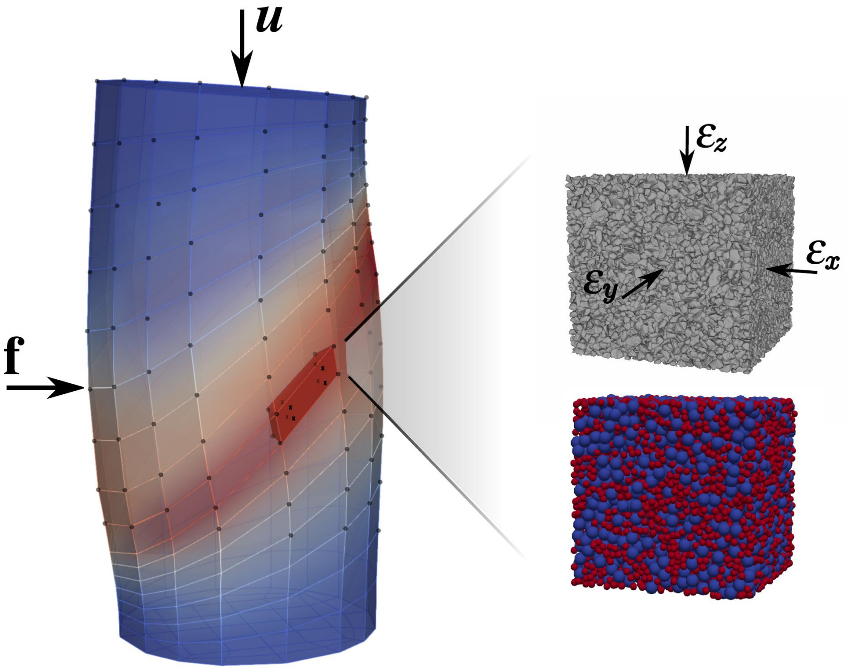


CIVIL-408 Multiscale Modeling in Mechanics

Prof. Kostas Karapiperis

Week 11

Quiz

Which of the following are key characteristics of **Data-Driven Computational Mechanics (DDCM)**? Select all that apply.

a. It replaces constitutive models with a material dataset.

b. It enforces equilibrium and compatibility through numerical solvers.

c. It requires training a neural network on large datasets.

d. It projects strain–stress states onto the closest admissible data point in phase space.

e. It extrapolates well beyond the range of provided data.

Quiz

Which statements accurately describe **ML-based surrogate modeling** in solid mechanics? Select all that apply.

a. It can approximate nonlinear constitutive behavior using neural networks

b. It often requires explicit enforcement of physical constraints such as symmetry or objectivity.

c. It may struggle with extrapolation outside the training domain.

d. It is inherently unable to model path-dependent behavior.

Today

Homogenization for structural elements

- Beams
- Shells

Homogenization for structural materials

- Concrete
- Wood
- Cellular/architected solids

Homogenization for geomaterials

- Jointed rocks
- Granular materials
- Clays

Today

K.Karapipieris

Homogenization for structural elements

- Beams
- Shells

Homogenization for structural materials

- Concrete
- Wood
- Cellular/architected solids

Homogenization for geomaterials

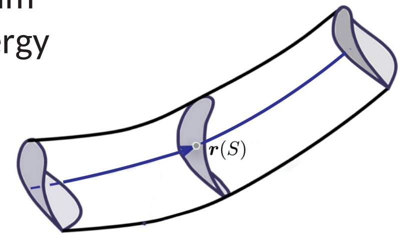
- Jointed rocks
- Granular materials
- Clays

Homogenization for structural elements

Beams under finite strains

Continuum strain energy

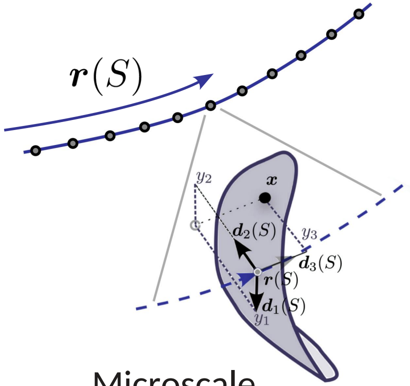
$\psi(\boldsymbol{F})$



Asymptotic dimension reduction

Le Clezio et al, 2023

Macroscale



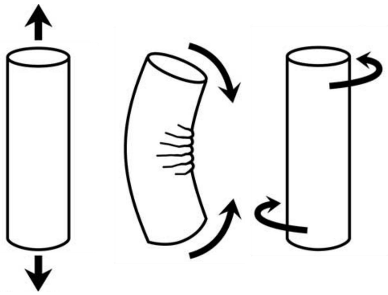
Microscale

Condensed beam energy

$\psi_{\text{eff}}\left(\varepsilon,\kappa_1,\kappa_2,\tau\right)$

$\boldsymbol{E}$

Beam kinematics

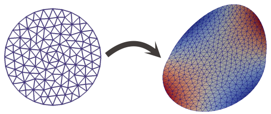


Stretching $\varepsilon(S)$ Bending $\kappa_1(S)\,\kappa_2(S)$ Twist $\tau(S)$

$$\boldsymbol{F}=\boldsymbol{F}(\boldsymbol{E}(S),\boldsymbol{y}(\boldsymbol{X},S)) \longrightarrow \min_{\boldsymbol{y}} \int_0^L \int_{\mathcal{A}} \psi(\boldsymbol{F}(\boldsymbol{E},\boldsymbol{y}))\,d\mathcal{A}\,dS \longrightarrow \psi_{\text{eff}}(\boldsymbol{E})$$

Microscopic coordinates

Condense out (FE^2)



Homogenization for structural elements

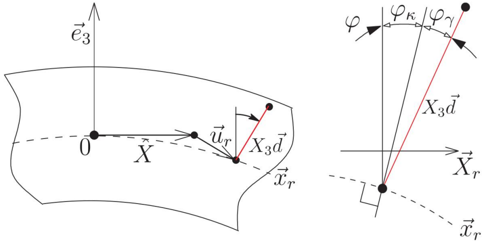
Shells

K.Karapiperis

Macroscale (Mindlin-Reisner shell)
Kinematics:

In-plane strains/Transverse shear — Out-of-plane curvature

$\varepsilon_{\alpha\beta}$ γ_α $\kappa_{\alpha\beta}$



Assumption: Directors remain straight and are inextensible

Special care needs to be taken for thick shells!

Microscale (3D continuum)
Enforcing macroscale averages:

Periodic fluctuations subject to kinematic constraints

$$u^z(x^r_\beta, z) = -\frac{1}{2} x^r_\alpha \kappa_{\alpha\beta} x^r_\beta + \tilde{u}^z$$

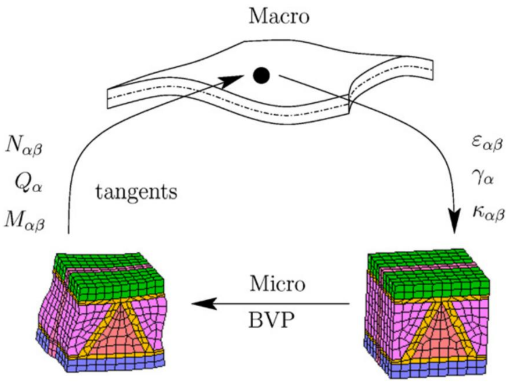
$$u^r_\alpha(x^r_\beta, z) = \varepsilon_{\alpha\beta} x^r_\beta + z\kappa_{\alpha\beta} x^r_\beta + \tilde{u}^r_\alpha$$

Computing macroscale generalized forces:

$$N_{\alpha\beta} = \int_{-H/2}^{H/2} \sigma_m^{\alpha\beta} dh$$

$$V_\alpha = \frac{1}{2}\int_{-H/2}^{H/2} (\sigma_m^{3\alpha} + \sigma_m^{\alpha 3}) dh$$

$$M_{\alpha\beta} = \int_{-H/2}^{H/2} h\sigma_m^{\alpha\beta} dh$$



M G D Geers et al 2007 Modelling Simul. Mater. Sci. Eng

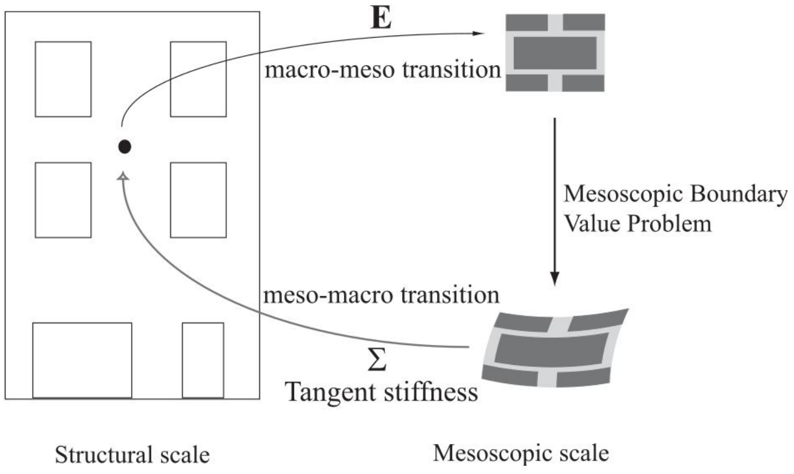
Homogenization for masonry

Masonry flat shells - Case of *homogeneous* deformation

Macroscale (Mindlin-Reisner shell)
Kinematics:

In-plane strains/Transverse shear   Out-of-plane curvature

$\varepsilon_{\alpha\beta}$ γ_α $\kappa_{\alpha\beta}$



Microscale (3D continuum)

Energy consistency between scales:

$$N_{\alpha\beta}\varepsilon_{\alpha\beta} + M_{\alpha\beta}\kappa_{\alpha\beta} + V_\alpha\gamma\alpha$$
$$= \frac{1}{V}\int_V \sigma_{ij}\varepsilon_{ij}dV$$

What if there is **bifurcation** from a homogeneous deformation state?

Then it should be detected, and a new upscaling procedure is needed that accounts for the correct dissipated energy/mode.

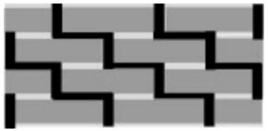
Massart, Peerlings and Geers 2007 Int. J. Num Meth. Eng

Homogenization for masonry

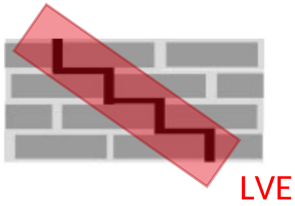
Masonry flat shells - Case of *localized* deformation

The bifurcation from a macroscopically homogeneous deformation state manifests itself as a discrete localized band. Generally hierarchical techniques have trouble accounting for true localized displacement fields.

Periodic



True/Realistic



Energy consistency between scales needs to account now also the localized contribution.

Localization can be handled by appropriate kinematic enrichment at the macroscale, where the jump happens across a cohesive zone:

$$u^r = u^r + [[u_d^r]]\Psi^r$$

$$u^z = u^z + [[u_d^z]]\Psi^z$$

unit jumps along discontituity lines

Can obtain new generalized strains accounting for the discontinuities

$$\varepsilon_{\alpha\beta} \qquad \gamma_\alpha \qquad \kappa_{\alpha\beta}$$

At the microscale, one needs to consider also a localized volume element (LVE).

Mercatoris and Massart 2012 Int. J. Fract.
Massart, Peerlings and Geers 2007 Int. J. Num Meth. Eng

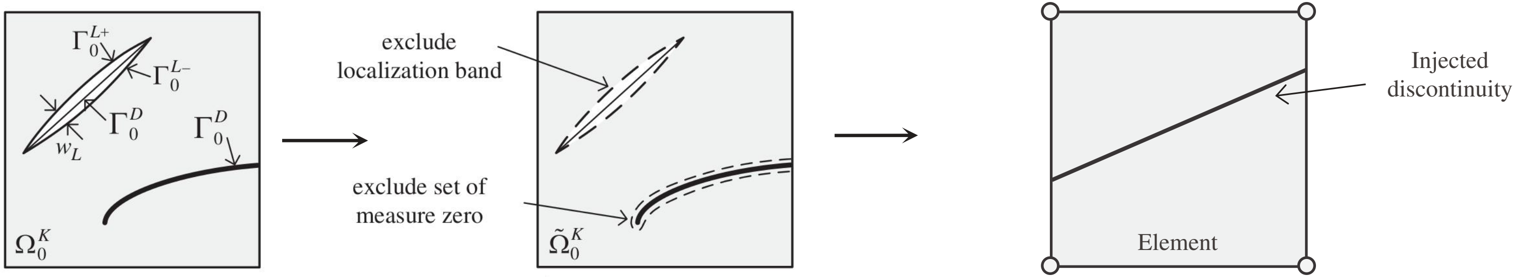
Continuous-discontinuous homogenization

Overcoming the lack scale separation

The previous example represents a case of a more general continuous-discontinuous homogenization approach in the presence of interfaces/cracks, e.g. via the Multiscale Aggregating Discontinuities method.

Microscale
A material instability is detected
(loss of ellipticity)

Macroscale
Inject discontinuity to the macroscale
guaranteeing material stability (ellipticity)



- Compute stress on a modified "perforated" unit cell that excludes cracks $\langle \mathbf{P}^K \rangle = \frac{1}{|\tilde{\Omega}_0^K|} \int_{\tilde{\Omega}_0^K} \mathbf{P}^K \, d\Omega$

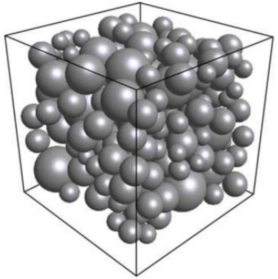
- Compute orientation/magnitude of discontinuity $(\bar{\mathbf{U}}^{K-1}, \bar{\mathbf{N}}^{K-1}) = \arg\left(\min_{\bar{\mathbf{U}},\bar{\mathbf{N}}} (\bar{\mathbf{U}} \otimes \bar{\mathbf{N}} - \mathscr{F}^{K-1} + \langle \mathbf{F}^K \rangle)^2 \right)$

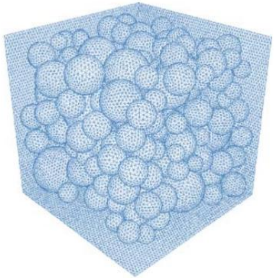
Belytschko, Loehnert and Song 2008 Int. J. Num Meth. Eng

Homogenization for concrete

A damage-based approach

Mesostructure generation (generation of aggregates and their placement within the matrix)





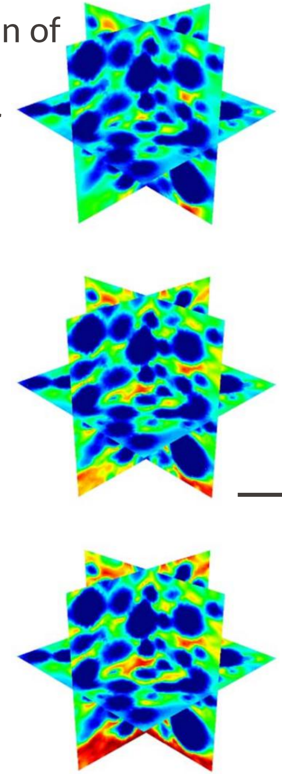
FEM simulations using damaging material

$$\boldsymbol{\sigma} = (1-D)\mathbb{C}\boldsymbol{\varepsilon}$$

$$\rho\psi = \frac{1}{2}\boldsymbol{\sigma} = (1-D)\boldsymbol{\varepsilon}\mathbb{C}\boldsymbol{\varepsilon}$$

$$\dot{\phi} = -\rho\frac{\partial\psi}{\partial D}\dot{D}$$

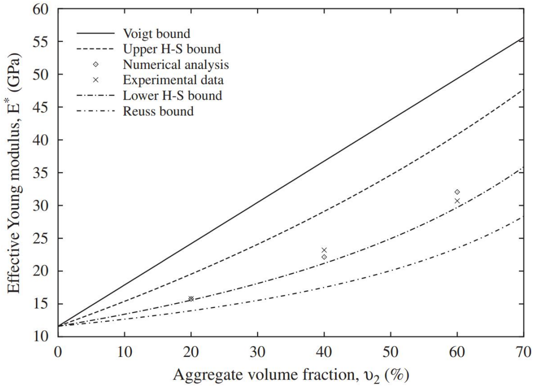
Distribution of damage parameter



Calculation of effective stiffness

$$\begin{Bmatrix} \langle\sigma_{11}\rangle_\Omega \\ \langle\sigma_{22}\rangle_\Omega \\ \langle\sigma_{33}\rangle_\Omega \\ \langle\sigma_{12}\rangle_\Omega \\ \langle\sigma_{23}\rangle_\Omega \\ \langle\sigma_{31}\rangle_\Omega \end{Bmatrix} = \begin{bmatrix} \mathbb{C}^*_{11} & \mathbb{C}^*_{12} & \mathbb{C}^*_{13} & \mathbb{C}^*_{14} & \mathbb{C}^*_{15} & \mathbb{C}^*_{16} \\ \mathbb{C}^*_{21} & \mathbb{C}^*_{22} & \mathbb{C}^*_{23} & \mathbb{C}^*_{24} & \mathbb{C}^*_{25} & \mathbb{C}^*_{26} \\ \mathbb{C}^*_{31} & \mathbb{C}^*_{32} & \mathbb{C}^*_{33} & \mathbb{C}^*_{34} & \mathbb{C}^*_{35} & \mathbb{C}^*_{36} \\ \mathbb{C}^*_{41} & \mathbb{C}^*_{42} & \mathbb{C}^*_{43} & \mathbb{C}^*_{44} & \mathbb{C}^*_{45} & \mathbb{C}^*_{46} \\ \mathbb{C}^*_{51} & \mathbb{C}^*_{52} & \mathbb{C}^*_{53} & \mathbb{C}^*_{54} & \mathbb{C}^*_{55} & \mathbb{C}^*_{56} \\ \mathbb{C}^*_{61} & \mathbb{C}^*_{62} & \mathbb{C}^*_{63} & \mathbb{C}^*_{64} & \mathbb{C}^*_{65} & \mathbb{C}^*_{66} \end{bmatrix} \begin{Bmatrix} \langle\epsilon_{11}\rangle_\Omega \\ \langle\epsilon_{22}\rangle_\Omega \\ \langle\epsilon_{33}\rangle_\Omega \\ 2\langle\epsilon_{12}\rangle_\Omega \\ 2\langle\epsilon_{23}\rangle_\Omega \\ 2\langle\epsilon_{31}\rangle_\Omega \end{Bmatrix}$$

Comparison against experiments

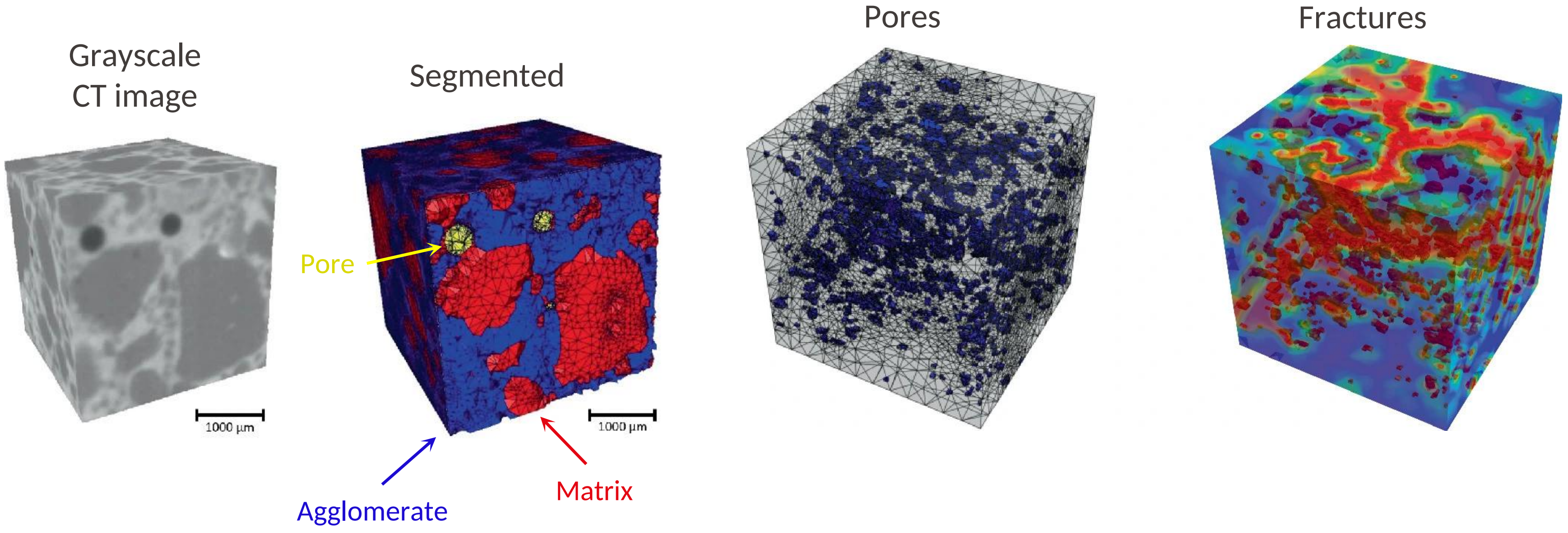


P. Wriggers and S.O. Moftah, 2005 Fin. El. Anal. Des.

Homogenization for concrete

A damage-based approach

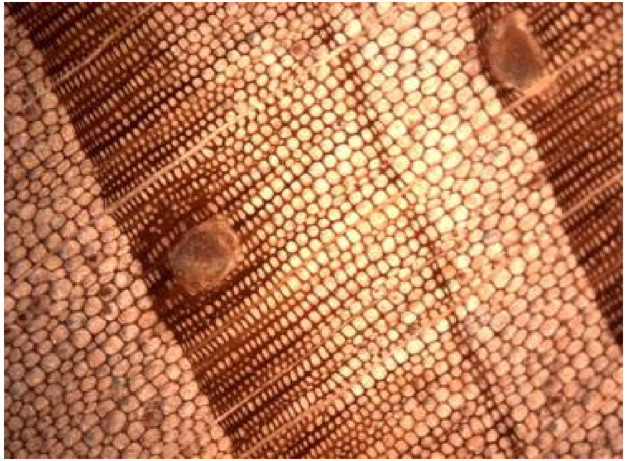
Studies also apply these ideas to digital twins from X-ray Computed Tomography



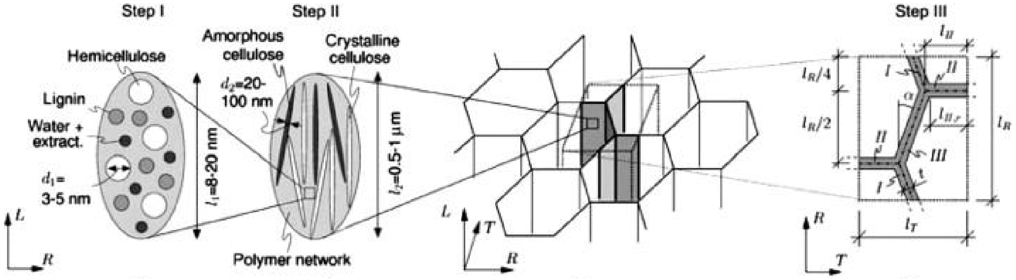
Wessels et al, 2022 Current Trends and Open Problems in Computational Mechanics

Homogenization for wood

Cellular microstructure revealed from micrograph of structural wood



Three-step homogenization procedure



$$\mathbb{C}^{SCI}_{polynet} = \left\{\sum_r \tilde{f}_r \mathbb{c}_r : [\mathbb{I} + \mathbb{P}^{polynet}_{sph} : (\mathbb{c}_r - \mathbb{C}^{SCI}_{polynet})]^{-1}\right\} : \left\{\sum_s \tilde{f}_s [\mathbb{I} + \mathbb{P}^{polynet}_{sph} : (\mathbb{c}_s - \mathbb{C}^{SCI}_{polynet})]^{-1}\right\}^{-1}$$

$$\mathbb{C}^{MTI}_{cwm} = \left\{f_{polynet}\mathbb{C}^{SCI}_{polynet} + \sum_r f_r \mathbb{c}_r : [\mathbb{I} + \mathbb{P}^{polynet}_{cyl} : (\mathbb{c}_r - \mathbb{C}^{SCI}_{polynet})]^{-1}\right\}$$

$$: \left\{f_{polynet}\mathbb{I} + \sum_s f_s : [\mathbb{I} + \mathbb{P}^{polynet}_{cyl} : (\mathbb{c}_s - \mathbb{C}^{SCI}_{polynet})]^{-1}\right\}^{-1}, \quad r, s \in [\text{crycel}, \text{amocel}].$$

$$\mathbb{C}^{MTII}_{SW} = \{(1 - \hat{f}_{lum})\mathbb{C}^{MTI}_{cwm}\} : \{(1 - \hat{f}_{lum})\mathbb{I} + \hat{f}_{lum} : [\mathbb{I} - \mathbb{P}^{cwm}_{cyl} : \mathbb{C}^{MTI}_{cwm}]^{-1}\}^{-1}$$

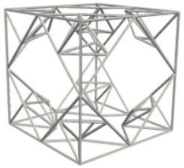
Hofstetter, C. Hellmich and J. Eberhardsteiner , 2007 Holzforschung

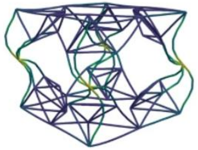
Homogenization for architected/cellular solids

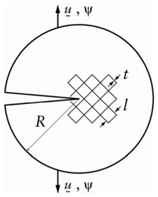
The future of structural materials

Lattice materials furnish nowadays a manufacturable solution to near-optimal structural material properties (stiff, light, strong and damage-tolerant)

Homogenization of single unit cells composed of beam elements:





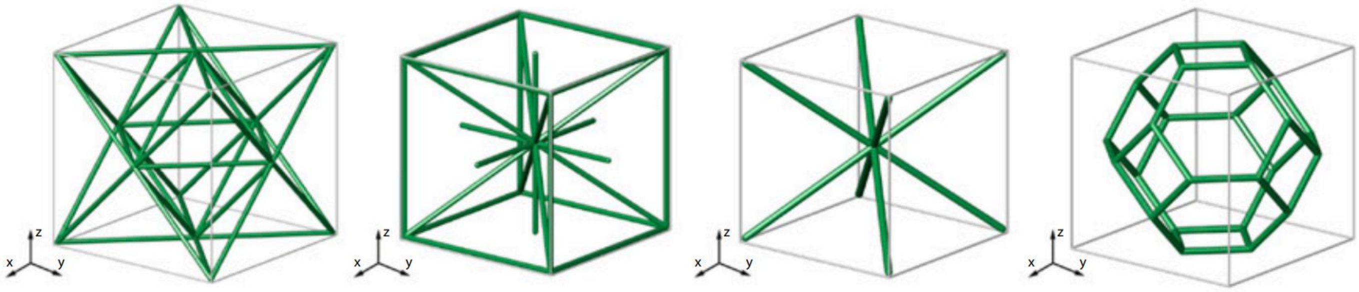


Can be used to derive scaling laws of their properties

Elasticity: $E/E_s = B\bar{\rho}^b$

Strength: $\sigma_C/\sigma_{cs} = C\bar{\rho}^c$

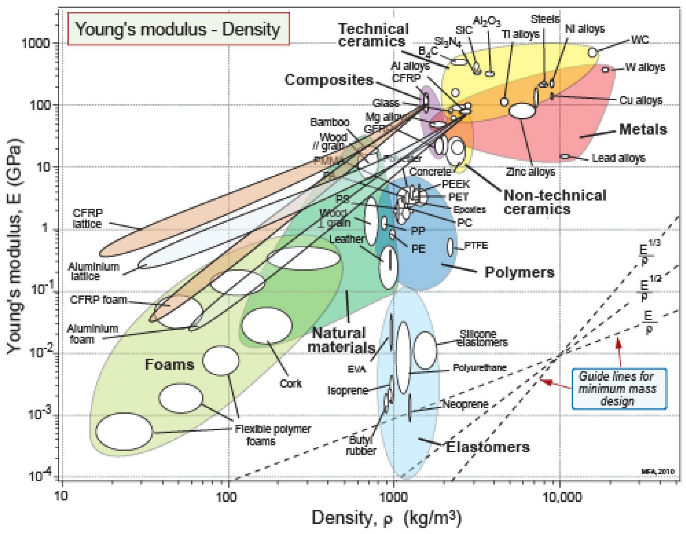
Fracture toughness: $K_{IC}/\sigma_{cs}\sqrt{l} = D\bar{\rho}^d$

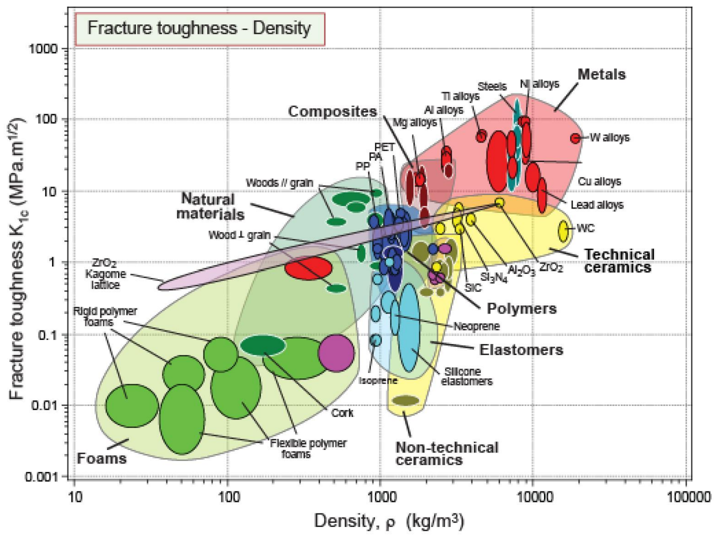


K.Karapiperis

Homogenization for architected/cellular solids

Expanding the boundaries of material property space





NA Fleck, VS Deshpande, MF Ashby, 1999 Proc. R. Soc. A

Today

Homogenization for structural elements

- Beams
- Shells

Homogenization for structural materials

- Concrete
- Wood
- Cellular/architected solids

Homogenization for geomaterials

- Jointed rocks
- Granular materials
- Clays

Application to geomaterials

Homogenization of jointed-rock mass

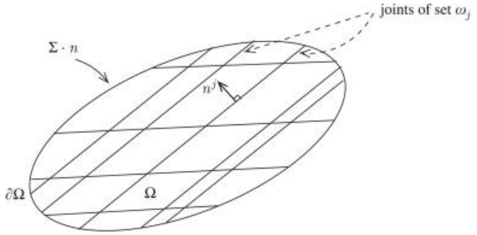
Effective medium theory under non-interacting assumptions may be used to capture rock elasticity. The effective compliance tensor is represented as the sum of a background compliance tensor and contributions related to individual non-interacting fractures

Rock:

$$\boldsymbol{\varepsilon} = \boldsymbol{s}^m : \boldsymbol{\sigma}$$

Joints:

$$[\boldsymbol{\xi}] = \boldsymbol{s}^j : \boldsymbol{T}, \quad \boldsymbol{T} = \boldsymbol{\Sigma} \cdot \boldsymbol{n}^j$$



Total strain derived from the bulk and the joints

$$\boldsymbol{E} = \langle \boldsymbol{\varepsilon} \rangle + \frac{1}{|\Omega|} \int_\Omega \boldsymbol{n} \otimes [\boldsymbol{\xi}] dS$$

$$\boldsymbol{E} = \boldsymbol{s}^m : \Sigma + a^j (\boldsymbol{s}^j \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{n}^j) \otimes \boldsymbol{n}^j$$

Rewritten as

$$\boldsymbol{E} = \boldsymbol{S}^{\text{hom}} : \Sigma$$

$$\boldsymbol{S}^{\text{hom}} = \boldsymbol{s}^{\text{m}} + a^j s^j_{\alpha\beta} \boldsymbol{e}^j_\alpha \otimes \boldsymbol{n}^j \otimes \boldsymbol{e}^j_\beta \otimes \boldsymbol{n}^j$$

Can be extended to an elastoplastic formulation (plastic sliding of joints)

Maghus, Bernaud, Freard and Garnier, 2008 Int. J. Rock. Mech. Min. Sci.

Application to geomaterials

FEMxDEM for localization in granular materials

With appropriate choice of RVEs, FEMxDEM may also simulate shear banding in these materials

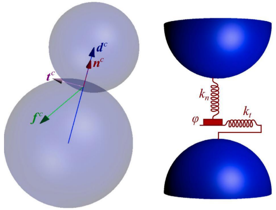
Microscale (RVE)

Love-Weber formula

$$\boldsymbol{\sigma} = \frac{1}{V}\sum_c \boldsymbol{l}^c \otimes \boldsymbol{f}^c$$

Tangent operator

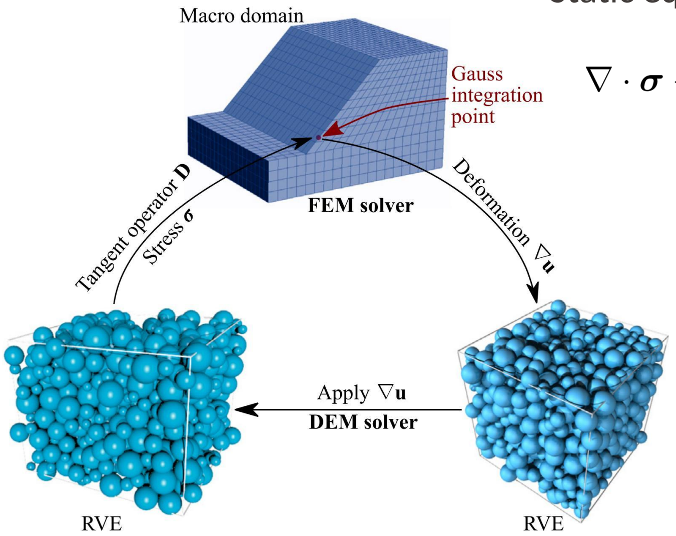
$$\boldsymbol{C} = \frac{1}{V}\sum_c k_n \boldsymbol{n}^c \otimes \boldsymbol{l}^c \otimes \boldsymbol{n}^c \otimes \boldsymbol{l}^c + \frac{1}{V}\sum_c k_t \boldsymbol{t}^c \otimes \boldsymbol{l}^c \otimes \boldsymbol{t}^c \otimes \boldsymbol{l}^c$$



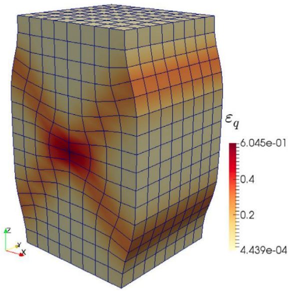
Macroscale (Continuum)

Static equilibrium

$$\nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{b} = \boldsymbol{0}$$



Guo and Zhao, 2016 Comp. Geotech.



Application to geomaterials

Granular micromechanics

Analytical homogenization techniques furnish a useful efficient alternative beyond FEMxDEM.

Contact scale

Relative displacement
betwen two particles (m,n):

$$\delta_i^{mn} = u_i^m - u_i^n + e_{ijk}(\omega_j^m r_k^m - \omega_j^n r_k^n)$$

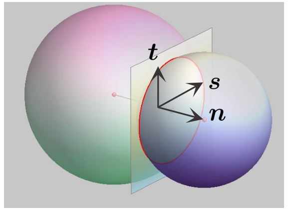
Rewrite using mean strain and
fluctuation (w/ equilibrium closure):

$$\delta_i^{mn} = (\delta_{jl} l_k^{mn} - \Gamma_{jkl}^n)\varepsilon_{kl}^n$$

Ensuing contact force:

$$f_i = K_{ij}\delta_j$$

$$K_{ij} = K_n n_i n_j + K_s(s_i s_j + t_i t_j)$$



Cell scale

Split system into cells s.t.
the stress of each cell:

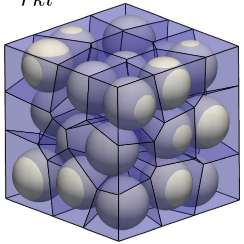
$$\sigma_{ij}^n = \frac{1}{2V^n}\sum_m l_i^{nm} f_j^{nm}$$

relates to the cell strain via:

$$\sigma_{ij}^n = C_{ijkl}^n \varepsilon_{kl}^n$$

Combining everything:

$$C_{ijkl}^n = \frac{1}{2V^n}\sum_m l_i^{nm} K_{jl}^{nm} l_k^{nm} - \frac{1}{2V^n}\sum_m l_i^{nm} K_{jr}^{nm}\Gamma_{rkl}^n$$



A Misra and C.S. Chang, 1992 Int. J. Sol. Struct.

Assembly (macro) scale

By volume averaging

$$\bar{\sigma}_{ij} = \frac{1}{V}\sum_n V^n \sigma_{ij}^n$$

$$\bar{\varepsilon}_{ij} = \frac{1}{V}\sum_n V^n \varepsilon_{ij}^n$$

Derive concentration
tensor by solving an
Eshelby-like problem:

$$\varepsilon_{kl}^n = H_{mnkl}^n \bar{\varepsilon}_{kl}$$

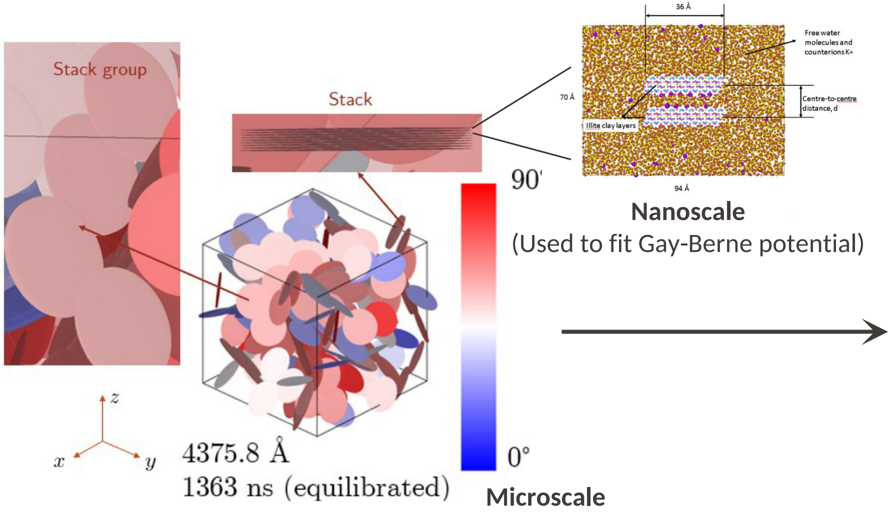
Obtain in the end:

$$\bar{\sigma}_{ij} = C_{ijkl}\bar{\varepsilon}_{kl} = \left(\frac{1}{V}\sum_n V^n C_{ijmn}^n H_{mnkl}^n\right)\bar{\varepsilon}_{kl}$$

Application to geomaterials

Homogenization for clays

Coarse-grained Molecular Dynamics simulations, with fitted MD potential from nanoscale models



Macroscale

The consider a macroscopic model where the energy of the system U is divided into:

- *interstack* potential energy
- *intrastack* potential energy

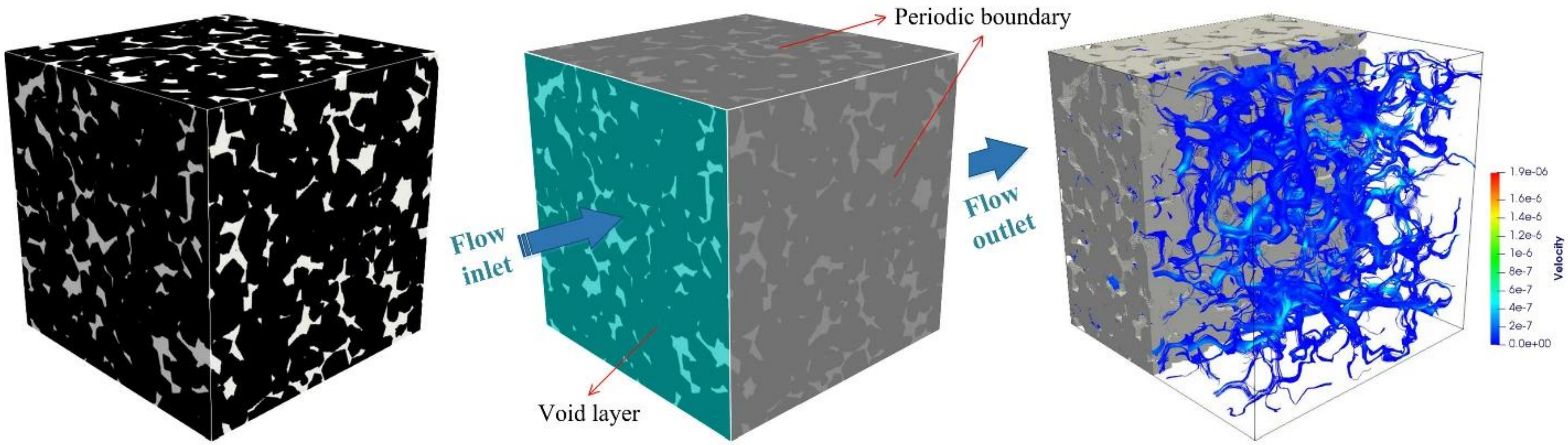
These are derived from system parameters (stack density, average stack size, interstack pair correlation function, fabric tensor, …)

Zhu, Whittle and Pellenq, 2025 J. Mech. Phys. Sol.

Outlook

Rarely are these materials interacting only mechanically. Multiphysics interactions matter, e.g.:

Poromechanical effects



Discussion

That's what I prepared for you today.

What would you like to discuss?

Reading for next class:

Collection of research articles

(Week 12 - Reading Assignments)