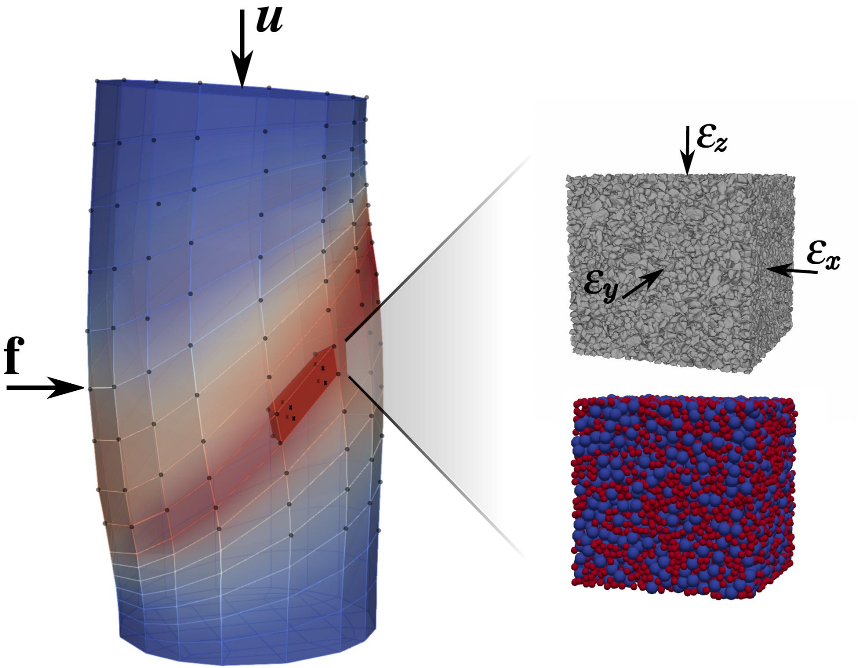

CIVIL-408 Multiscale Modeling in Mechanics

Prof. Kostas Karapiperis

Week 5

Numerical vs Analytical Homogenization

Computational homogenization can be very accurate yet computationally expensive!

Alternative homogenization techniques rely on analytical constructions at the expense of generality.

We discuss the most prominent techniques:

- Dilute mean-field methods (**Eshelby**, **Mori-Tanaka** method)
- Asymptotic **Hashin-Shtrikman** bounds
- **Cauchy-Born** rule

Dilute Composites

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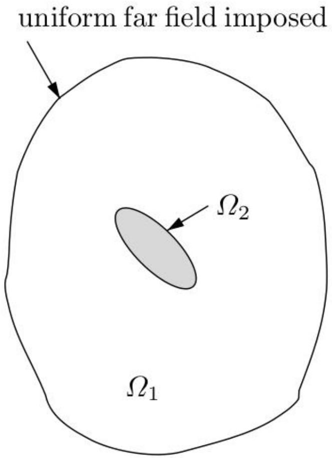
Composites with **non-interacting/weakly interacting inclusions**.

Eshelby (1957) studied a linearly elastic ellipsoidal particle embedded into an infinite matrix. Under uniform far field, the stress/strain in the particle is constant.

He derived the so-called **Eshelby tensor** (*S*) which relates the actual strain inside the inclusion to the eigenstrain **ε*** i.e. the strain that the inclusion would undergo if unconstrained:

$$\langle \boldsymbol{\varepsilon} \rangle_{\Omega_2} = \boldsymbol{S} : \langle \boldsymbol{\varepsilon}^* \rangle_{\Omega_2}$$

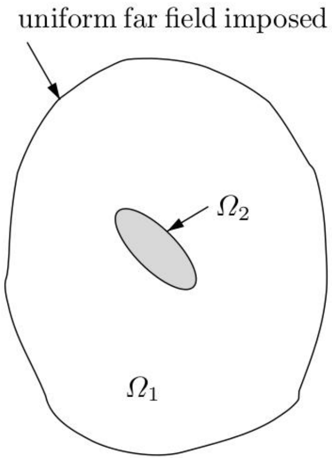


Dilute Composites

The Eshelby tensor can in turn be used to calculate the **strain concentration tensor *A*** which relates the actual strain inside the inclusion to the uniform applied far-field strain i.e. the average strain in $\Omega = \Omega_1 \cup \Omega_2$:

$$\boldsymbol{A} = [\boldsymbol{I} + \boldsymbol{S} : \mathbb{C}_1^{-1} : (\mathbb{C}_2 - \mathbb{C}_1)]^{-1}$$

$$\langle \boldsymbol{\varepsilon} \rangle_{\Omega_2} = \boldsymbol{A} : \langle \boldsymbol{\varepsilon} \rangle_{\Omega}$$



where $\mathbb{C}_1$ and $\mathbb{C}_2$ are the stiffness tensors of the matrix and the inclusion respectively.

Dilute Composites

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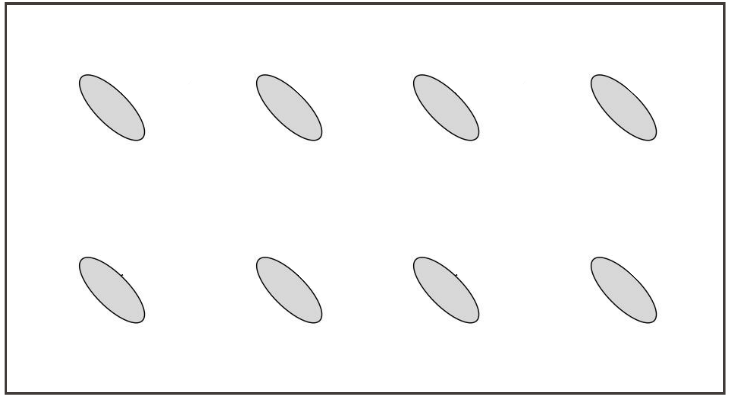
The homogenized stiffness tensor of the dilute composite can be obtained (upon algebraic manipulations) as :

$$\langle \mathbb{C} \rangle_\Omega = \mathbb{C}_1 + \phi \, (\mathbb{C}_2 - \mathbb{C}_1) : \boldsymbol{A}$$

where ϕ is the packing fraction of the inclusion phase.

Assumptions:

- Low volume fractions (ϕ << 1)
- No inclusion-inclusion interactions
- Exact for ellipsoidal inclusions



The Mori-Tanaka Method

Non-interaction of particles is an **unrealistic** assumption for materials with randomly dispersed particulate microstructure at even a few percent volume fraction.

Mori-Tanaka (1973) modified the dilute method to account for ***weak* interaction** between particles/inclusions. The point of departure of the Eshelby solution is:

$$\langle \boldsymbol{\varepsilon} \rangle_{\Omega_2} = \boldsymbol{A} : \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1} \quad \text{(instead of } \langle \boldsymbol{\varepsilon} \rangle_{\Omega_2} = \boldsymbol{A} : \langle \boldsymbol{\varepsilon} \rangle_{\Omega} \text{)}$$

due to the fact that the matrix strain itself is altered by the effect of inclusions.

By definition of the average strain of the two-phase composite:

$$\langle \boldsymbol{\varepsilon} \rangle_{\Omega} = (1-\phi)\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1} + \phi \langle \boldsymbol{\varepsilon} \rangle_{\Omega_2}$$

Hence:

$$\langle \boldsymbol{\varepsilon} \rangle_{\Omega} = (1-\phi)\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1} + \phi \boldsymbol{A} : \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}$$

The Mori-Tanaka Method

This allows us to write:

$$\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1} = [\boldsymbol{I} + \phi(\boldsymbol{A} - \boldsymbol{I})]^{-1} \langle \boldsymbol{\varepsilon} \rangle_{\Omega}$$

$$\langle \boldsymbol{\varepsilon} \rangle_{\Omega_2} = \boldsymbol{A}[\boldsymbol{I} + \phi(\boldsymbol{A} - \boldsymbol{I})]^{-1} \langle \boldsymbol{\varepsilon} \rangle_{\Omega} = \boldsymbol{A}^{M-T} \langle \boldsymbol{\varepsilon} \rangle_{\Omega}$$

In terms of the **Mori-Tanaka concentration tensor**:

$$\boldsymbol{A}^{M-T} = \boldsymbol{A}[\boldsymbol{I} + \phi(\boldsymbol{A} - \boldsymbol{I})]^{-1}$$

Finally, the Mori-Tanaka estimate of the composite stiffness tensor is:

$$\langle \mathbb{C} \rangle_{\Omega}^{\text{M-T}} = \mathbb{C}_1 + \phi\left(\mathbb{C}_2 - \mathbb{C}_1\right) : \boldsymbol{A}^{\text{M-T}}$$

- Good for **moderate volume fractions** of aligned ellipsoidal inclusions.
- Less accurate for high contrast in phase stiffness or non-ellipsoidal shapes.

Asymptotic Hashin-Shtrikman Bounds

Until 1963, the best estimates for the effective behavior of isotropic composites were the Voigt and Reuss bounds we discussed previously.

In 1963, Hashin and Shtrikman used **variational principles** and concept of **'polarization'** of micromechanical variables to derive the **tightest possible bounds on isotropic composites**, where the only known information is the volume fractions and the moduli of each phase (matrix, inclusions).

For the heterogeneous and the spatially averaged quantities we have respectively:

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbb{C}(\boldsymbol{x}) : \boldsymbol{\varepsilon}(\boldsymbol{x}) \qquad \langle \boldsymbol{\sigma} \rangle = \langle \mathbb{C} \rangle : \langle \boldsymbol{\varepsilon} \rangle$$

We can define the polarization fields by comparing to a homogeneous reference material of stiffness $\mathbb{C}_0$:

$$\boldsymbol{\sigma}'(\boldsymbol{x}) = (\mathbb{C}(\boldsymbol{x}) - \mathbb{C}_0) : \boldsymbol{\varepsilon}(\boldsymbol{x}) \qquad \boldsymbol{\varepsilon}'(\boldsymbol{x}) = \boldsymbol{\varepsilon}(\boldsymbol{x}) - \langle \boldsymbol{\varepsilon} \rangle$$

Asymptotic Hashin-Shtrikman Bounds

We can rewrite the total potential energy

$$\Pi[\boldsymbol{u}] = \frac{1}{2}\int_{\Omega} \langle \boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon} \rangle \, dV$$

in terms of the polarization (fluctuation) field:

$$\Pi[\boldsymbol{u}'] = \frac{1}{2}\int_{\Omega} \left[\langle \boldsymbol{\varepsilon} \rangle : \mathbb{C}_0 : \langle \boldsymbol{\varepsilon} \rangle + (\boldsymbol{\varepsilon} - \langle \boldsymbol{\varepsilon} \rangle) : \mathbb{C}_0 : (\boldsymbol{\varepsilon} - \langle \boldsymbol{\varepsilon} \rangle) + 2\boldsymbol{\varepsilon} : \boldsymbol{\sigma}' \right] dV$$

and define a variational principle over admissible polarization fields.

Assuming isotropy and following calculus of variations arguments, we can eventaully obtain tight bounds for the homogenized bulk and shear modulus.

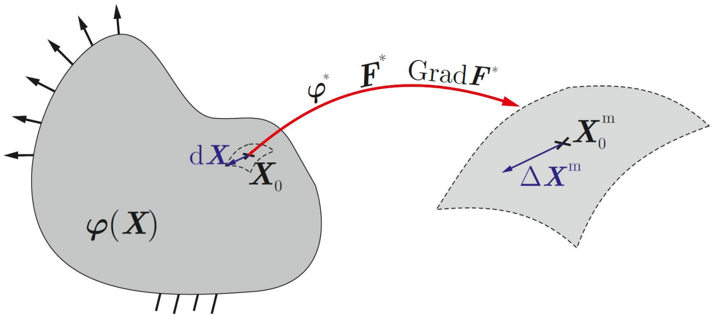
Asymptotic Hashin-Shtrikman Bounds

$$\underbrace{\kappa_1 + \frac{\phi}{\frac{1}{\kappa_2-\kappa_1} + \frac{3(1-\phi)}{3\kappa_1+4\mu_1}}}_{\text{Bulk modulus H-S lower bound}} \leq \kappa^* \leq \underbrace{\kappa_2 + \frac{1-\phi}{\frac{1}{\kappa_1-\kappa_2} + \frac{3\phi}{3\kappa_2+4\mu_2}}}_{\text{Bulk modulus H-S upper bound}}$$

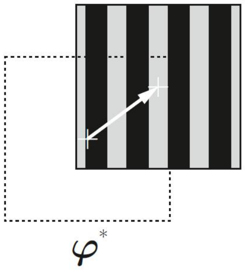
$$\underbrace{\mu_1 + \frac{\phi}{\frac{1}{\mu_2-\mu_1} + \frac{6(1-\phi)(\kappa_1+2\mu_1)}{5\mu_1(3\kappa_1+4\mu_1)}}}_{\text{Shear modulus H-S lower bound}} \leq \mu^* \leq \underbrace{\mu_2 + \frac{1-\phi}{\frac{1}{\mu_1-\mu_2} + \frac{6\phi(\kappa_2+2\mu_2)}{5\mu_2(3\kappa_2+4\mu_2)}}}_{\text{Shear modulus H-S upper bound}}$$

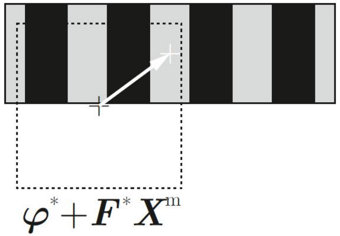
- Applicable for any microstructure
- Bounds sensitive to sample size, valid only asymptotically (large samples sizes)!

The Cauchy-Born rule



macroscale problem RVE problem

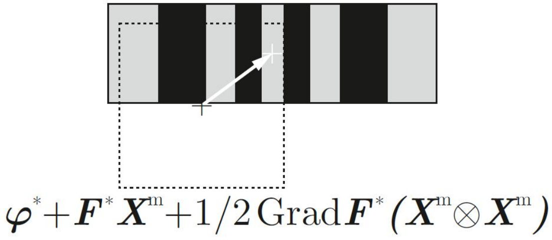




Taylor expansion of the deformation around a **macroscale point**:

$$\varphi_i(\boldsymbol{X}) = \varphi_i(\boldsymbol{X}_0) + \frac{\partial \varphi_i}{\partial X_J}(\boldsymbol{X}_0)\,\mathrm{d}X_J + \frac{1}{2}\frac{\partial^2 \varphi_i}{\partial X_J\,\partial X_K}(\boldsymbol{X}_0)\,\mathrm{d}X_J\,\mathrm{d}X_k + \text{h.o.t.}$$

$$= \varphi_i(\boldsymbol{X}_0) + F_{iJ}(\boldsymbol{X}_0)\,\mathrm{d}X_J + \frac{1}{2}F_{iJ,K}(\boldsymbol{X}_0)\,\mathrm{d}X_J\,\mathrm{d}X_k + \text{h.o.t.},$$



Application to the deformation in a **unit cell** on the microscale:

$$\varphi_i(\boldsymbol{X}^{\mathrm{m}}) \approx \varphi_i^* + F_{iJ}^*\Delta X_J^{\mathrm{m}} + \frac{1}{2}F_{iJ,K}^*\Delta X_J^{\mathrm{m}}\,\Delta X_k^{\mathrm{m}} + \text{h.o.t.}$$

The Cauchy-Born rule - 1st-order

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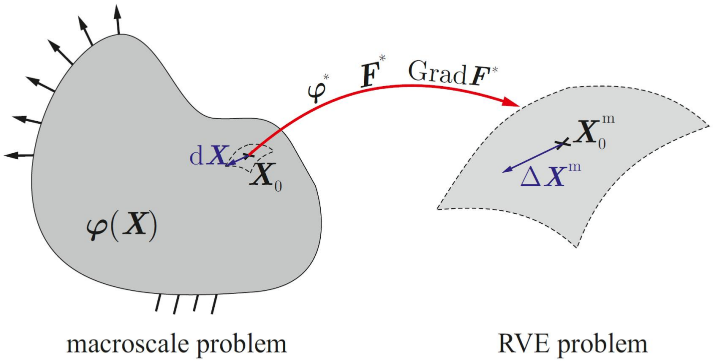


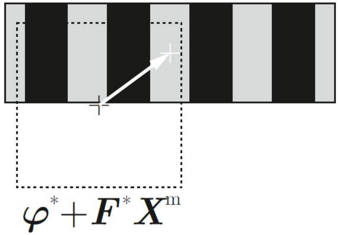
Application to the deformation in a **unit cell** on the microscale:

$$\varphi_i(\boldsymbol{X}^{\mathrm{m}}) \approx \varphi_i^* + F_{iJ}^* \Delta X_J^{\mathrm{m}} + \frac{1}{2} F_{iJ,K}^* \Delta X_J^{\mathrm{m}} \Delta X_k^{\mathrm{m}} + \mathrm{h.o.t.}$$

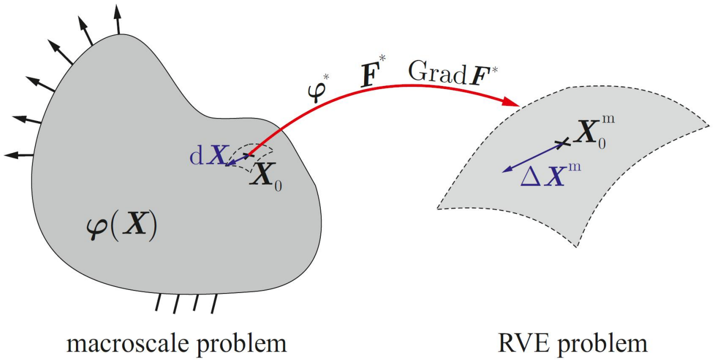
Extracting the effective response by averaging:

$$W^*(\boldsymbol{F}^*) = \frac{1}{V} \int_\Omega W(\boldsymbol{F}^*, \boldsymbol{X}) \, \mathrm{d}V = \langle W(\boldsymbol{F}^*, \boldsymbol{X}) \rangle$$

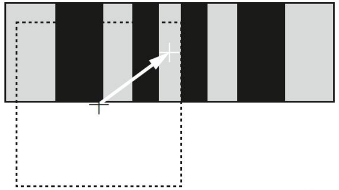
$$\Longrightarrow \quad \boldsymbol{P}^* = \frac{\partial W^*}{\partial \boldsymbol{F}^*}(\boldsymbol{F}^*) = \langle \frac{\partial W}{\partial \boldsymbol{F}}(\boldsymbol{F}^*, \boldsymbol{X}) \rangle = \langle \boldsymbol{P}(\boldsymbol{F}^*, \boldsymbol{X}) \rangle$$



The Cauchy-Born rule - 2nd-order



Application to the deformation in a **unit cell** on the microscale:



$$\varphi^* + F^* X^{\mathrm{m}} + 1/2\, \mathrm{Grad}\, F^* \, (X^{\mathrm{m}} \otimes X^{\mathrm{m}})$$

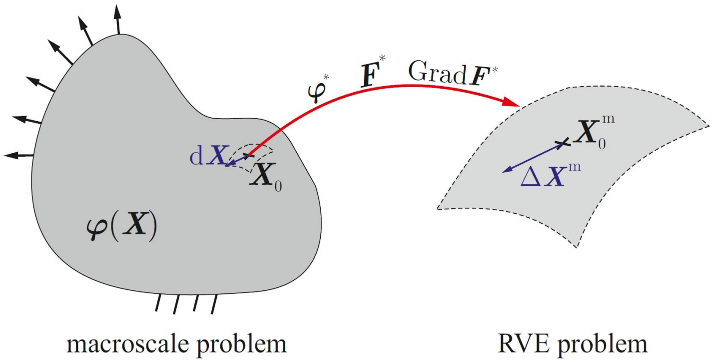
$$\varphi_i(\boldsymbol{X}^{\mathrm{m}}) \approx \varphi_i^* + F_{iJ}^* \Delta X_J^{\mathrm{m}} + \frac{1}{2} F_{iJ,K}^* \Delta X_J^{\mathrm{m}} \Delta X_k^{\mathrm{m}} + \mathrm{h.o.t.}$$

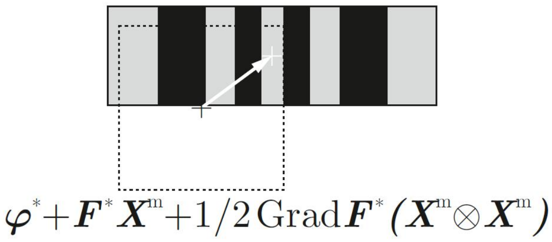
Extracting the effective response by averaging:

$$W^*(\boldsymbol{F}^*, \mathrm{Grad}\, \boldsymbol{F}^*) = \frac{1}{V} \int_\Omega W(\boldsymbol{F}^* + (\mathrm{Grad}\, \boldsymbol{F}^*)\boldsymbol{X}^{\mathrm{m}}, \boldsymbol{X}^{\mathrm{m}})\, \mathrm{d}V = \langle W(\boldsymbol{F}^* + \mathrm{Grad}\, \boldsymbol{F}^* \boldsymbol{X}^{\mathrm{m}}, \boldsymbol{X}^{\mathrm{m}}) \rangle$$

$$\longrightarrow \quad \boldsymbol{P}^* = \frac{\partial W^*}{\partial \boldsymbol{F}^*}$$

The Cauchy-Born rule - 2nd-order





This construction also gives rise to a **couple-stress tensor**:

$$\boldsymbol{Y}^* = \frac{\partial W^*}{\partial(\nabla \boldsymbol{F}^*)}$$

The macroscale variational problem must also be revised:

$$I[\varphi] = \int_\Omega W(\phi, \boldsymbol{F}, \nabla \boldsymbol{F})\, dV$$

becoming **nonlocal**, and allowing us to capture material length-scales.

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The Cauchy-Born rule - Discrete systems

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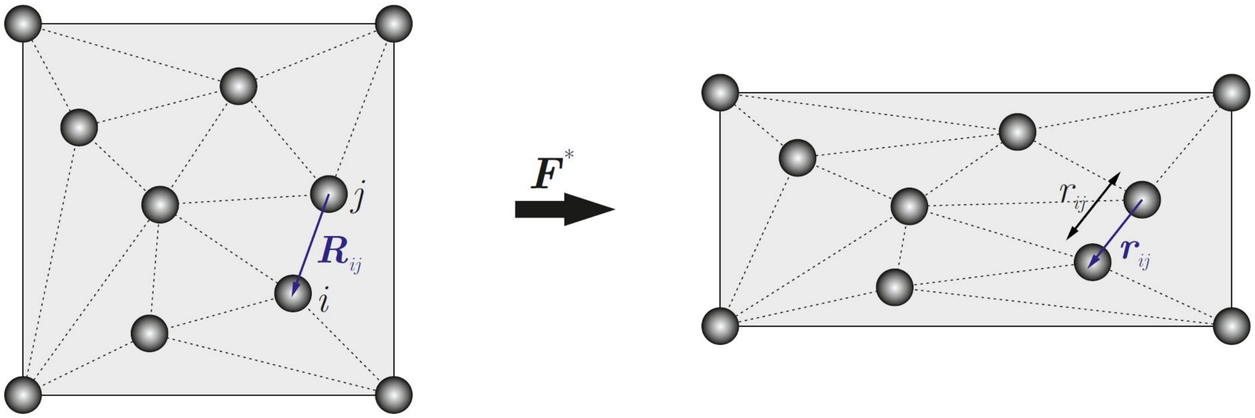
Application of **affine deformation** to **particle interactions** on the microscale:



$$W^*(\boldsymbol{F}^*) = \frac{1}{2V}\sum_{i=1}^{N}\sum_{j\neq i} V\left(r_{ij}\right) \qquad \text{with} \qquad r_{ij} = \left\|\boldsymbol{x}_i^{\mathrm{m}} - \boldsymbol{x}_j^{\mathrm{m}}\right\|, \quad \boldsymbol{x}_i^{\mathrm{m}} = \boldsymbol{F}^*\boldsymbol{X}_i^{\mathrm{m}}$$

$$W^*(\boldsymbol{F}^*) = \frac{1}{2V}\sum_{i=1}^{N}\sum_{j\neq i} V\left(\left\|\boldsymbol{F}^*\boldsymbol{X}_i^{\mathrm{m}} - \boldsymbol{F}^*\boldsymbol{X}_j^{\mathrm{m}}\right\|\right) \longrightarrow \boldsymbol{P}^*(\boldsymbol{F}^*) = \frac{1}{2V}\sum_{i=1}^{n}\sum_{j\neq i} \boldsymbol{f}_{ij}\otimes\boldsymbol{R}_{ij}$$

(We will come back to this approach when talking about discrete systems)

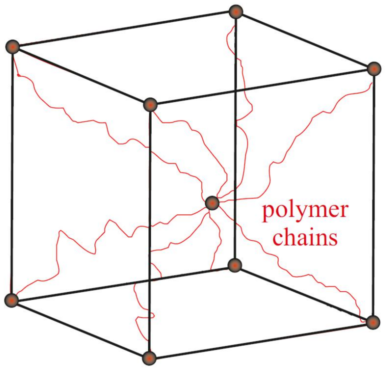
The Cauchy-Born rule - Polymers

Define the **energy density of a polymer** by affinely deforming the eight diagonal chains in a cubic unit cell:

$$W^*(\boldsymbol{F}^*) = \frac{1}{2V}\sum_{i=1}^{8} V\left(\|\boldsymbol{F}^*\boldsymbol{X}_i^{\mathrm{m}}\|\right) = \frac{1}{2L^3}\sum_{i=1}^{8} V\left(\sqrt{\boldsymbol{X}_i^{\mathrm{m}}\cdot(\boldsymbol{F}^*)^{\mathrm{T}}\boldsymbol{F}^*\boldsymbol{X}_i^{\mathrm{m}}}\right)$$

Leads to a popular **hyperelastic model**:

$$W(\boldsymbol{F}^*) = C_1\sum_{i=1}^{5}\alpha_i\beta^{2(i-1)}(I_1^i - 3^i)$$

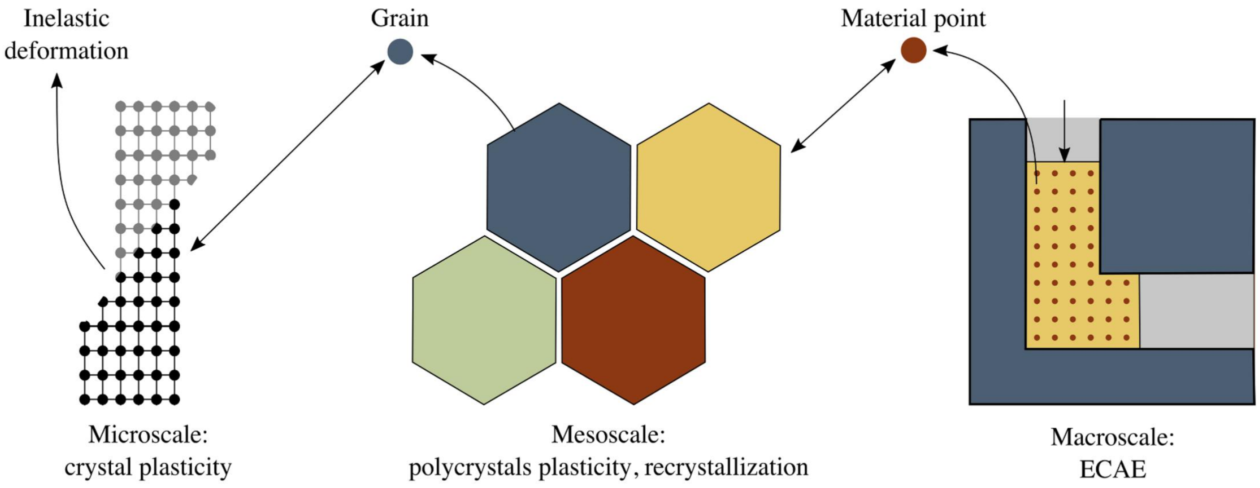


J. Mech. Phys. Solids Vol. 41, No. 2, pp. 389 412, 1993.
Printed in Great Britain.
0022 5096/93 $6.00 + 0.00

A THREE-DIMENSIONAL CONSTITUTIVE MODEL FOR THE LARGE STRETCH BEHAVIOR OF RUBBER ELASTIC MATERIALS

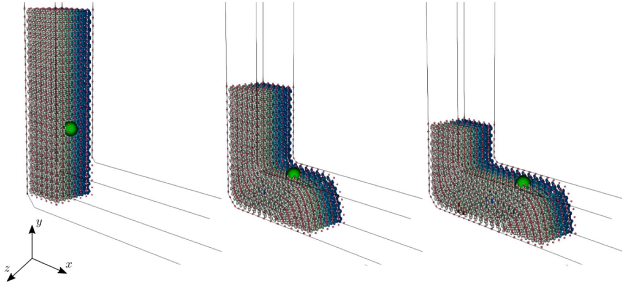
Ellen M. Arruda and Mary C. Boyce
The Department of Mechanical Engineering, The Massachusetts Institute of Technology

The Cauchy-Born rule - Polycrystals

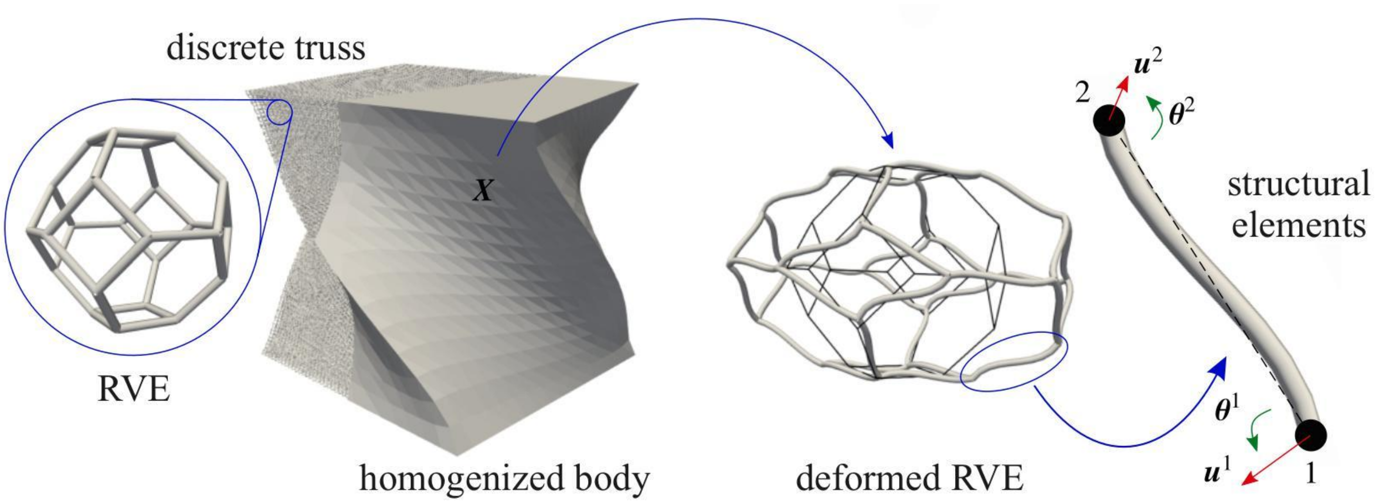


Constitutive response obtained from averaging over all grains, which all experience the same deformation:

$$\langle \boldsymbol{P} \rangle = \frac{1}{V} \int_{\Omega} \boldsymbol{P}(\boldsymbol{X}, \boldsymbol{F}^*) = \frac{1}{V} \sum_i V_i \boldsymbol{P}_i(\boldsymbol{F}^*) = \sum_i v_i \boldsymbol{P}_i(\boldsymbol{F}^*)$$



The nonlocal Cauchy-Born rule - Trusses

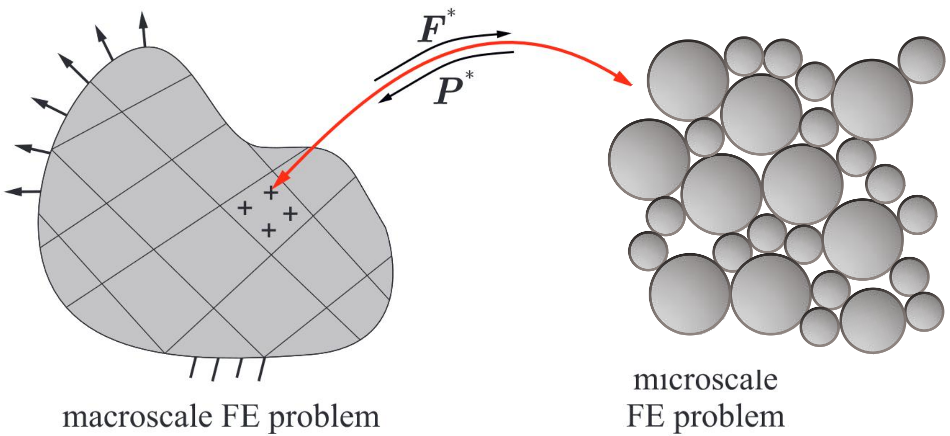


In this case, the need for higher-order terms arise from **rotational degrees of freedom**

$$I[\varphi, \boldsymbol{\theta}] = \int_{\Omega} W(\phi, \boldsymbol{F}, \boldsymbol{\theta}, \boldsymbol{\kappa})\, dV \quad \rightarrow \quad \min$$

Outlook

Discrete Element Modeling and Computational Homogenization



Discussion

That's what I prepared for you today.

What would you like to discuss?

Reading for next class:

Particulate Discrete Element Modeling, C. O'Sullivan

(available from EPFL Library)

Chapters 1-4