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Computational homogenization of higher-order continua

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Introduction

Additive manufacturing allows for lightweight construction of sophisticated geometries using complex micro-morphologies, changing the macro-properties of the produced parts. To simulate such materials, multiscale methods are required. Here, we introduce a novel computational framework for the multiscale simulation of higher-order continua that allows for the consideration of first-, second-, and third-order effects at micro- and macro-level. In line with classical two-scale approaches, we describe the microstructure via representative volume elements that are attached to each integration point of the macroscopic problem.

Mesoscopic boundary value problem for second-gradient media

We start with the mapping for the microscopic relative position of the material points $\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X})$ using the macro values $\bar{\boldsymbol{F}} = \nabla\bar{\boldsymbol{\varphi}}$ and $\bar{\mathfrak{F}} = \nabla^2\bar{\boldsymbol{\varphi}}$ and obtain

$$\boldsymbol{\varphi}(\boldsymbol{X}) = \bar{\boldsymbol{F}}\,\boldsymbol{X} + \frac{1}{2}\bar{\mathfrak{F}} : (\boldsymbol{X}\otimes\boldsymbol{X}) + \tilde{\boldsymbol{w}}\,.$$

Here, $\tilde{\boldsymbol{w}}$ describes the unknown microscopic fluctuation field, which includes all higher-order terms of the Taylor series expansion.

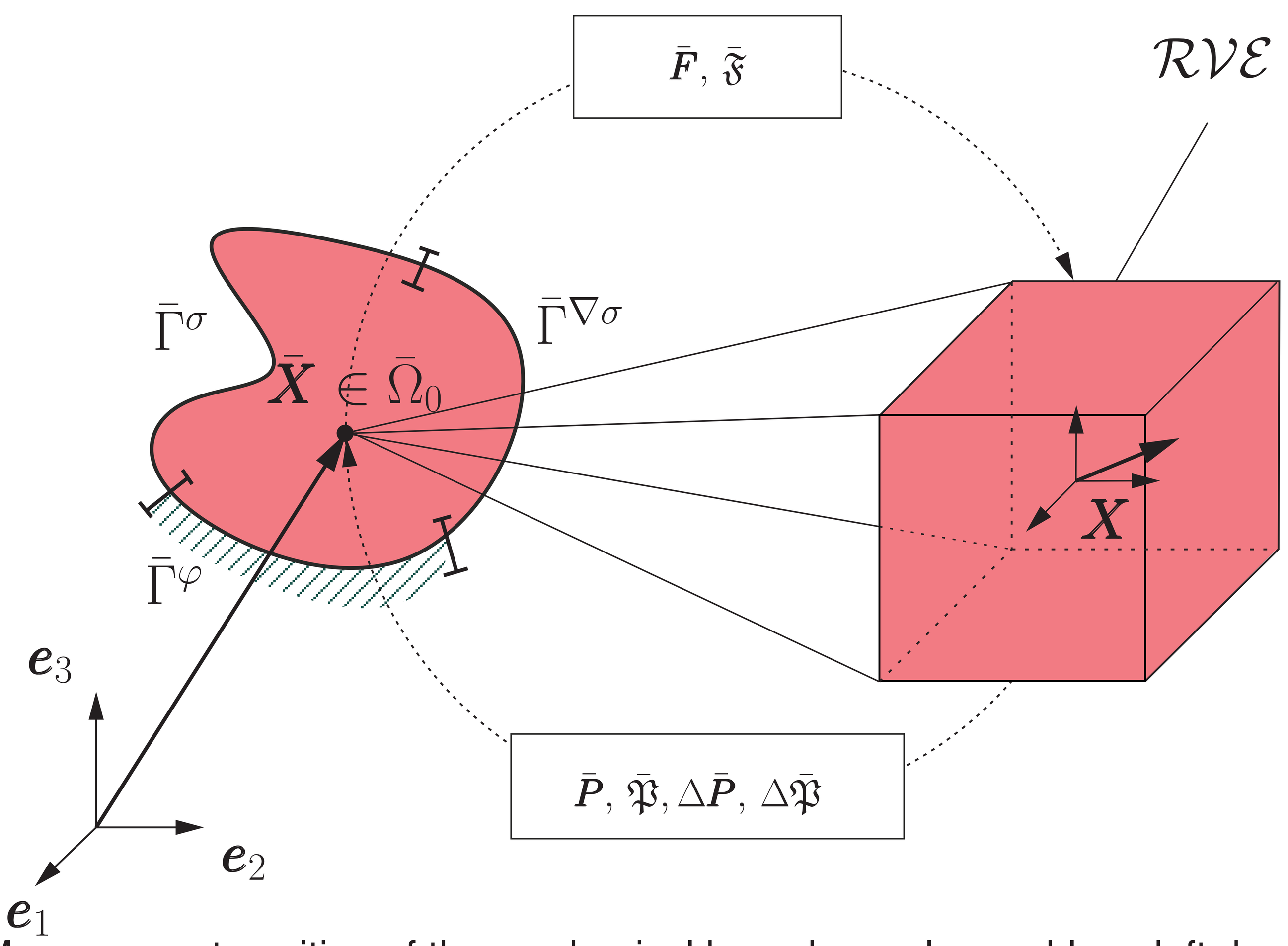

Figure: Meso-macro transition of the mechanical boundary value problem, left: boundary decomposition of the macroscopic continuum in Dirichlet boundaries $\bar{\Gamma}^{\varphi}$ and Neumann boundaries $\bar{\Gamma}^{\sigma}$, $\bar{\Gamma}^{\nabla\sigma}$ of the traction force and the hyperstress traction force, right: $\mathcal{RVE}$ as defined for every macroscopic point.

Third-gradient media

Energetic criterion for equal virtual work of the macro- and microscale

$$\frac{1}{V}\int_{\mathcal{RVE}} \left(\boldsymbol{P} : \nabla\delta\boldsymbol{\varphi} + \mathfrak{P} \,\vdots\, \nabla^2\delta\boldsymbol{\varphi}\right)\,\mathrm{d}V = \bar{\boldsymbol{P}} : \delta\bar{\boldsymbol{F}} + \bar{\mathfrak{P}} \,\vdots\, \delta\bar{\mathfrak{F}} + \bar{\mathbb{P}} :: \delta\bar{\mathbb{F}}\,.$$

where $\bar{\mathbb{F}} = \nabla^3\bar{\boldsymbol{\varphi}}$. The mapping of the microscopic position reads

$$\boldsymbol{\varphi}(\boldsymbol{X}) = \bar{\boldsymbol{F}}\,\boldsymbol{X} + \frac{1}{2}\bar{\mathfrak{F}} : (\boldsymbol{X}\otimes\boldsymbol{X}) + \frac{1}{6}\bar{\mathbb{F}} \,\vdots\, (\boldsymbol{X}\otimes\boldsymbol{X}\otimes\boldsymbol{X}) + \tilde{\boldsymbol{w}}\,.$$

Insertion yields the relations

$$\bar{\boldsymbol{P}} = \frac{1}{V}\int_{\mathcal{RVE}} \boldsymbol{P}\;\mathrm{d}V, \quad \bar{\mathfrak{P}} = \underbrace{\frac{1}{V}\int_{\mathcal{RVE}} \boldsymbol{P}\otimes\boldsymbol{X}\;\mathrm{d}V}_{\bar{\mathfrak{P}}^{P}} + \underbrace{\frac{1}{V}\int_{\mathcal{RVE}} \mathfrak{P}\;\mathrm{d}V}_{\bar{\mathfrak{P}}^{\mathfrak{P}}},$$

$$\bar{\mathbb{P}} = \underbrace{\frac{1}{V}\int_{\mathcal{RVE}} \frac{1}{2}\boldsymbol{P}\otimes\boldsymbol{X}\otimes\boldsymbol{X}\;\mathrm{d}V}_{\bar{\mathbb{P}}^{P}} + \underbrace{\frac{1}{V}\int_{\mathcal{RVE}} \mathfrak{P}\otimes\boldsymbol{X}\;\mathrm{d}V}_{\bar{\mathbb{P}}^{\mathfrak{P}}},$$

where we have made use of $\int_{\mathcal{RVE}} \boldsymbol{X}\,\mathrm{d}V = \boldsymbol{0}$.

Boundary conditions

Dirichlet boundary conditions

$$\bar{\boldsymbol{F}}\,\boldsymbol{X} + \frac{1}{2}\bar{\mathfrak{F}} : (\boldsymbol{X}\otimes\boldsymbol{X}) + \frac{1}{6}\bar{\mathbb{F}} \,\vdots\, (\boldsymbol{X}\otimes\boldsymbol{X}\otimes\boldsymbol{X}) - \boldsymbol{\varphi} = \boldsymbol{0},$$

$$\bar{\boldsymbol{F}} + \bar{\mathfrak{F}}\,\boldsymbol{X} + \frac{1}{2}\bar{\mathbb{F}} : (\boldsymbol{X}\otimes\boldsymbol{X}) - \boldsymbol{F} = \boldsymbol{0},$$

Periodic boundary conditions

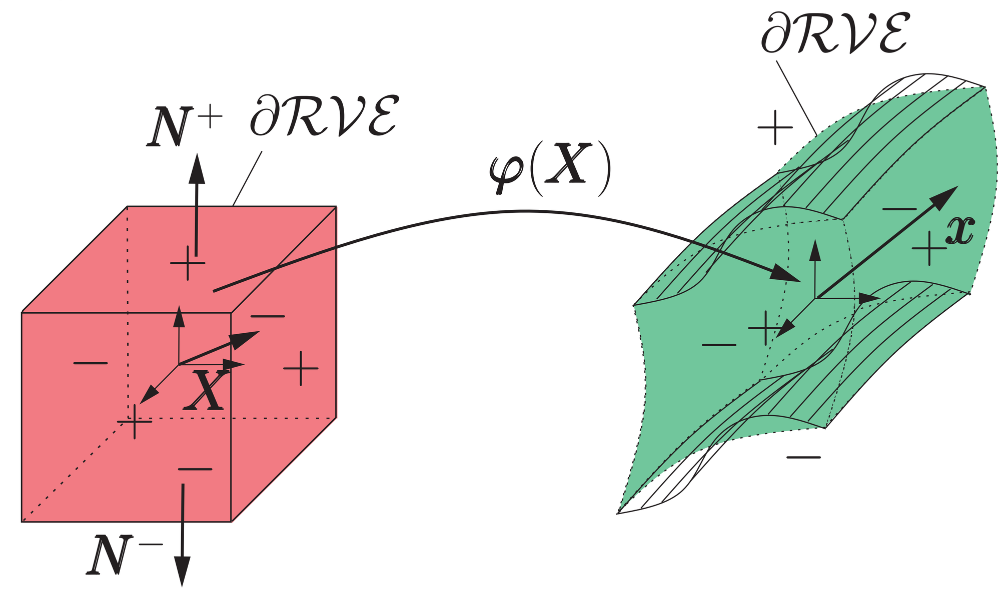

Figure: Mesoscopic boundary value problem, periodic boundary conditions on $\partial\mathcal{RVE}$, here only displayed for top and bottom for better understanding.

Cook's membrane

We examine Cook's membrane as macroscopic system, using a second-gradient model for the microscopic system inheriting a void.

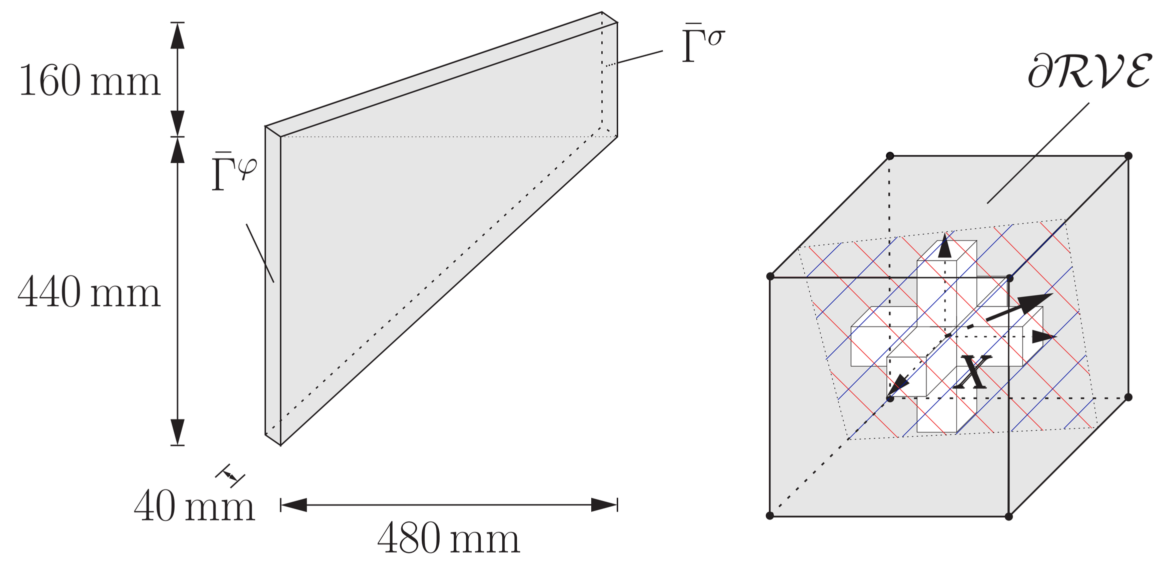

Figure: Left: Cook's membrane with boundary conditions, right: Fiber-reinforced polymers surrounding a void with applied Dirichlet conditions for the $\mathcal{RVE}$.

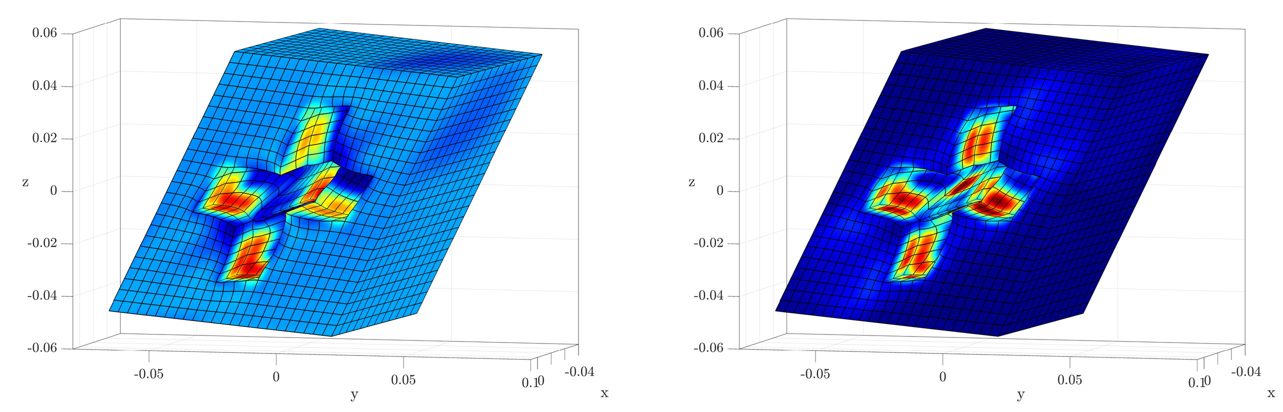

Figure: Exemplary deformed $\mathcal{RVE}$ with second-gradient material, sliced at the midplane. Left: Von Mises stress distribution, right: $||\mathfrak{P}||$ distribution.

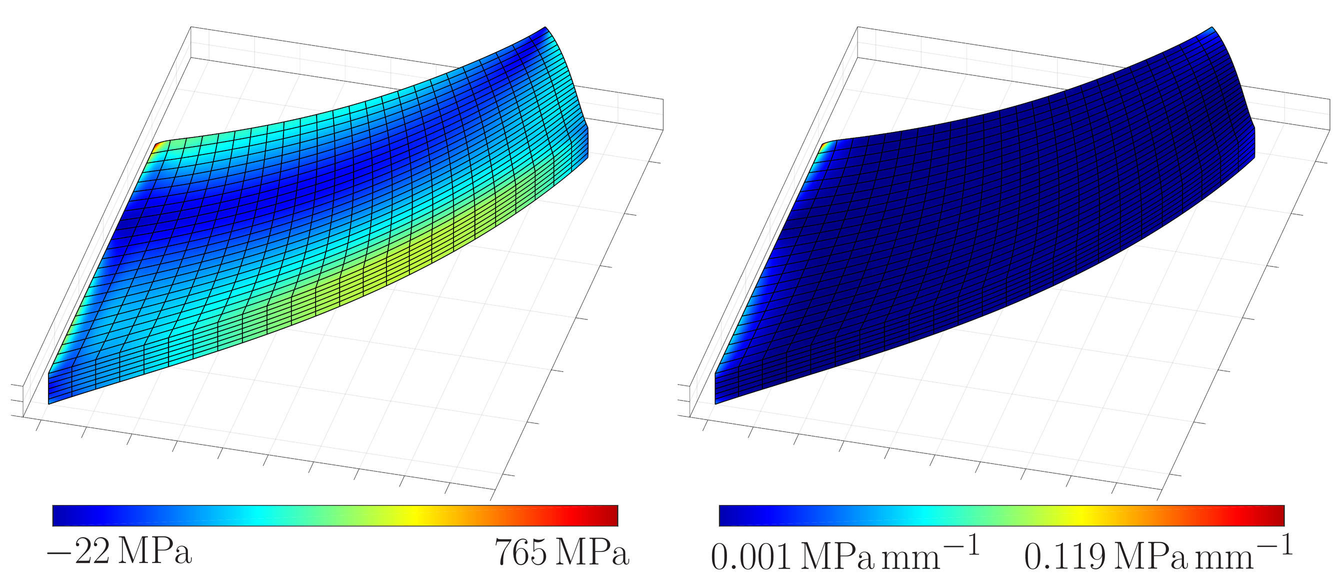

Figure: Cook's membrane. Stresses at different resolutions with a scaled displacement using the factor 5. Left: Von Mises stress distribution, right: $||\mathfrak{P}||$ distribution.

References:

[1] F. Schmidt, M. Krüger, M.-A. Keip and C. Hesch. *Computational homogenization of higher-order continua.* International Journal for Numerical Methods in Engineering, 123:2499-2529, 2022.

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