite structure with inclusions/interfaces
- Time-dependence/material nonlinearity
- Large deformations

$$\int \underbrace{\psi(\overbrace{\mathbf{M}}^{\text{Fiber orientation}})}_{\text{Probability density of fiber orientation}} \phi_f \underbrace{\overline{W}_f}_{\text{Energy density}}(\overbrace{\bar{\mathbf{C}}}^{\text{deformation}}, \overbrace{\mathbf{A}}^{\text{structure}})\,dS$$



Arrangement of structural elements
in articular cartilage

S. Federico, W. Herzog (2008), *J. Biomech*. 41, 3309.

MICROSTRUCTURAL MODELS
ISSUES AND CHALLENGES

- Integrated modeling of all "essential" structural elements in the complex microstructure

  - *Selection of model parameters*
  - *Mathematical modeling of each family of structural elements*
  - *Interactions of the structural elements within and across scales*
  - *Integrated in a framework for solving problems of large domain (???)*

PHENOMENOLOGICAL MODELING

- Motivated by:

  - Large domains (three-dimensional)
  - Complex microstructure
  - Complex boundary conditions
  - Complex domain shape and loading

Techniques for large scale problems require simple models – complex microstructural models will overwhelm the solution process

PHENOMENOLOGICAL MODELING

SOFT TISSUES

$$W = \sum_{i+j=1}^{N} C_{ij} (I_1 - 3)^i (I_2 - 3)^j$$

Brain tissue: K. Miller, K. Chinzei (1982), *J. Biomech*. 30, 1115.

$$W = c(I_1 - 3)^n$$

Elastinous tissue: Watton et al. (2009), *J. Biomech*. 42, 1320.

$$W = \frac{C}{2}(e^Q - 1)$$

$$Q = 2c_1(E_{11} + E_{22} + E_{33}) + c_2 E_{11}^2 + c_3(E_{22}^2 + E_{33}^2 + E_{23}^2) + 2c_4(E_{12}^2 + E_{13}^2)$$

Gastroesophageal junction: Yassi et al. (2009), *J. Biomech*. 42, 1604.

Major advantage:

Reduction in the number of parameters

Issue:

Determination of parameters via comparison of model predictions to whole field measurements made by various imaging techniques

What is the link between microstructural and phenomenological parameters?

PHENOMENOLOGICAL MODELING

GELS

Microstructural modeling:

Hong et al. (2008), *J. Mech Phys. Solids 56*, 1779.

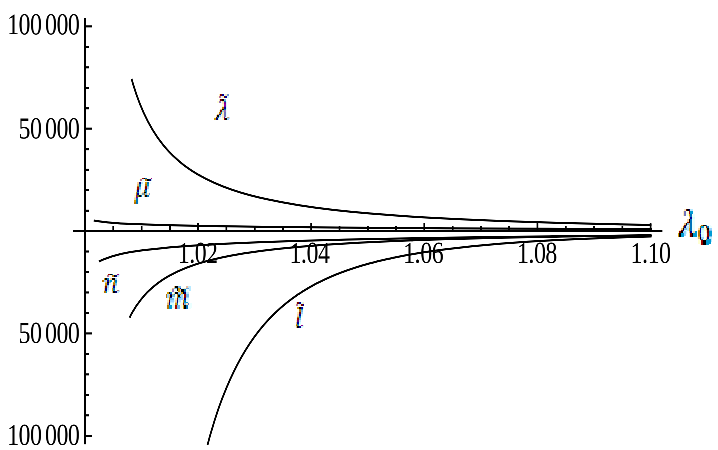
$$W = \frac{NkT}{2}\left(I_1^2 - 2I_2 - 3 - 2\log I_3\right) + \frac{kT}{v}\left(vC\log\frac{vC}{1+vC} - \frac{\chi}{1+vC}\right)$$

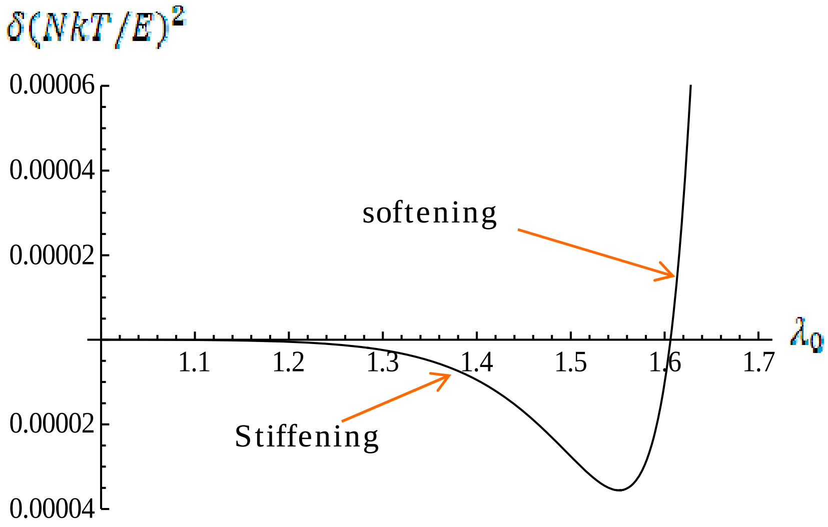
Phenomenological modeling: second-order nonlinear elasticity model

M.S. Wu and H.O.K. Kirchner (2010), *J. Mech. Phys. Solids* 58, 300.

$$W = \alpha J_1 + \frac{\lambda + 2\mu}{2} J_1^2 - 2\mu J_2 + \frac{l + 2m}{3} J_1^3 - 2m J_1 J_2 + n J_3$$

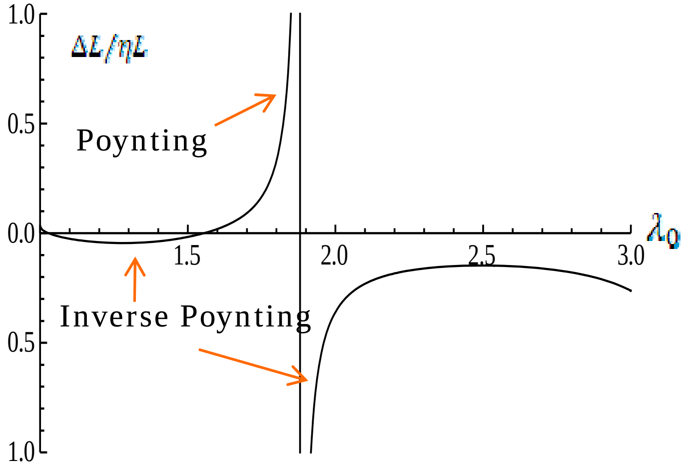
PHENOMENOLOGICAL MODELING GELS





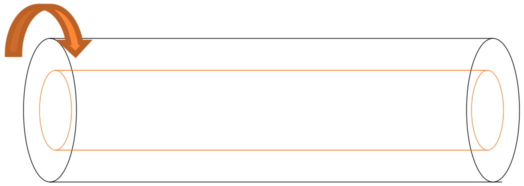
softening

Stiffening



Poynting

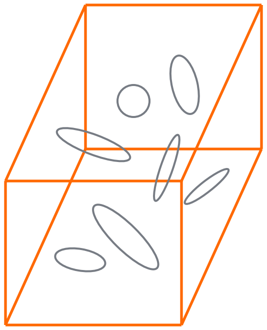
Inverse Poynting



CHALLENGES

MODELING OF CROSS-PROPERTY CORRELATIONS

- Different physical properties such as elastic stiffness and electrical conductivity may be correlated via their dependence on microstructure (Sevostianov and Kachanov, Adv. Appl. Mech. 42, 69)



$$\frac{E_0 - E}{E} = \frac{16}{45}\frac{\left(1-\nu_0^{\,2}\right)\left(10-3\nu_0\right)}{2-\nu_0}\rho$$

Stiffness-Crack Density

$$\frac{k_0 - k}{k} = \frac{8}{9}\rho$$

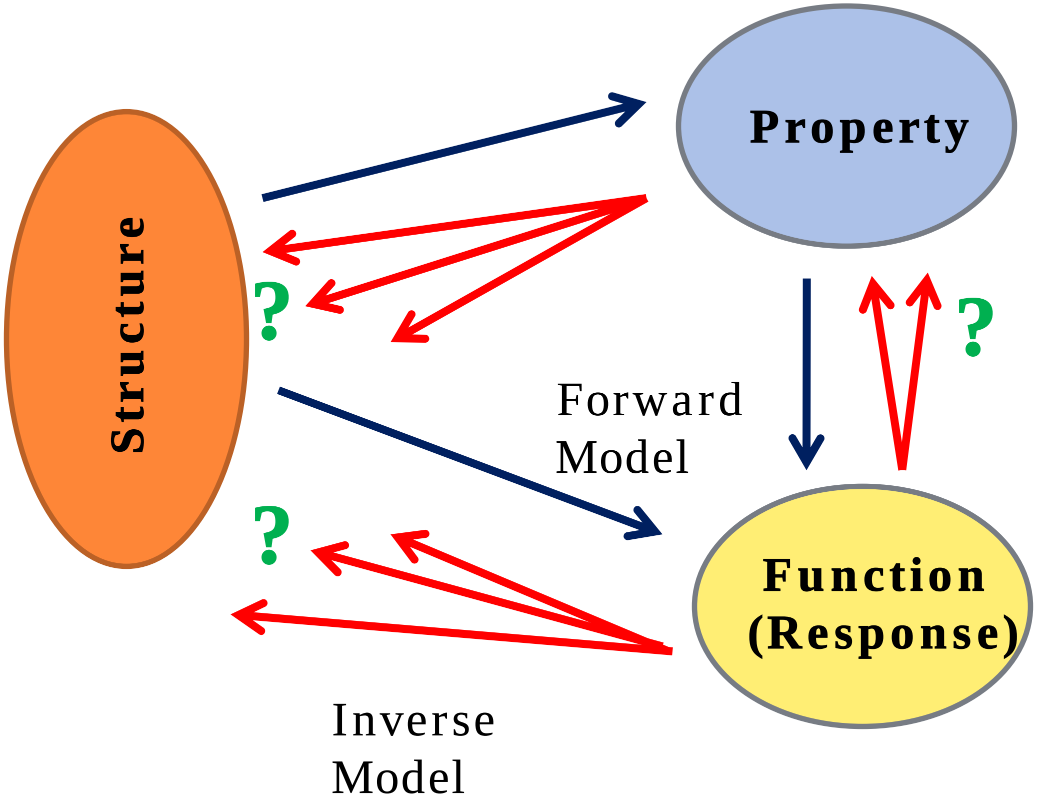
Conductivity-Crack Density

$$\boxed{\frac{E_0 - E}{E} = \frac{2}{5}\frac{\left(1-\nu_0^{\,2}\right)\left(10-3\nu_0\right)}{2-\nu_0}\frac{k_0 - k}{k}}$$

Stiffness-Conductivity

CHALLENGES: INVERSE MODELING

STRUCTURE-PROPERTY-FUNCTION



A PROPERTY-FUNCTION INVERSE MODEL

ELASTICITY IMAGING

Tissue deformation + Image acquisition

⇓

Displacement field computation via image processing

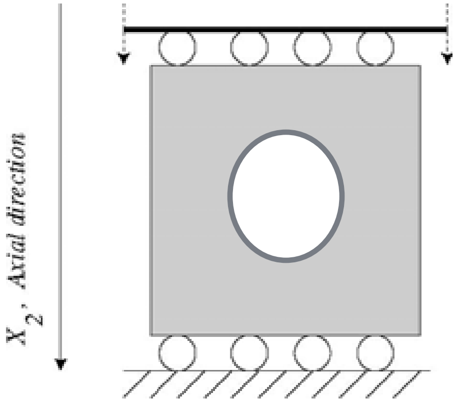
⇓

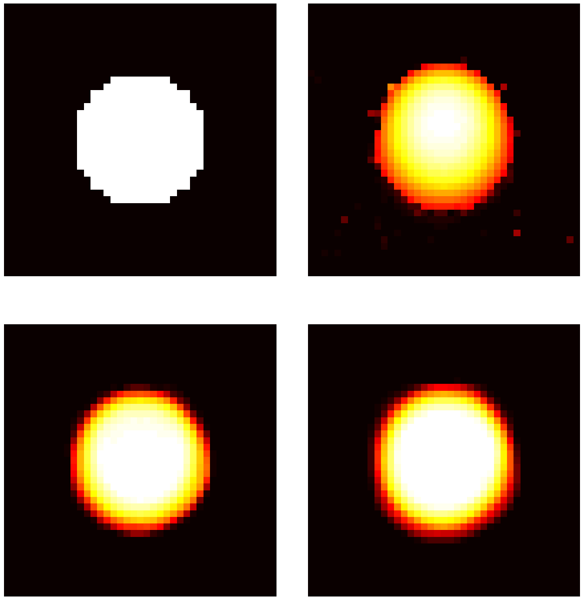
Inverse problem solved to determine spatial distribution of material properties

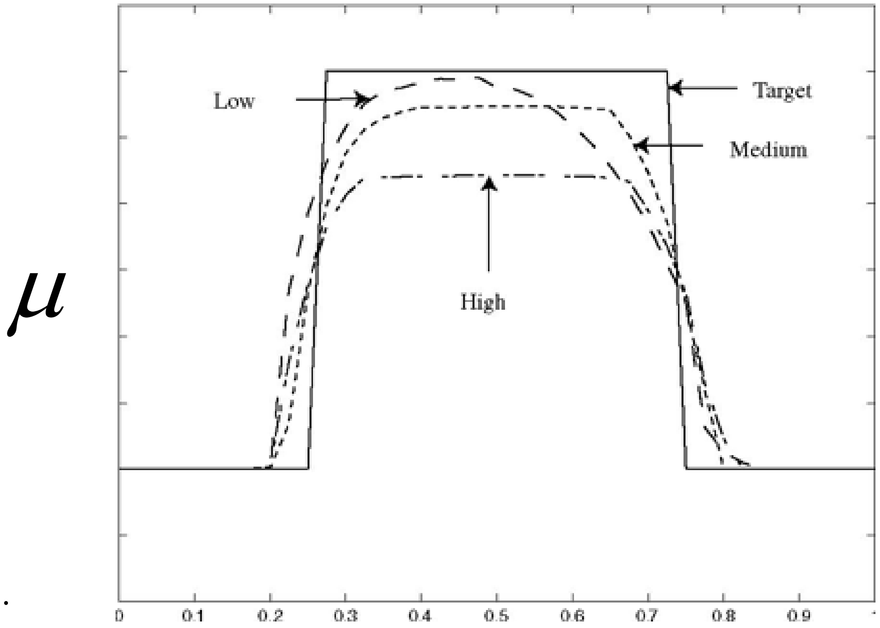
A PROPERTY-FUNCTION INVERSE MODEL

ELASTICITY IMAGING

$$W = \frac{\lambda}{4}(I_2 - 1) - (\frac{\lambda}{4} + \frac{\mu}{2})\ln I_2 + \frac{\mu}{2}(I_1 - 2)$$







Gokhale et al. (2008), *Inverse Problems* 24, 045010.

CONCLUSIONS

- Strategies for modeling biological and bionspired materials can be broadly classified in various ways; particularly:
  - Multiscale/single scale models
  - Phenomenological/microstructural models

- Challenges include:
  - Further development of multiscale models, tackling issues such as *scale bridging*, *concurrent hybrid techniques*, solution accuracy and stability
  - Modeling of microstructure: *hierarchical architecture, inclusions, inhomogeneity and anisotropy, material and geometrical nonlinearity, etc.*

- Development of forward and inverse models to design new bio-inspired materials with targeted properties and functions
- Modeling of cross-property correlations