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Center for Integrative Multiscale Modeling and Simulation

## UP-SCALING AND POROELASTICITY

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# **BRIEF HISTORY OF POROELASTICITY**

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- 1941 – Biot (quasi-statics, theory and analysis)
- 1944 – Frenkel (electroseismics and waves)
- 1951 – Gassmann (undrained behavior, theory)
- 1954 – Skempton (undrained behavior, experiments in soil)
- 1956 – Biot (waves, Lagrangian app., prediction of the slow wave)
- 1957 – Biot and Willis (coefficients from experiment)
- 1962 – Biot (reformulation of wave theory, Hamiltonian app.)
- 1976 – Rice and Cleary (quasi-statics, numerical methods)
- 1980 – Plona (slow wave first observed!)
- 1980 – Berryman, Brown, Johnson (eff. mass, tortuosity, liquid He)
- 1980 – Drumheller and Bedford (mixture theory)
- 1981 – Burridge and Keller (homogenization theory)

# OUTLINE

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- Biot's Poroelasticity Theory Is Correct!
  - Laboratory data
  - Finite element approach to modeling
- Four Methods for Up-Scaling
  - Effective medium theories
  - Mixture theory
  - Homogenization theory
  - Volume averaging methods
- New Model: "Random Polycrystals of Laminates"
- Conclusions

## Biot's (1962) Strain Energy Functional

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$$2E = He^2 - 2Ce\zeta + M\zeta^2 - 4\mu I_2$$

where  $H$ ,  $C$ ,  $M$ , and  $\mu$  are poroelastic constants,

$e = \nabla \cdot \vec{u}$  = frame dilatation,

$\zeta = -\nabla \cdot \vec{w}$  = increment of fluid content,

$\phi$  = porosity,

$\vec{u}$  = solid frame displacement,

$\vec{u}_f$  = pore fluid displacement,

$\vec{w} = \phi(\vec{u}_f - \vec{u})$  = relative displacement, and

$I_2 = e_x e_y + e_y e_z + e_z e_x - \frac{1}{4}(\gamma_x^2 + \dots)$  = a strain invariant.

# Biot's Equations of Dynamic Poroelasticity



$$\omega^2 \rho \vec{u} + (H - \mu) \nabla e + \mu \nabla^2 \vec{u} = -\omega^2 \rho_f \vec{w} + C \nabla \zeta,$$

$$\omega^2 q(\omega) \vec{w} - M \nabla \zeta = -\omega^2 \rho_f \vec{u} - C \nabla e,$$

where

$\omega = 2\pi f$  = angular frequency,

$\rho = \phi \rho_f + (1 - \phi) \rho_m$  = the average density,

$q(\omega) = \rho_f [\tau / \phi + i F(\xi) \eta / \kappa \omega]$ , and

$p_f = -M \nabla \cdot \vec{w} - C \nabla \cdot \vec{u}$  = fluid pressure.

## Some Relations Among Poroelastic Constants



$$\begin{aligned}H &= K_u + \frac{4}{3}\mu, \\K_u &= K_d/(1 - \alpha B), \\K_u &= K_d + \alpha^2 M, \\M &= BK_u/\alpha, \\C &= \alpha M = BK_u,\end{aligned}$$

where

$\alpha = 1 - K/K_m$  = the effective stress coefficient, and

$K_u$  is undrained or Gassmann bulk modulus of system,

$K_d$  is drained modulus,  $B$  is Skempton's coefficient.

# Dispersion Relations



- For shear wave:

$$k_s^2 = \omega^2(\rho - \rho_f^2/q)/\mu$$

- For fast and slow compressional waves:

$$k_{\pm}^2 = \frac{1}{2} [b + f \mp [(b - f)^2 + 4cd]^{1/2}]$$

$$b = \omega^2(\rho M - \rho_f C)/\Delta, \quad c = \omega^2(\rho_f M - qC)/\Delta$$

$$d = \omega^2(\rho_f H - \rho C)/\Delta, \quad f = \omega^2(qH - \rho_f C)/\Delta$$

where

$$\Delta = HM - C^2.$$

## SOME UP-SCALING RESULTS

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via effective medium theory or homogenization methods

- Electrical Conductivity (scale invariant)

$$J = \sigma E \rightarrow \langle J \rangle = \sigma^* \langle E \rangle$$

- Navier-Stokes equation  $\rightarrow$  Darcy's equation

definitely not scale invariant!

- Linear elasticity + Navier-Stokes equations  $\rightarrow$

Biot's equations of poroelasticity

- Heterogeneous Biot  $\rightarrow$  ????

Possibly to a double-porosity model in a variety of circumstances, but there are some other choices as well.

# First Method: Effective Medium Theory

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Effective medium theory is designed to produce estimates of coefficients in the equations of motion.

Various good alternatives are available:

- Average T-matrix (Mori-Tanaka, Kuster-Toksöz)
- Self-consistent (SC or CPA)
- Differential effective medium (DEM)
- Also, rigorous bounding methods are known.

# Eshelby and Poroelasticity



Eshelby's main result in elasticity states that  
for ellipsoidal inclusions:

$$\varepsilon_{pq}^{(i)} = T_{pqrs} \varepsilon_{rs}^*$$

relating inclusion strain to strain at the boundary.

Generalizing to poroelasticity (and similar results hold  
for thermoelasticity):

$$\varepsilon_{pq}^{(i)} - e_{pq}(p_f) = T_{pqrs} [\varepsilon_{rs}^* - e_{rs}(p_f)]$$

where

$$e_{pq} = \left( \frac{\alpha^{(h)} - \alpha^{(i)}}{K^{(h)} - K^{(i)}} \right) \frac{p_f}{3} \delta_{pq}.$$

## Example: Coherent Potential Approximation



If  $C^{(i)}$  is the stiffness tensor of an inclusion,  $C^{(h)}$  is stiffness of a host, and  $C^*$  is stiffness of the effective medium, then within the coherent potential approximation (CPA) we have

$$\sum v^{(i)} (C^{(i)} - C_{CPA}^*) T^{*i} = 0.$$

Similarly, for the Biot-Willis parameter:

$$\sum v^{(i)} (1 - P^{*i}) \frac{\alpha^{(i)} - \alpha_{CPA}^*}{K^{(i)} - K_{CPA}^*} = 0.$$

## Second Method: Mixture Theory

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Mixture theory is designed to keep careful track of the energy in the system. So this approach includes:

- Hamiltonian and Lagrangian methods
- Biot's original method
- Drumheller and Bedford's method

This method is especially powerful for nonlinear problems, but also provides a good method to derive Biot's linear equations.

## Third Method: Homogenization Theory

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Homogenization theory is probably the newest of the methods, being first developed in the 1970s. Other methods can be traced back to earlier periods of history. Periodic boundary conditions are normally used to implement the method.

Development is designed to determine rigorously *the form of the equations* in some fixed frequency regime. So it may not determine how the equations change as frequency is varied widely.

## Fourth Method: Volume Averaging

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Volume averaging was apparently first developed in the 1960s for application to Darcy flow.

There are similarities to homogenization theory, but does not require periodic boundary conditions.

Uses rigorous identities concerning volume integration in 3D to smooth the equations of interest.

Not restricted to a fixed frequency domain, but requires supplementary information to obtain estimates of the coefficients.

# Random Polycrystals of Laminates (1)

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- Assume building blocks (crystalline grains) composed of layers
  - Use Backus averaging scheme to compute effective properties of these grains
  - Use Hashin-Shtrikman bounds based on layer properties to estimate behavior using only volume fraction and layer property information

## Random Polycrystals of Laminates (2)

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- Assume also that the grains are equi-axed: when all grains are considered, the axis of anisotropic grain symmetry due to the layering has no preferred direction
  - Use bounds based on these “anisotropic crystals” to estimate overall behavior of the resulting random polycrystal
  - Use self-consistent method to provide one type of direct estimate of the overall behavior

## Random Polycrystals of Laminates (3)

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- For poroelasticity, we also have two kinds of exact results:
  - If layers are poroelastic (Gassmann – i.e., microhomogeneous) materials, then with just two types of layers exact results are available for Biot-Willis parameter and Skempton's coefficient.
  - If, in addition, the permeability of these two types of layers are very different, then double-porosity modeling can also be pursued and this also gives exact results for two components.
  - The exact results do not predict the drained constants, but the random polycrystals of laminates model gives very close bounds.

# Uniaxial Shear Energy per Unit Volume and the Product Formula

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For an applied uniaxial shear *strain* applied along the symmetry axis

$$\text{i.e., } (e_{11}, e_{22}, e_{33}) = (1, 1, -2)/\sqrt{6}$$

$$G_{eff}^v \equiv (c_{11} + c_{33} - 2c_{13} - c_{66})/3$$

For an applied uniaxial shear *stress* applied along the symmetry axis

$$\text{i.e., } (\sigma_{11}, \sigma_{22}, \sigma_{33}) = (1, 1, -2)/\sqrt{6}$$

$$G_{eff}^r \equiv K_{Reuss} G_{eff}^v / K_{Voigt}.$$

The latter expression is the product formula, relating the shear energies per unit volume to Voigt and Reuss bounds on  $K$ .

## SPIN-OFFS OF THIS WORK

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### ELASTIC CONSTANT BOUNDS FOR POLYCRYSTALS

Important for:

hexagonal, trigonal, tetragonal, and cubic symmetries

Hashin-Shtrikman bounds also lead to self-consistent estimates.

# BOUNDS ON K FOR POLYCRYSTALS

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Hashin-Shtrikman-type bounds for elastic constants of isotropic random polycrystals are known, given first by Peselnick and Meister (1965), later improved by Watt and Peselnick (1980).

The bounds for the bulk modulus can be expressed in terms of these uniaxial shear energies per unit volume as

$$K_{PM}^{\pm} = K_V \frac{G_{eff}^r + \zeta_{\pm}}{G_{eff}^v + \zeta_{\pm}}$$

where

$$\zeta_{\pm} = \frac{G_{\pm}}{6} \left( \frac{9K_{\pm} + 8G_{\pm}}{K_{\pm} + 2G_{\pm}} \right).$$

Parameters  $G_{\pm}$ ,  $K_{\pm}$  were defined by Watt and Peselnick.

# BOUNDS ON G FOR POLYCRYSTALS



The bounds on shear modulus can be expressed similarly as

$$\frac{5}{G_{PM}^{\pm} + \zeta_{\pm}} = \frac{1 - X_{\pm}}{G_{eff}^v + \zeta_{\pm} + Y_{\pm}} + \frac{2}{c_{44} + \zeta_{\pm}} + \frac{2}{c_{66} + \zeta_{\pm}}$$

where  $X_{\pm}$  and  $Y_{\pm}$  are additional parameters depending on  $G_{\pm}$  and  $K_{\pm}$ .

Note that in both cases when  $\zeta_{-} \rightarrow 0$  the bounds go to the Reuss average (lower bound), and when  $\zeta_{+} \rightarrow \infty$  the bounds go to the Voigt average (upper bound). For example,

$$K_{PM}^{-} \rightarrow K_V G_{eff}^r / G_{eff}^v \equiv K_R$$

from the product formulas.

# DOUBLE-POROSITY APPLICATIONS



$$\begin{pmatrix} e \\ -\zeta^{(1)} \\ -\zeta^{(2)} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} \begin{pmatrix} -p_c \\ -p_f^{(1)} \\ -p_f^{(2)} \end{pmatrix},$$

where

$$a_{11} = \frac{1}{K_d^*},$$

$$a_{22} = \frac{v^{(1)}\alpha^{(1)}}{K^{(1)}} \left( \frac{1}{B^{(1)}} - \frac{\alpha^{(1)}(1-Q_1)}{1-K^{(1)}/K^{(2)}} \right),$$

$$a_{12} = -\frac{v^{(1)}Q_1}{K^{(1)}}\alpha^{(1)},$$

$$a_{23} = \frac{\alpha^{(1)}\alpha^{(2)}K^{(1)}K^{(2)}}{[K^{(2)}-K^{(1)}]^2} \left[ \frac{v^{(1)}}{K^{(1)}} + \frac{v^{(2)}}{K^{(2)}} - \frac{1}{K_d^*} \right],$$

## **DOUBLE-POROSITY APPLICATIONS (2)**

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and where

$$v^{(1)}Q_1 = \frac{1 - K^{(2)}/K_d^*}{1 - K^{(2)}/K^{(1)}}.$$

The remaining coefficients can be found using phase-interchange symmetry.

## Other Methods: Were Any Left Out?

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- There are other methods I have not talked about today, including:
  - Double-porosity up-scaling
  - Numerical methods
  - Hybrid methods — using two or more methods simultaneously: for example, mixture theory supplemented with effective medium theory was a very powerful combination in 1980.
  - More work to do on all the methods, including the random polycrystals of laminates model.

# CONCLUSIONS

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I take a very democratic viewpoint concerning all these methods. I have never seen an up-scaling method I did not like. (Well, almost never!)

All these up-scaling methods have some advantages and some disadvantages.

I have stressed the advantages today.

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