On computational modeling of sintering based on homogenization

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2014-07-22

Motivation

- Challenge in computational homogenization: Seamless transition of macroscale compressibility $\rightarrow$ 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

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

- Prototype material model: isotropic linear elasticity

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

$$\hat{\boldsymbol{\sigma}}_{\mathrm{d}}(\boldsymbol{\epsilon}_{\mathrm{d}}) = \boldsymbol{\sigma} + p\boldsymbol{I}, \quad \boldsymbol{\epsilon}_{\mathrm{d}} \overset{\text{def}}{=} [\boldsymbol{u} \otimes \boldsymbol{\nabla}]_{\mathrm{d}}^{\mathrm{sym}}$$

$$\hat{e}(p) \overset{\text{def}}{=} -C\,p$$

- 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 $\Omega_\square$

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

- 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

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

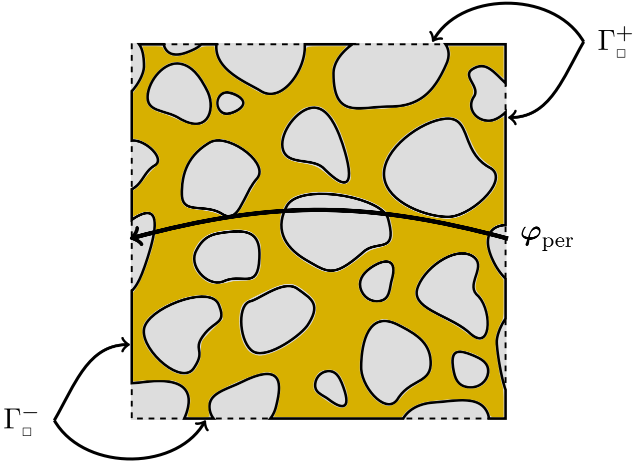
$$\int_\Omega [-\bar{\boldsymbol{u}} \cdot \boldsymbol{\nabla} + \bar{e}\{\bar{\boldsymbol{\epsilon}}_\mathrm{d}, \bar{p}\}] \delta\bar{p} \,\mathrm{d}V = 0 \quad \forall \delta\bar{p} \in \bar{\mathbb{P}}$$

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

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

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

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

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

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

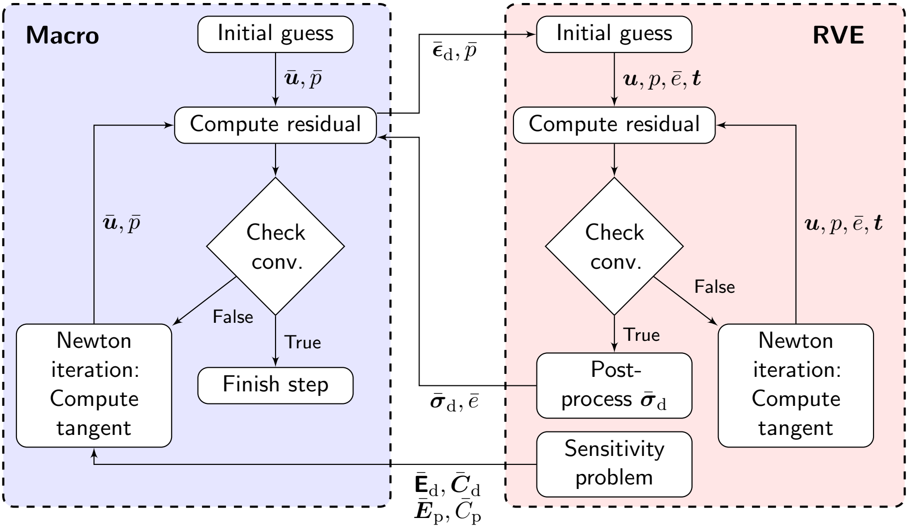
$$-\int_{\Gamma_\square^+} \delta\boldsymbol{t} \cdot [\![\boldsymbol{u} - \bar{e}\frac{1}{3}\boldsymbol{x}]\!] \,\mathrm{d}S = -\int_{\Gamma_\square^+} \delta\boldsymbol{t} \cdot [\![\bar{\boldsymbol{\epsilon}}_\mathrm{d} \cdot \boldsymbol{x}]\!] \,\mathrm{d}S \qquad \forall\, \delta\boldsymbol{t} \in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

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

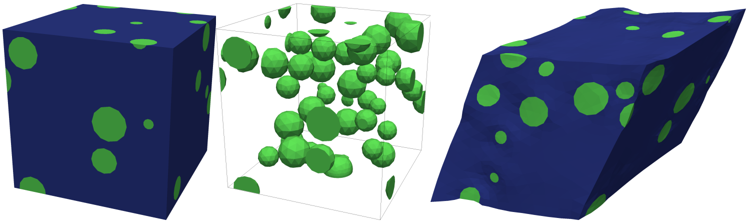
RVE problem

- For given macroscale variables $\bar{\boldsymbol{\epsilon}}_{\mathrm{d}}$ and $\bar{p}$, obtain $\bar{\boldsymbol{\sigma}}_{\mathrm{d}}$ and $\bar{e}$ as output from the RVE problem:
  - Dirichlet b.c.: find $(\boldsymbol{u}, p, \bar{e}) \in \mathbb{U}_{\square}^{D'} \times \mathbb{P}_{\square} \times \mathbb{R}$
    - Note: $\bar{e}$ (volumetric part of macroscopic strain) is not controlled.
    - $\bar{\boldsymbol{\sigma}}_{\mathrm{d}}$ is obtained from post-processing reaction forces on RVE-boundary.
  - Neumann b.c.: find $(\boldsymbol{u}, p, \bar{\boldsymbol{\sigma}}_{\mathrm{d}}) \in \mathbb{U}_{\square} \times \mathbb{P}_{\square} \times \mathbb{R}_{\mathrm{d}}^{3\times 3}$.
    - Note: $\bar{p}$ (volumetric part of macroscopic stress) is controlled.
    - $\bar{e}$ is obtained from post-processing displacements on RVE-boundary.
- Remarks:
  - Dirichlet/Neumann b.c. represent upper/lower bound of macroscale strain energy
  - Weakly periodic b.c. has been enforced approximately by polynomial basis for tractions in $\mathbb{T}_{\square}$ (costly, implemented but no results shown in this presentation).

FE^2 summarized



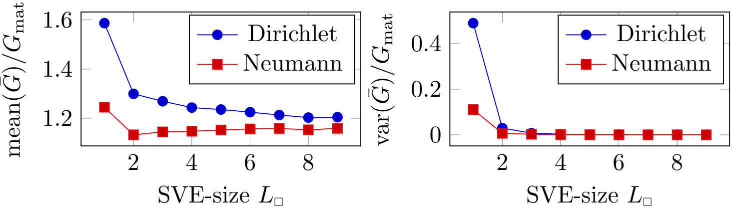
Numerical examples



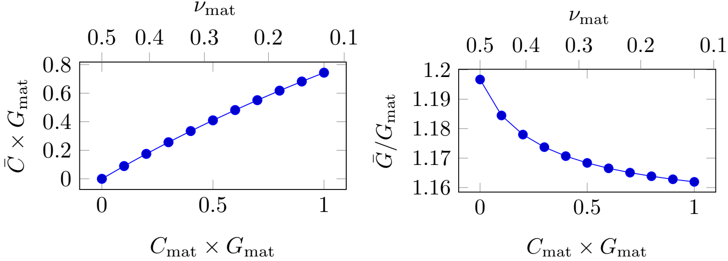
$$\hat{\boldsymbol{\sigma}}_{\mathrm{d}}(\boldsymbol{\epsilon}_{\mathrm{d}}) = 2G\boldsymbol{\epsilon}_{\mathrm{d}}$$

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

Numerical examples



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



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

Conclusions

- Multiscale problem derived from fine-scale problem with VCH
- Seamless transition to macroscopic incompressibility
- Methodology is extendable to include pores and surface tension
- Implementation of RVE boundary conditions is available in the open source code OOFEM `www.oofem.org`