Computational homogenization of incompressible microstructures

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2014-08-29

Motivation

- Challenge in computational homogenization: Seamless transition of macroscale compressibility → incompressibility.
- Practical application: Meltphase sintering of hardmetal producs: 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

$$-[\hat{\boldsymbol{\sigma}}_{\mathrm{d}}(\boldsymbol{\epsilon}_{\mathrm{d}}) - p\boldsymbol{I}] \cdot \boldsymbol{\nabla} = \boldsymbol{0} \text{ in } \Omega$$
$$\hat{e}(p) - \boldsymbol{u} \cdot \boldsymbol{\nabla} = 0 \text{ in } \Omega$$

- Prototype material model: isotropic linear elasticity

$$\hat{\boldsymbol{\sigma}}_{\mathrm{d}}(\boldsymbol{\epsilon}_{\mathrm{d}}) \stackrel{\mathrm{def}}{=} 2G\boldsymbol{\epsilon}_{\mathrm{d}}$$
$$\hat{\boldsymbol{\sigma}}_{\mathrm{d}}(\boldsymbol{\epsilon}_{\mathrm{d}}) = \boldsymbol{\sigma} + p\boldsymbol{I}, \quad \boldsymbol{\epsilon}_{\mathrm{d}} \stackrel{\mathrm{def}}{=} [\boldsymbol{u} \otimes \boldsymbol{\nabla}]_{\mathrm{d}}^{\mathrm{sym}}$$
$$\hat{e}(p) \stackrel{\mathrm{def}}{=} -C\,p$$

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

Weak form of "fine-scale" problem

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

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

$$\int_\Omega [\hat{e}(p) - \boldsymbol{u} \cdot \boldsymbol{\nabla}]\delta p\,\mathrm{d}v = 0 \qquad \forall \delta p \in \mathbb{P}$$

Variationally Consistent Homogenization (VCH)

- Volume average operators over the RVE-window $\Omega_\square$

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

- Decompose the fields into macroscopic and fluctuating parts:

$$\boldsymbol{u} = \boldsymbol{u}^{\mathrm{M}} + \boldsymbol{u}^{\mathrm{s}}$$
$$p = p^{\mathrm{M}} + p^{\mathrm{s}}$$

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

Variationally Consistent Homogenization (VCH)

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

$$\boldsymbol{u}^{\mathrm{M}} = \bar{\boldsymbol{u}} + [\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}] \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]$$
$$p^{\mathrm{M}} = \bar{p}$$

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

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

$$\langle \boldsymbol{u} \otimes \boldsymbol{\nabla} \rangle_{\square} = \bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}$$
$$\langle p \rangle_{\square} = \bar{p}$$

Macroscale problem

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

$$\int_{\Omega} [\bar{\boldsymbol{\sigma}}_{\mathrm{d}}\{\bar{\boldsymbol{\epsilon}}_{\mathrm{d}}, \bar{p}\} - \bar{p}\boldsymbol{I}] : [\delta\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}] \,\mathrm{d}V = 0 \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0$$

$$\int_{\Omega} [-\bar{\boldsymbol{u}} \cdot \boldsymbol{\nabla} + \bar{e}\{\bar{\boldsymbol{\epsilon}}_{\mathrm{d}}, \bar{p}\}]\delta\bar{p} \,\mathrm{d}V = 0 \quad \forall \delta\bar{p} \in \bar{\mathbb{P}}$$

- RVE-input: $\bar{\boldsymbol{\epsilon}}_{\mathrm{d}} \overset{\text{def}}{=} [\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}]_{\mathrm{d}}^{\mathrm{sym}}$ and $\bar{p}$.

- Homogenized response variables identified as

$$\bar{\boldsymbol{\sigma}}_{\mathrm{d}} \overset{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \left[\int_{\Gamma_{\square}} \boldsymbol{t} \otimes [\boldsymbol{x} - \bar{\boldsymbol{x}}] \,\mathrm{d}S \right]_{\mathrm{d}}$$

$$\bar{e} \overset{\text{def}}{=} \frac{1}{|\Omega_{\square}|} \int_{\Gamma_{\square}} \boldsymbol{u} \cdot \boldsymbol{n} \,\mathrm{d}S$$

Weak periodicity on RVE
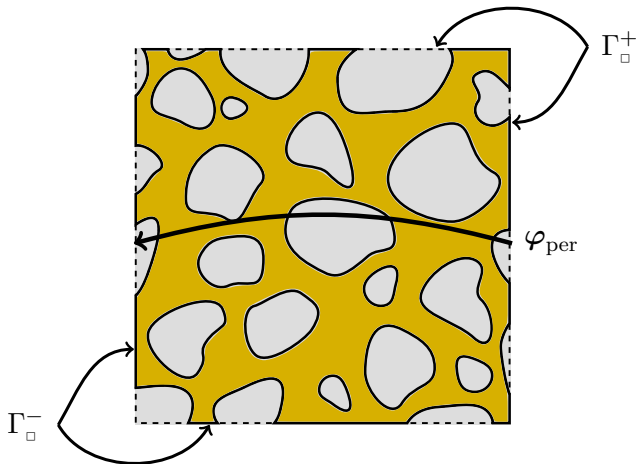
- $[\![\bullet]\!]$ = difference of $\bullet$ between $\Gamma_\square^+$ and $\Gamma_\square^-$ (mirror point)

RVE problem — Weakly Periodic b.c.

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

$$\int_{\Omega_{\square}} [\hat{\boldsymbol{\sigma}}_{\mathrm{d}}([\boldsymbol{u} \otimes \boldsymbol{\nabla}]_{\mathrm{d}}^{\mathrm{sym}}) - p\boldsymbol{I}] : [\delta\boldsymbol{u} \otimes \boldsymbol{\nabla}] \, \mathrm{d}V - \int_{\Gamma_{\square}^+} \boldsymbol{t} \cdot [\![\delta\boldsymbol{u}]\!] \, \mathrm{d}S = 0$$

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

$$\int_{\Omega_{\square}} -\delta p [\boldsymbol{u} \cdot \boldsymbol{\nabla} - \hat{e}(p)] \, \mathrm{d}V = 0 \qquad\qquad \forall \, \delta p \in \mathbb{P}_{\square}$$

$$-\int_{\Gamma_{\square}^+} \delta\boldsymbol{t} \cdot [\![\boldsymbol{u} - \bar{e}\frac{1}{3}\boldsymbol{x}]\!] \, \mathrm{d}S = -\int_{\Gamma_{\square}^+} \delta\boldsymbol{t} \cdot [\![\bar{\boldsymbol{\epsilon}}_{\mathrm{d}} \cdot \boldsymbol{x}]\!] \, \mathrm{d}S \qquad \forall \, \delta\boldsymbol{t} \in \mathbb{T}_{\square}$$

$$\int_{\Gamma_{\square}^+} \boldsymbol{t} \cdot [\![\frac{1}{3}\boldsymbol{x}]\!] \, \mathrm{d}S \, \delta\bar{e} = -\bar{p}\,\delta\bar{e} \qquad\qquad \forall \, \delta\bar{e} \in \mathbb{R}$$

Pore space and surface tension

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

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

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

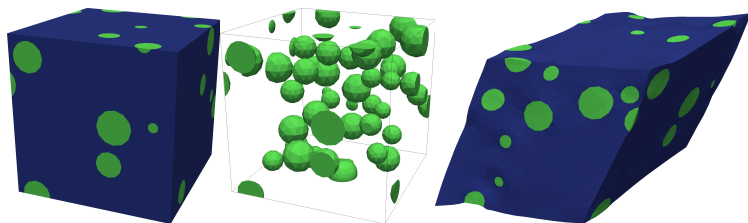- For scale transitions, we choose the expansion and constraints

$$\boldsymbol{u}^{\mathrm{M}} = \bar{\boldsymbol{u}} + [\bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}] \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}], \qquad \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{u} \otimes \boldsymbol{n} \, \mathrm{d}A = \bar{\boldsymbol{u}} \otimes \boldsymbol{\nabla}$$

$$p^{\mathrm{M}} = \frac{|\Omega_\square|}{|\Omega_\square^{\mathrm{part}}|} [\bar{p} + \frac{2}{3} \langle\!\langle \gamma_{\mathrm{s}} \rangle\!\rangle_\square], \qquad -\frac{1}{3}\frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \, \mathrm{d}A = \bar{p}$$

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

FE^2 summarized
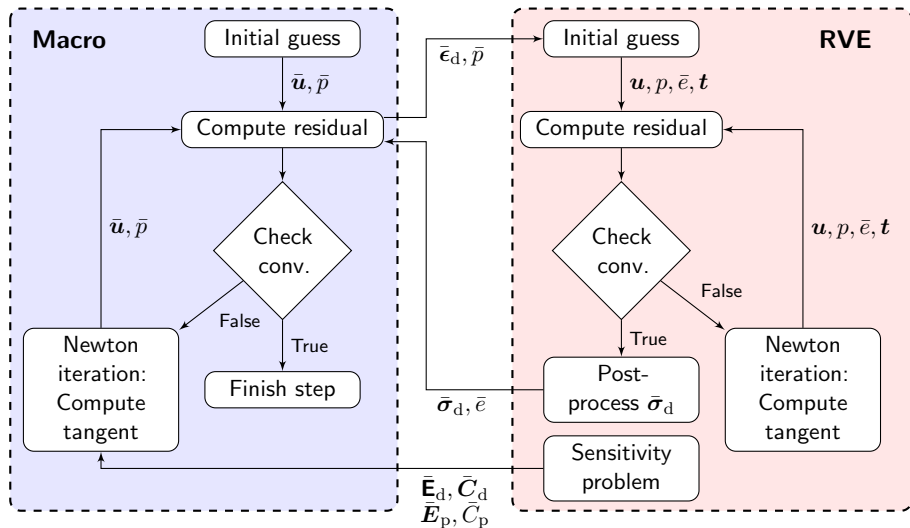
Numerical examples
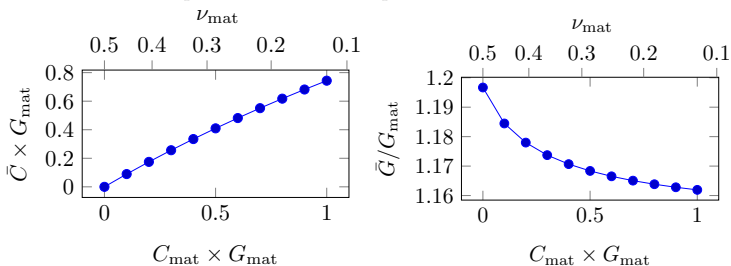

$$\hat{\boldsymbol{\sigma}}_{\mathrm{d}}(\boldsymbol{\epsilon}_{\mathrm{d}}) = 2G\boldsymbol{\epsilon}_{\mathrm{d}}$$

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

Numerical examples
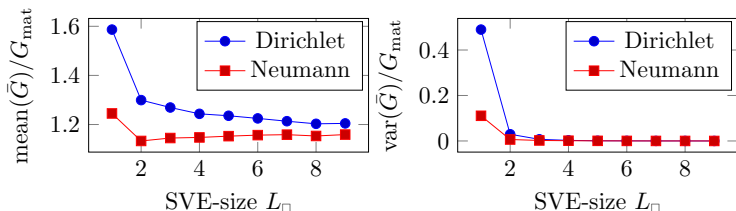
$$G_{\mathrm{part}} = 5G_{\mathrm{mat}},\ C_{\mathrm{part}} = C_{\mathrm{mat}} = 0$$

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

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

Initial

Dirichlet

Neumann

CHALMERS
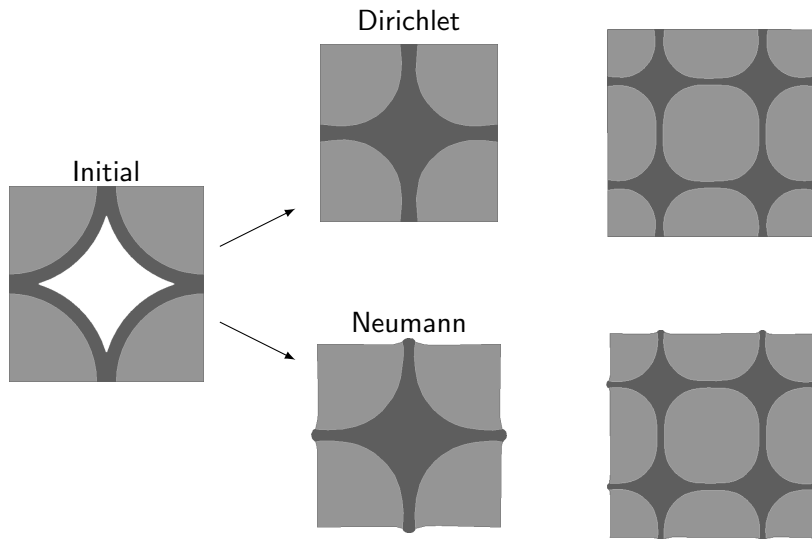
Conclusions

- 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