Computational homogenization of incompressible microstructures

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Outline

- Mixed formulation for incompressible elasticity
- Problem with traditional boundary conditions
- Macroscale problem
- Weakly periodic boundary condition
- Conclusions

Fine-scale problem

- Mixed displacement-pressure formulation

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

- Example material model, isotropic linear elasticity

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

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

$$
\hat{e}(p) \stackrel{\mathrm{def}}{=} -C\,p
$$

- For compressible cases, 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

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

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

Problem with classical boundary conditions

- As $C \to 0$, the volumetric part of the macroscopic strain can no longer be controlled in an RVE. Classical (Dirichlet and Neumann) boundary conditions for homogenization breaks down.
- Solution presented:

Mikael Öhman, Kenneth Runesson, and Fredrik Larsson.
On the variationally consistent computational homogenization of elasticity in the incompressible limit.
Advanced Modeling and Simulation in Engineering Sciences (2014).
Under review

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

Variationally Consistent Macrohomogenity Condition

- Variationally Consistent Macrohomogeneity condition (VCMC):

$$
\begin{tikzcd}
\min\limits_{z} \Pi(z) \arrow[r, "\text{(I)}", "\text{stat}"'] \arrow[d, "\text{VCH}"', "\text{(II)}"] & \Pi'(z;\delta z) = 0 \quad \forall \delta z \arrow[d, "\text{VCH}"', "\text{(I)}"] \\
\min\limits_{\bar{z}} \bar{\Pi}\{\bar{z}\} \arrow[r, "\text{(II)}", "\text{stat+VCMC}"'] & \bar{\Pi}'\{\bar{z};\delta\bar{z}\} = \bar{R}\{\bar{z};\delta\bar{z}\} = 0 \quad \forall \delta\bar{z}
\end{tikzcd}
$$

- $\rightsquigarrow$ restrictions on microscale boundary conditions
- $z = (\boldsymbol{u}, p)$
- A generalized Hill-Mandel condition

Hierarchical split

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

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

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

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

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

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

RVE problem — Weakly Periodic b.c.

- For given macroscale variables $\bar{\epsilon}_{\mathrm{d}}$ 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

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

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

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

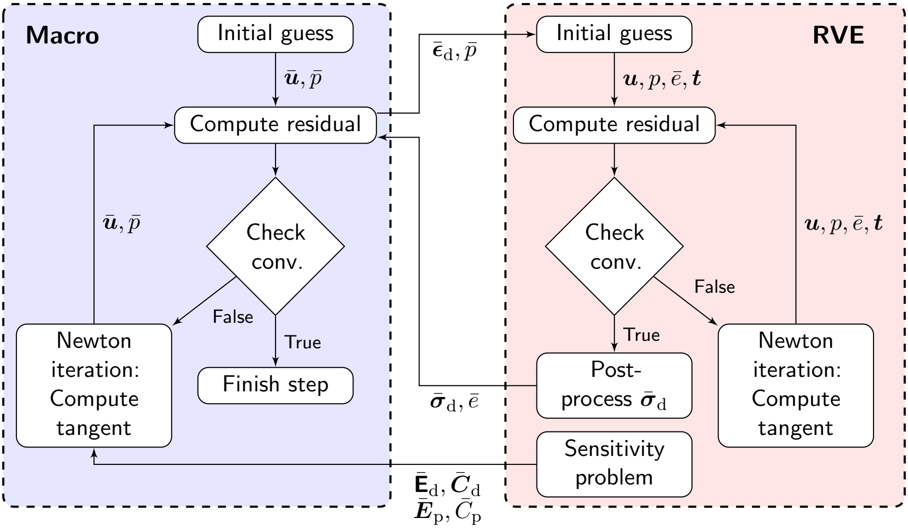
$$\int_{\Gamma^+_{\square}} \boldsymbol{t} \cdot [\![\frac{1}{3}\boldsymbol{x}]\!] \,\mathrm{d}S \,\delta\bar{e} = -\bar{p}\,\delta\bar{e} \qquad \forall\, \delta\bar{e} \in \mathbb{R}$$

- $[\![\bullet]\!]$ = difference of $\bullet$ between $\Gamma^+_{\square}$ and $\Gamma^-_{\square}$ (mirror point)

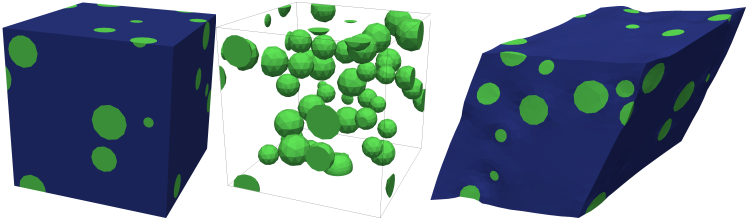
RVE problem — Dirichlet and Neumann b.c.

- For given macroscale variables $\bar{\boldsymbol{\epsilon}}_{\mathrm{d}}$ and $\bar{p}$ obtain $\bar{\boldsymbol{\sigma}}_{\mathrm{d}}$ and $\bar{e}$:
  - Dirichlet b.c.: find $(\boldsymbol{u}, p, \bar{e}) \in \mathbb{U}'_{\square} \times \mathbb{P}_{\square} \times \mathbb{R}$
    - Similar implementation to traditional Dirichlet b.c. only $\bar{e}$ is not controlled.
    - $\bar{\boldsymbol{\sigma}}_{\mathrm{d}}$ response is post-processed reaction forces on RVE-boundary.
  - Neumann b.c.: find $(\boldsymbol{u}, p, \bar{\boldsymbol{\sigma}}_{\mathrm{d}}) \in \mathbb{U}_{\square} \times \mathbb{P}_{\square} \times \mathbb{R}^{3\times 3}_{\mathrm{d}}$.
    - Similar implementation to traditional Neumann b.c. only $\bar{p}$ is controlled.
    - $\bar{e}$ response is post-processed from displacement on RVE-boundary.

FE^2 summarized



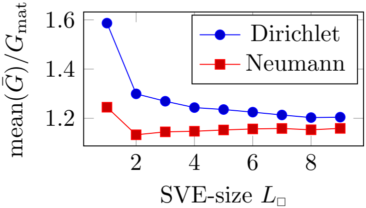
Statistical Volume Element (SVE)

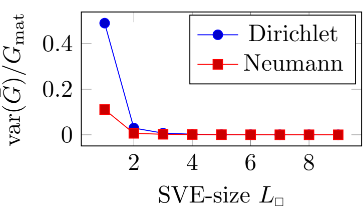


$$\hat{\boldsymbol{\sigma}}_{\mathrm{d}}(\boldsymbol{\epsilon}_{\mathrm{d}}) = 2G\boldsymbol{\epsilon}_{\mathrm{d}}$$

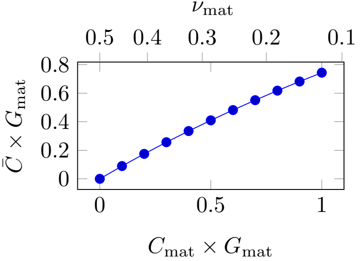
$$\hat{e}(p) = -Cp = -\frac{1}{K}p$$

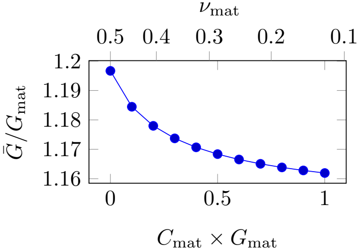
Homogenized shear and bulk modulus





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





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

Conclusions

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