

# Homogenization estimates for the macroscopic response and field statistics in viscoplastic polycrystals

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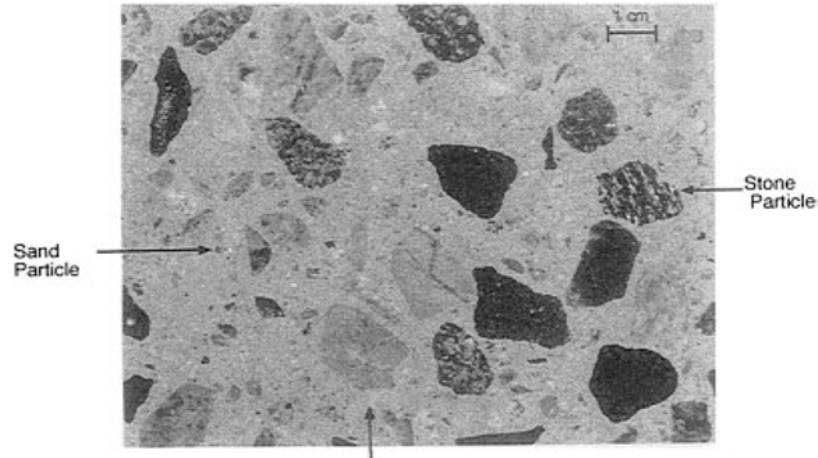
Applied Mathematics and Computational Science

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# MOTIVATION

# Examples of Microstructures

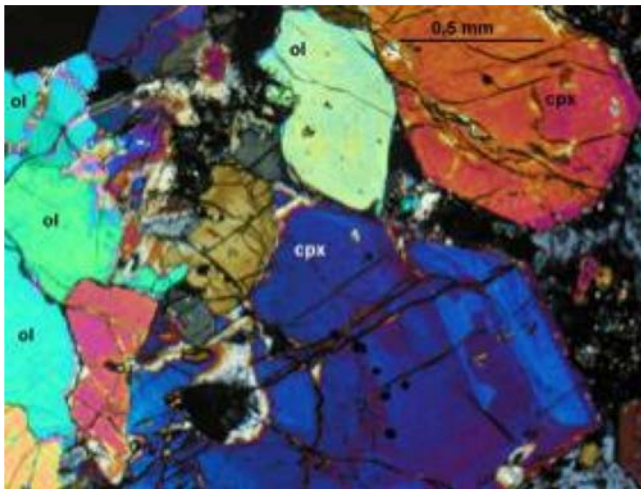
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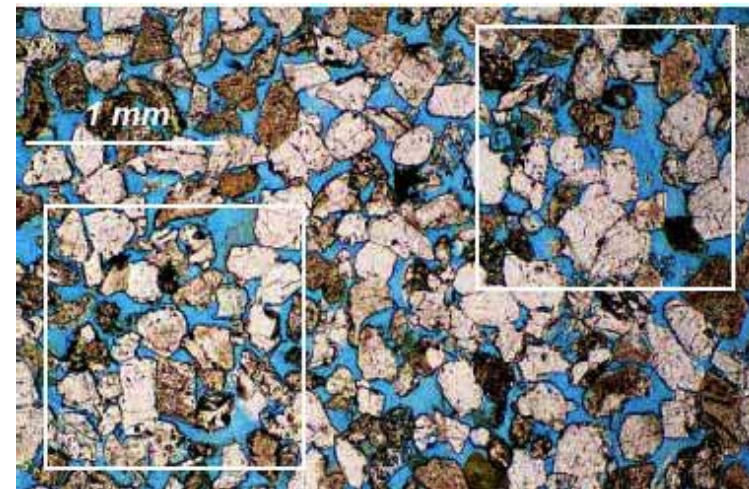
Cement Paste Matrix  
concrete



Polycrystalline ice

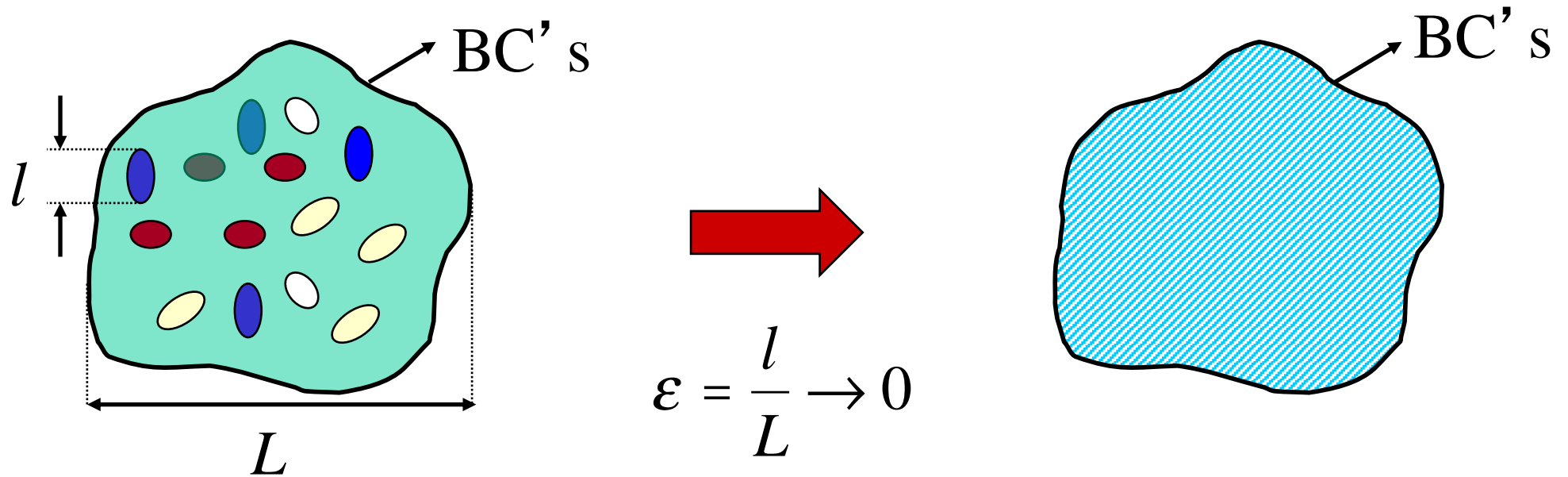


Polycrystalline olivine



Fluid-impregnated sandstone

# Homogenization



- If there is a wide separation of length scales and the boundary conditions vary “slowly” relative to the micro-scale, then an RVE of the composite behaves like a **homogeneous** material with **effective properties** depending on the properties and distribution of the constituent phases (i.e., **microstructure**), but **not** on the specific boundary conditions.

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# BACKGROUND

# Nonlinear Elasticity/Viscoplasticity

- Strain-displacement (strain-rate/velocity) relation

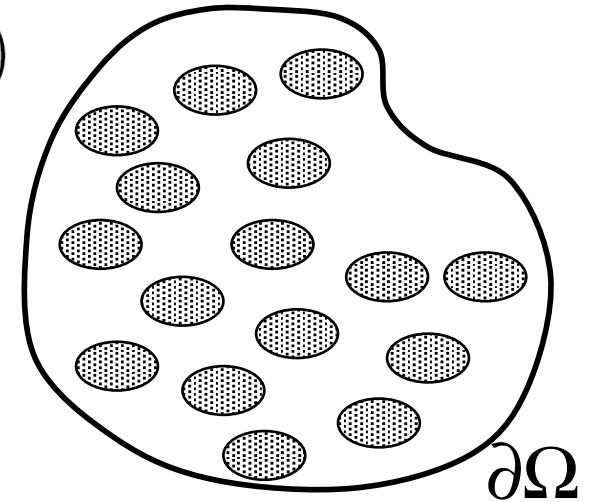
$$\boldsymbol{\varepsilon} = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \quad \varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i})$$

- Equilibrium

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0}, \quad \text{or} \quad \sigma_{ij,j} + b_i = 0$$

- Constitutive relation

$$\boldsymbol{\varepsilon} = \frac{\partial u^{(r)}(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}}$$



Eulerian

where  $u^{(r)}$  is a **convex** stress potential, which may be isotropic or anisotropic

$$u^{(r)}(\boldsymbol{\sigma}) = \phi^{(r)}(\sigma_e) \quad u^{(r)}(\boldsymbol{\sigma}) = \sum_{k=1}^{K^{(r)}} \phi_{(k)}^{(r)}(\tau_{(k)}^{(r)})$$

# Homogenization: Effective Properties

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- *Local* behavior:

$$\boldsymbol{\epsilon} = \frac{\partial u}{\partial \boldsymbol{\sigma}}, \quad u(\mathbf{x}, \boldsymbol{\sigma}) = \sum_{r=1}^N \chi^{(r)}(\mathbf{x}) u^{(r)}(\boldsymbol{\sigma})$$

where the  $\chi^{(r)}$  characterize the microstructure.

- *Effective or macroscopic* behavior:

$$\bar{\boldsymbol{\epsilon}} = \frac{\partial \tilde{U}}{\partial \bar{\boldsymbol{\sigma}}} \quad \tilde{U}(\bar{\boldsymbol{\sigma}}) = \min_{\boldsymbol{\sigma} \in \mathcal{S}} \langle u(\mathbf{x}, \boldsymbol{\sigma}) \rangle$$

where  $\mathcal{S} = \{ \boldsymbol{\sigma}, \operatorname{div} \boldsymbol{\sigma} = \mathbf{0} \text{ in } \Omega, \boldsymbol{\sigma} \mathbf{n} = \bar{\boldsymbol{\sigma}} \mathbf{n} \text{ on } \partial\Omega \}$  and  $\langle \boldsymbol{\sigma} \rangle = \bar{\boldsymbol{\sigma}}$  and  $\bar{\boldsymbol{\epsilon}} = \langle \boldsymbol{\epsilon} \rangle$  are average stress and strain (rate).

Hashin (1964); Hill (1965); Hutchinson (1976); Willis (1983)



# Homogenization: Field Statistics

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- Phase averages:

$$\overline{\boldsymbol{\epsilon}}^{(r)} = \langle \boldsymbol{\epsilon} \rangle^{(r)} \quad \overline{\boldsymbol{\sigma}}^{(r)} = \langle \boldsymbol{\sigma} \rangle^{(r)}$$

- Second moments/covariance tensors:

$$\langle \boldsymbol{\epsilon} \otimes \boldsymbol{\epsilon} \rangle^{(r)} \quad \langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle^{(r)} \quad \mathbb{C}_{\boldsymbol{\sigma}}^{(r)} = \langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle^{(r)} - \overline{\boldsymbol{\sigma}}^{(r)} \otimes \overline{\boldsymbol{\sigma}}^{(r)}$$

- Results can be obtained via identities of the type

$$\overline{\boldsymbol{\sigma}}^{(r)} = \frac{1}{c^{(r)}} \partial_{\boldsymbol{\eta}^{(r)}} \tilde{U}_{\boldsymbol{\eta}} \Big|_{\boldsymbol{\eta}^{(r)} = \mathbf{0}}$$
$$u_{\boldsymbol{\eta}}(\mathbf{x}, \boldsymbol{\sigma}) = \sum_{s=1}^N \chi^{(s)}(\mathbf{x}) u^{(s)}(\boldsymbol{\sigma}) + \chi^{(r)}(\mathbf{x}) \boldsymbol{\eta}^{(r)} \cdot \boldsymbol{\sigma}$$



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# EFFECTIVE BEHAVIOR & FIELD FLUCTUATIONS FOR 3-D, POWER-LAW POLYCRYSTALS

Liu & PC (2004) JMPS

Song & PC (2018) IJP