



Computational homogenization of incompressible microstructures



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Motivation

- Challenge in computational homogenization: Seamless transition of macroscale compressibility \rightarrow incompressibility.
- Practical application: Meltphase sintering of hardmetal products:
Porosity vanishes



Motivation

- Prototype problem (this presentation): Solid phase microstructure with heterogeneous subscale compressibility.
Extreme situation: Uniform incompressibility \rightarrow macroscale incompressibility
- Need for comprehensive variational framework for homogenization.
Reference: Öhman et al. *On the variationally consistent computational homogenization of elasticity in the incompressible limit*. AMSE (2014).
Conditionally accepted

Outline

- Mixed formulation for incompressible elasticity
- Variationally consistent homogenization
- Macroscale problem
- Subscale problem
- Numerical examples
- Conclusions

Fine-scale problem

- Mixed displacement-pressure formulation

$$\begin{aligned} -[\hat{\boldsymbol{\sigma}}_d(\boldsymbol{\epsilon}_d) - p\mathbf{I}] \cdot \boldsymbol{\nabla} &= \mathbf{0} \text{ in } \Omega \\ \hat{e}(p) - \mathbf{u} \cdot \boldsymbol{\nabla} &= 0 \text{ in } \Omega \end{aligned}$$

- Prototype material model: isotropic linear elasticity

$$\begin{aligned} \hat{\boldsymbol{\sigma}}_d(\boldsymbol{\epsilon}_d) &\stackrel{\text{def}}{=} 2G\boldsymbol{\epsilon}_d \\ \hat{\boldsymbol{\sigma}}_d(\boldsymbol{\epsilon}_d) &= \boldsymbol{\sigma} + p\mathbf{I}, \quad \boldsymbol{\epsilon}_d \stackrel{\text{def}}{=} [\mathbf{u} \otimes \boldsymbol{\nabla}]_d^{\text{sym}} \\ \hat{e}(p) &\stackrel{\text{def}}{=} -C p \end{aligned}$$

- In the case of local compressibility, the bulk modulus is $K = C^{-1}$
- Subscript d denotes deviatoric tensor: $\bullet_d = \bullet - \frac{1}{3}[\bullet : \mathbf{I}]\mathbf{I}$

Weak form of “fine-scale” problem

- Find $(\mathbf{u}, p) \in \mathbb{U} \times \mathbb{P}$ such that

$$\int_{\Omega} [\hat{\boldsymbol{\sigma}}_{\text{d}}([\mathbf{u} \otimes \boldsymbol{\nabla}]_{\text{d}}^{\text{sym}}) - p\mathbf{I}] : [\delta \mathbf{u} \otimes \boldsymbol{\nabla}] \, dv = 0 \quad \forall \delta \mathbf{u} \in \mathbb{U}^0$$

$$\int_{\Omega} [\hat{e}(p) - \mathbf{u} \cdot \boldsymbol{\nabla}] \delta p \, dv = 0 \quad \forall \delta p \in \mathbb{P}$$

Variationally Consistent Homogenization (VCH)

- Volume average operators over the RVE-window Ω_{\square}

$$\langle \bullet \rangle_{\square} \stackrel{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \int_{\Omega_{\square}} \bullet \, dV$$

- Decompose the fields into macroscopic and fluctuating parts:

$$\mathbf{u} = \mathbf{u}^{\text{M}} + \mathbf{u}^{\text{s}}$$

$$p = p^{\text{M}} + p^{\text{s}}$$

- Variationally Consistent Homogenization \leadsto macroscale problem
- Generalized Hill-Mandel condition \leadsto subscale modeling requirements

Variationally Consistent Homogenization (VCH)

- First order Taylor expansion of the displacement, and zeroth order expansion of the pressure

$$\begin{aligned}\mathbf{u}^M &= \bar{\mathbf{u}} + [\bar{\mathbf{u}} \otimes \nabla] \cdot [\mathbf{x} - \bar{\mathbf{x}}] \\ p^M &= \bar{p}\end{aligned}$$

where $(\bar{\mathbf{u}}, \bar{p})$ are macroscale fields with induced regularity requirements.

- Constraints on the fluctuations \mathbf{u}^s and p^s within each RVE via the conditions

$$\begin{aligned}\langle \mathbf{u} \otimes \nabla \rangle_{\square} &= \bar{\mathbf{u}} \otimes \nabla \\ \langle p \rangle_{\square} &= \bar{p}\end{aligned}$$

Macroscale problem

- Find $(\bar{\mathbf{u}}, \bar{p}) \in \bar{\mathcal{U}} \times \bar{\mathcal{P}}$ such that

$$\int_{\Omega} [\bar{\boldsymbol{\sigma}}_d \{\bar{\boldsymbol{\epsilon}}_d, \bar{p}\} - \bar{p} \mathbf{I}] : [\delta \bar{\mathbf{u}} \otimes \nabla] dV = 0 \quad \forall \delta \bar{\mathbf{u}} \in \bar{\mathcal{U}}^0$$

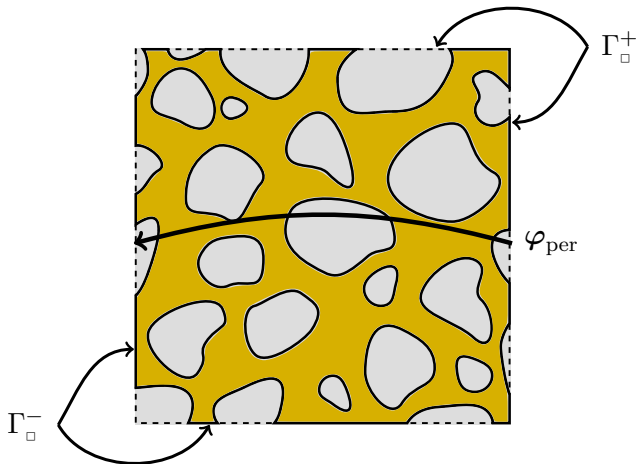
$$\int_{\Omega} [-\bar{\mathbf{u}} \cdot \nabla + \bar{e} \{\bar{\boldsymbol{\epsilon}}_d, \bar{p}\}] \delta \bar{p} dV = 0 \quad \forall \delta \bar{p} \in \bar{\mathcal{P}}$$

- RVE-input: $\bar{\boldsymbol{\epsilon}}_d \stackrel{\text{def}}{=} [\bar{\mathbf{u}} \otimes \nabla]_d^{\text{sym}}$ and \bar{p} .
- Homogenized response variables identified as

$$\bar{\boldsymbol{\sigma}}_d \stackrel{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \left[\int_{\Gamma_{\square}} \mathbf{t} \otimes [\mathbf{x} - \bar{\mathbf{x}}] dS \right]_d$$

$$\bar{e} \stackrel{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}} \mathbf{u} \cdot \mathbf{n} dS$$

Weak periodicity on RVE



- $\llbracket \bullet \rrbracket$ = difference of \bullet between Γ_{\square}^{+} and Γ_{\square}^{-} (mirror point)

RVE problem — Weakly Periodic b.c.

- For given macroscale variables $\bar{\epsilon}_d$ and \bar{p} , find $(\mathbf{u}, p, \mathbf{t}, \bar{e}) \in \mathbb{U}_\square \times \mathbb{P}_\square \times \mathbb{T}_\square \times \mathbb{R}$ that solve the system

$$\int_{\Omega_\square} [\hat{\boldsymbol{\sigma}}_d([\mathbf{u} \otimes \nabla]_d^{\text{sym}}) - p\mathbf{I}] : [\delta \mathbf{u} \otimes \nabla] dV - \int_{\Gamma_\square^+} \mathbf{t} \cdot \llbracket \delta \mathbf{u} \rrbracket dS = 0$$

$$\forall \delta \mathbf{u} \in \mathbb{U}_\square$$

$$\int_{\Omega_\square} -\delta p [\mathbf{u} \cdot \nabla - \hat{e}(p)] dV = 0$$

$$\forall \delta p \in \mathbb{P}_\square$$

$$-\int_{\Gamma_\square^+} \delta \mathbf{t} \cdot \llbracket \mathbf{u} - \bar{e} \frac{1}{3} \mathbf{x} \rrbracket dS = -\int_{\Gamma_\square^+} \delta \mathbf{t} \cdot \llbracket \bar{\epsilon}_d \cdot \mathbf{x} \rrbracket dS$$

$$\forall \delta \mathbf{t} \in \mathbb{T}_\square$$

$$\int_{\Gamma_\square^+} \mathbf{t} \cdot \llbracket \frac{1}{3} \mathbf{x} \rrbracket dS \delta \bar{e} = -\bar{p} \delta \bar{e}$$

$$\forall \delta \bar{e} \in \mathbb{R}$$

Pore space and surface tension

- Volume average operators over the particles $\Omega_{\square}^{\text{part}}$ inside the RVE-window Ω_{\square} :

$$\langle \bullet \rangle_{\square} \stackrel{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \int_{\Omega_{\square}^{\text{part}}} \bullet \, dV, \quad \Omega_{\square}^{\text{part}} \stackrel{\text{def}}{=} \Omega_{\square} \cap \Omega^{\text{part}}$$

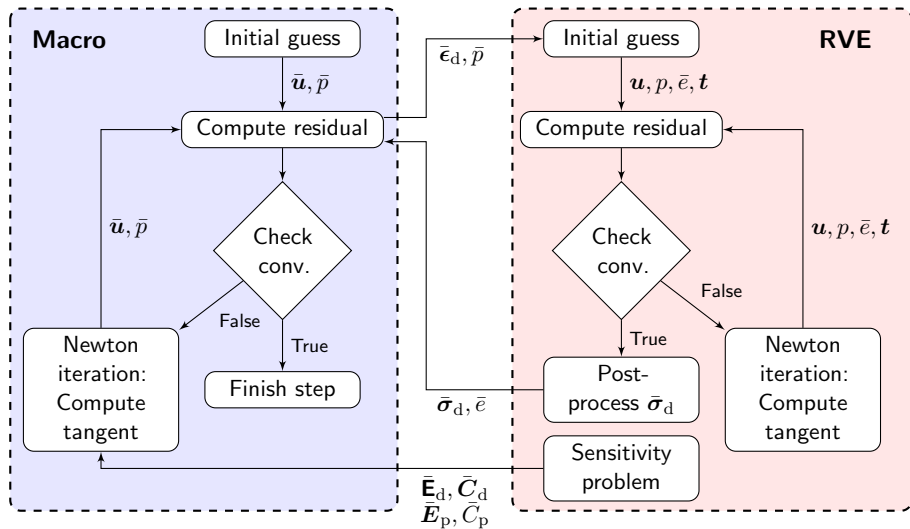
$$\langle\langle \bullet \rangle\rangle_{\square} \stackrel{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}^{\text{pore}}} \bullet \, dS, \quad \Gamma_{\square}^{\text{pore}} \stackrel{\text{def}}{=} \Omega_{\square} \cap \Gamma^{\text{pore}}$$

- For scale transitions, we choose the expansion and constraints

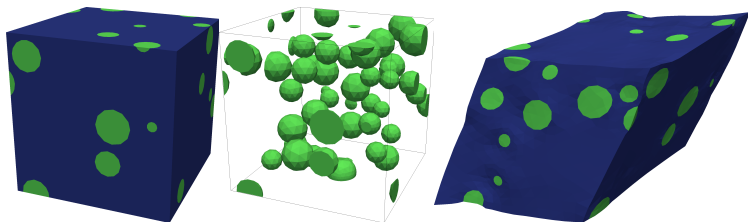
$$\mathbf{u}^{\text{M}} = \bar{\mathbf{u}} + [\bar{\mathbf{u}} \otimes \nabla] \cdot [\mathbf{x} - \bar{\mathbf{x}}], \quad \frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}} \mathbf{u} \otimes \mathbf{n} \, dA = \bar{\mathbf{u}} \otimes \nabla$$

$$p^{\text{M}} = \frac{|\Omega_{\square}|}{|\Omega_{\square}^{\text{part}}|} [\bar{p} + \frac{2}{3} \langle\langle \gamma_s \rangle\rangle_{\square}], \quad -\frac{1}{3} \frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}} \mathbf{t} \cdot [\mathbf{x} - \bar{\mathbf{x}}] \, dA = \bar{p}$$

- Note:** With pores, \bar{e} is generally nonzero even if $\hat{e}(p) = 0$.

FE² summarized

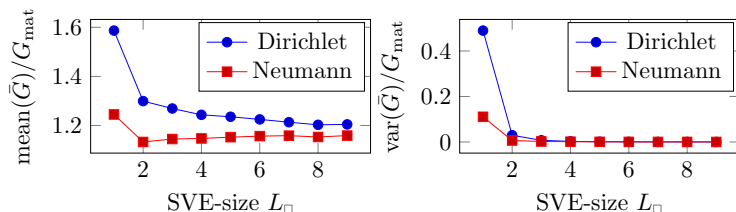
Numerical examples



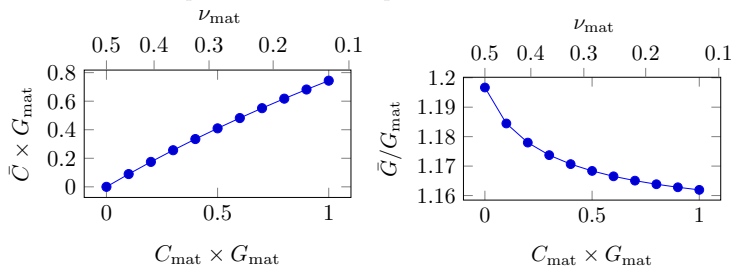
$$\hat{\sigma}_d(\epsilon_d) = 2G\epsilon_d$$

$$\hat{e}(p) = -Cp = -\frac{1}{K}p$$

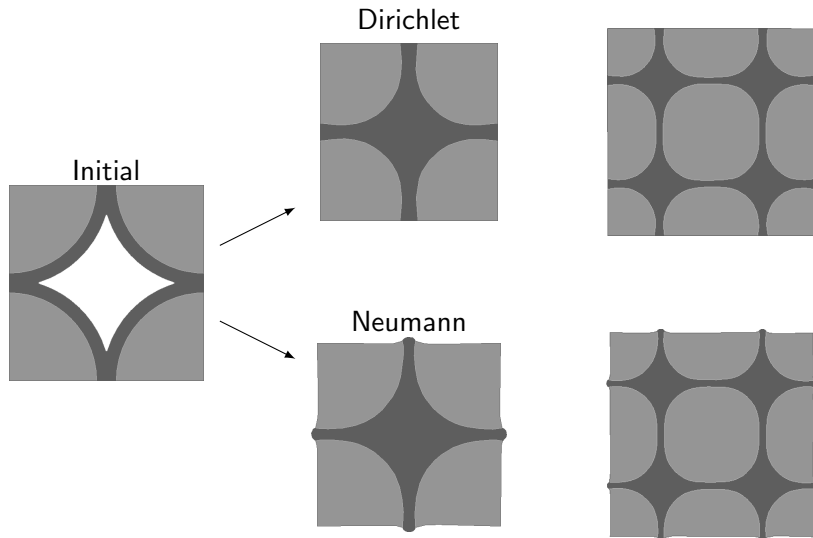
Numerical examples



$$G_{\text{part}} = 5G_{\text{mat}}, C_{\text{part}} = C_{\text{mat}} = 0$$



$$G_{\text{part}} = 5G_{\text{mat}}, C_{\text{part}} = 0$$

Numerical examples of free sintering ($\bar{p} = 0$)

Conclusions

- Multiscale problem derived from fine-scale problem with VCH
- Seamless transition to macroscopic incompressibility
- Methodology can include pores and surface tension (surface tension not shown in this presentation)
- Implementation of RVE boundary conditions is available in the open source code OOFEM www.oofem.org