Optimization of Robin-type problems of elasticity via homogenization and beam models with the application to medical textiles design.

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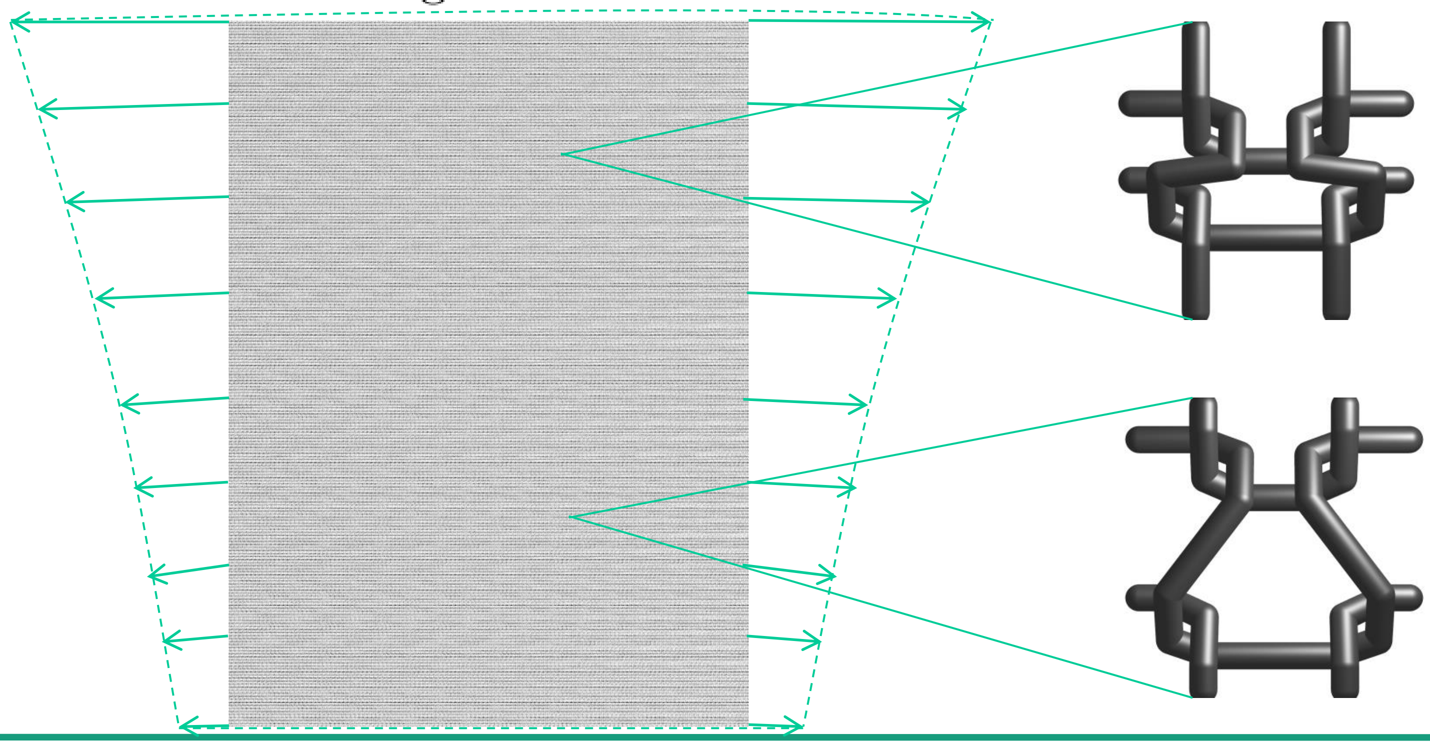
Motivation

Find the structure of the textile $g(x)$, which delivers the effective properties as close as possible to the desired values under prescribed displacement at the boundary of the fabric.

Parameters set $g(x)$ is controllable during the manufacturing process and can be varied along the fabric.



DIRECT PROBLEM

Statement of periodic problem

Consider the following problem in parameter-dependent ε-periodic domain Ω^ε:

1. Linear elasticity equation:

$$-\nabla \cdot (\boldsymbol{\sigma}^\varepsilon(\boldsymbol{x})) = 0,\ \boldsymbol{x} \in \Omega^\varepsilon,\ \boldsymbol{\sigma}^\varepsilon(\boldsymbol{x}) = \boldsymbol{A}^\varepsilon(\boldsymbol{x}) e(\boldsymbol{u}^\varepsilon(\boldsymbol{x})),$$

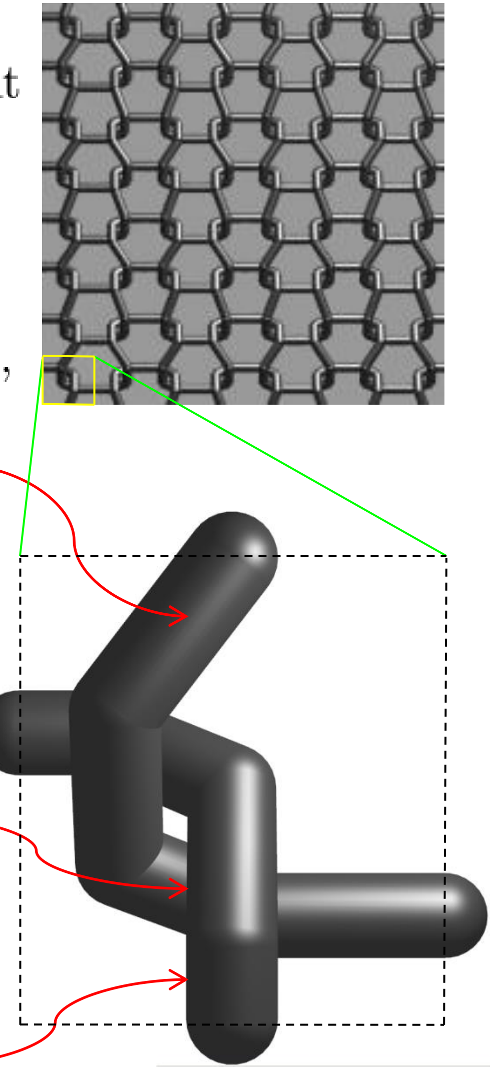
   $\boldsymbol{A}^\varepsilon(\boldsymbol{x})$ is symmetric uniformly positive-definite 4th order tensor, $e(\boldsymbol{u}) = \nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T$ is symmetrized displacement gradient.

2. Robin-type conditions at the contact interface:

$$(\boldsymbol{\sigma}^\varepsilon \boldsymbol{n}^\varepsilon)_n = \frac{1}{\varepsilon \delta_n} [\boldsymbol{u}^\varepsilon]_n, \quad (\boldsymbol{\sigma}^\varepsilon \boldsymbol{n}^\varepsilon)_t = \frac{1}{\varepsilon \delta_t} [\boldsymbol{u}^\varepsilon]_t,$$

3. Boundary conditions:

$$\boldsymbol{u}^\varepsilon(\boldsymbol{x}) = \boldsymbol{l}(\boldsymbol{x}),\ \boldsymbol{x} \in \partial\Omega^\varepsilon_D,\ \ \boldsymbol{\sigma}^\varepsilon \boldsymbol{n}^\varepsilon = 0,\ \boldsymbol{x} \in \partial\Omega^\varepsilon_N.$$



State of the art in homogenization

Cioranescu, D., Damlamian, A. and Orlik, J.: Homogenization via unfolding in periodic elasticity with contact on closed and open cracks, *Asymptotic Analysis*, **82**(3), 201–232, 2013.

Kikuchi, N., Oden J.T. *Contact Problems in Elasticity: A Study of Variatoinal Inequalities and Finite Elements Methods*, SIAM studies in applied mathematics. SIAM, 1987.

Hummel, H.-K.: Homogenization for heat transfer in polycrystals with interfacial resistances, *Applicable Analysis*, **75 (3–4)**, 403–424, 2000.

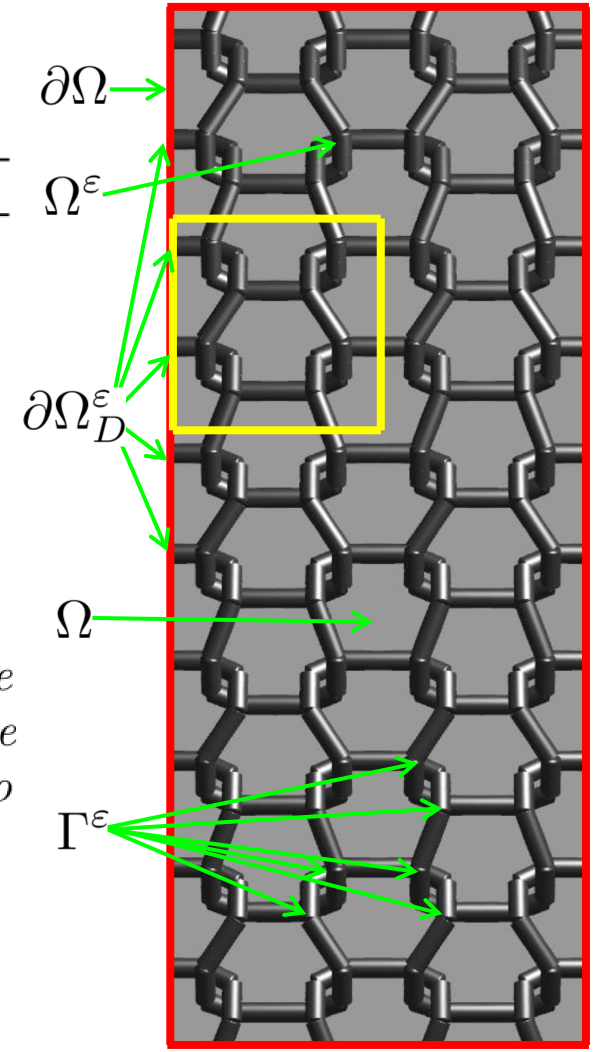
Homogenization

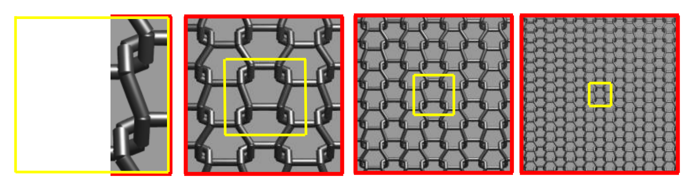
Consider periodic structure Ω^ε with period ε in domain Ω^ε and the following family of problems for displacement field $\boldsymbol{u}^\varepsilon \in H^1(\Omega^\varepsilon)$

$$\begin{gathered}
\nabla \cdot \boldsymbol{\sigma}^\varepsilon(\boldsymbol{x}) = 0,\ \boldsymbol{x} \in \Omega^\varepsilon,\ \boldsymbol{\sigma}^\varepsilon(\boldsymbol{x}) = \boldsymbol{A}^\varepsilon(\boldsymbol{x})e(\boldsymbol{u}^\varepsilon(\boldsymbol{x})),\\
\boldsymbol{u}^\varepsilon(\boldsymbol{x}) = \boldsymbol{l}(\boldsymbol{x}),\ \text{on } \partial\Omega^\varepsilon_D,\\
\boldsymbol{\sigma}^\varepsilon(\boldsymbol{x})\boldsymbol{n}^\varepsilon(\boldsymbol{x}) = 0,\ \boldsymbol{x} \in \partial\Omega^\varepsilon_N,\\
\boldsymbol{\sigma}^\varepsilon(\boldsymbol{x})\boldsymbol{n}^\varepsilon(\boldsymbol{x}) = \boldsymbol{R}^\varepsilon(\boldsymbol{x})[\boldsymbol{u}^\varepsilon],\ \text{on } \Gamma^\varepsilon.
\end{gathered}$$

Theorem. *Under proper conditions, as $\varepsilon \to 0$ there exist function $\boldsymbol{u}^0$ and 4th order symmetric positive-definite tensor $\boldsymbol{A}^{\mathrm{hom}}$ and extensions $\hat{\boldsymbol{u}}^\varepsilon$ of $\boldsymbol{u}^\varepsilon$ and $\hat{\boldsymbol{A}}^\varepsilon$ of $\boldsymbol{A}^\varepsilon$ into $\Omega^\varepsilon_{3\mathrm{D}}$ such that* $\left\|\hat{\boldsymbol{u}}^\varepsilon - \boldsymbol{u}^0\right\|_{L^2(\Omega^\varepsilon_{3\mathrm{D}})} \to 0$,

$$\begin{gathered}
\nabla \cdot \boldsymbol{\sigma}^0(\boldsymbol{x}) = 0,\ \boldsymbol{x} \in \Omega,\ \boldsymbol{\sigma}^0(\boldsymbol{x}) = \boldsymbol{A}^{\mathrm{hom}}(\boldsymbol{x})e(\boldsymbol{u}^0(\boldsymbol{x})),\\
\boldsymbol{u}^0(\boldsymbol{x}) = \boldsymbol{l}(\boldsymbol{x}),\ \text{on } \partial\Omega_D,\\
\boldsymbol{\sigma}^0(\boldsymbol{x})\boldsymbol{n}(\boldsymbol{x}) = 0,\ \text{on } \partial\Omega_N.
\end{gathered}$$





No Robin-type conditions in the limit problem.

Homogenization

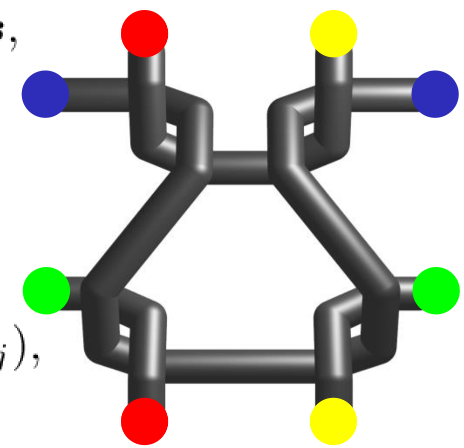
$$\text{In the limit problem } \nabla \cdot \boldsymbol{\sigma}^0(\boldsymbol{x}) = 0,\ \boldsymbol{x} \in \Omega,\ \boldsymbol{\sigma}^0(\boldsymbol{x}) = \boldsymbol{A}^{\text{hom}}(\boldsymbol{x}) e(\boldsymbol{u}^0(\boldsymbol{x})),$$
$$\boldsymbol{u}^0(\boldsymbol{x}) = \boldsymbol{l}(\boldsymbol{x}),\ \text{on } \partial\Omega_D,$$
$$\boldsymbol{\sigma}^0(\boldsymbol{x})\boldsymbol{n}(\boldsymbol{x}) = 0,\ \text{on } \partial\Omega_N,$$

the tensor $\boldsymbol{A}^{\text{hom}}$ is to be obtained from the solutions of the cell problems:

$$A^{\text{hom}}_{ijkl} = \frac{|\omega|}{|Y|} \int_\Omega (e(\boldsymbol{w}_{ij}) + \boldsymbol{e}_{ij}) : \boldsymbol{A}(\boldsymbol{x})(e(\boldsymbol{w}_{kl}) + \boldsymbol{e}_{kl})\, d\boldsymbol{x} +$$
$$+ \frac{|\omega|}{|Y|} \int_{\Gamma_C} \boldsymbol{C}(\boldsymbol{s})[\boldsymbol{w}_{ij}] : \boldsymbol{R}\boldsymbol{C}(\boldsymbol{s})[\boldsymbol{w}_{kl}]\, d\boldsymbol{s},$$
$$\boldsymbol{R} = \operatorname{diag}\left(\delta_n^{-1}, \delta_t^{-1}, \delta_t^{-1}\right),$$

where Y is the periodicity cell, $\boldsymbol{w}_{ij} \in H^1_\#(Y)$ satisfies

$$\nabla \cdot \boldsymbol{\sigma}_{ij}(\boldsymbol{x}) = 0,\ \boldsymbol{x} \in Y,\ \boldsymbol{\sigma}_{ij}(\boldsymbol{x}) = \boldsymbol{A}(\boldsymbol{x})(\boldsymbol{e}(\boldsymbol{w}_{ij}) + \boldsymbol{e}_{ij}),$$
$$\boldsymbol{\sigma}_{ij}(\boldsymbol{s})\boldsymbol{n}(\boldsymbol{s}) = \boldsymbol{R}\boldsymbol{C}(\boldsymbol{s})[\boldsymbol{w}_{ij}],\ \text{on } \Gamma_C.$$



Theorem. *The homogenized tensor is continuous w.r.t. the geometrical params.*

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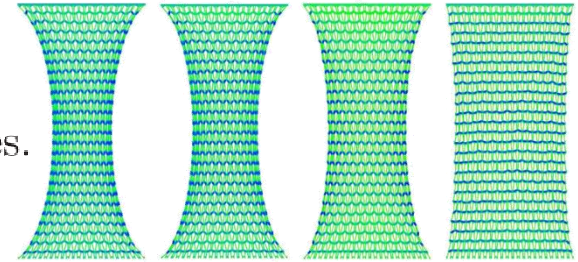
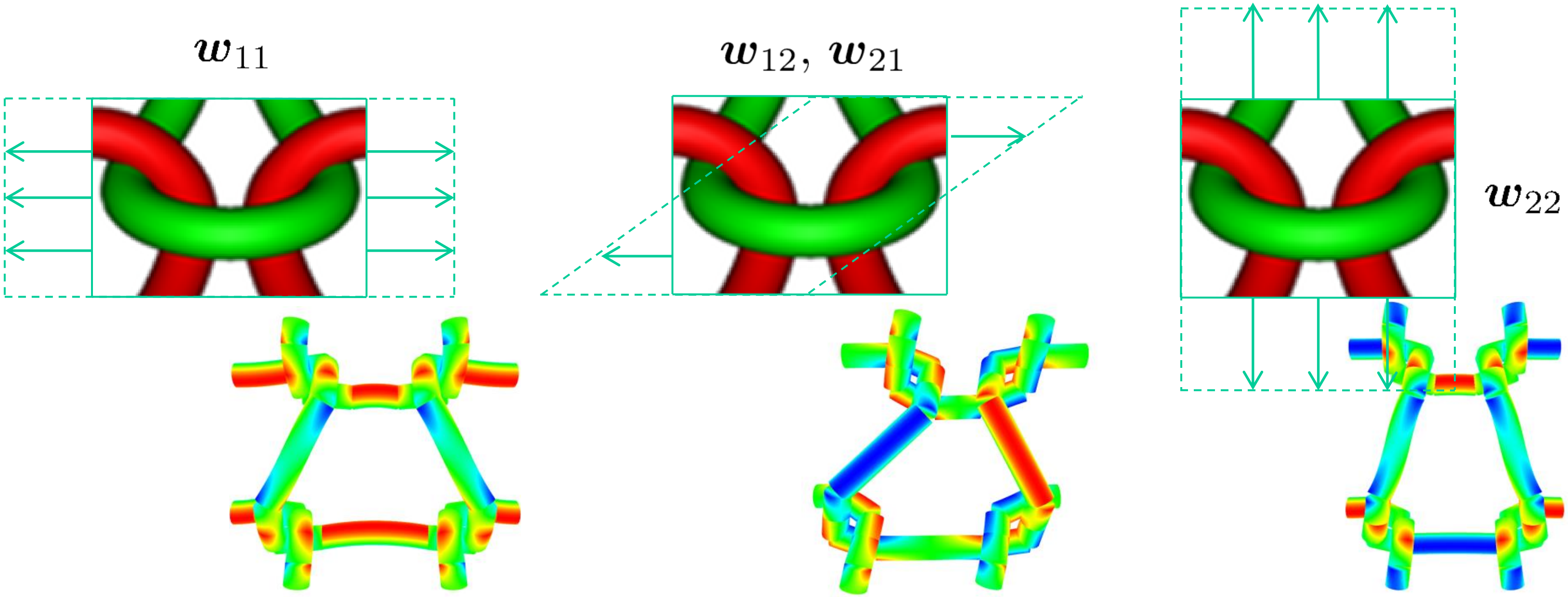
Plain strain motivation



We are concerned with only in-plane properties of textiles.

- cell geometries are essentially three-dimensional,
- 2D elasticity problem is desired in the limit.

Only in-plane homogenized properties are of interest. They are defined from the following 3 cell problems:



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REDUCTION TO BEAM MODELS IN THE CELL PROBLEMS

Cell problems: reduction to beam models

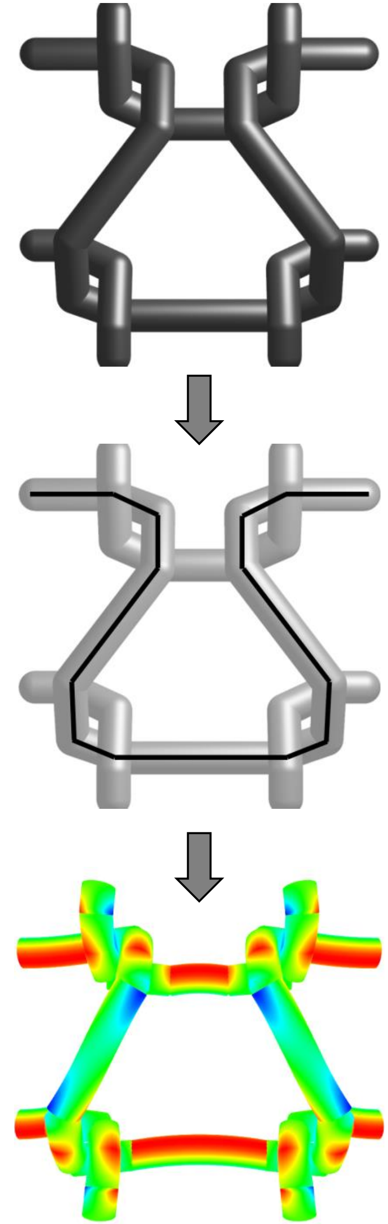
1D graph problem:

$$\begin{cases} EAu_1^{\mathrm{II}} = f_1, \\ EIu_{2,3}^{\mathrm{IV}} = f_{2,3}, \\ JGu_4^{\mathrm{II}} = f_4, \end{cases}$$

$$\left([EAu_1'] \quad [EIu_2'''] \quad [EIu_3'''] \quad [GJu_4'] \quad -[EIu_3''] \quad [EIu_2''] \quad \ldots\right)^T =$$
$$= -\boldsymbol{Q}^T \left(\boldsymbol{V}_f^T \boldsymbol{P}_f \boldsymbol{V}_f + \boldsymbol{V}_M^T \boldsymbol{P}_M \boldsymbol{V}_M\right) \boldsymbol{Q}\boldsymbol{w},$$
$$\boldsymbol{w} = \left(u_1, u_2, u_3, u_4, -u_3', u_2', v_1, v_2, v_3, v_4, -v_3', v_2'\right)^T,$$

+ boundary and force-moment transmission conditions.

1D-3D reconstruction formulas are used to compute the effective tensor from the set of four 1D functions.



Trabucho L., Viano J.M.: *Mathematical modelling of rods. Handbook of numerical analysis*, vol. 4, p. 487–974. Elsevier Science, 1996.

Baré D., Orlik J., and Panasenko G.: Asymptotic dimension reduction of a Robin-type elasticity boundary value problem in thin beams, *Applicable Analysis*, 2013.

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Cell problems: derivatives of the effective tensor

Further in optimization we'll need the derivatives of the cell problems' solutions with respect to $\boldsymbol{g}$ as a parameter.

- The exact solution of the cell graph 1D problem can be found from a linear algebraic system of equations similar to the standard finite element method systems. The direct FEM system is

$$\boldsymbol{K}_{ij}(\boldsymbol{g})\boldsymbol{q}_{ij}(\boldsymbol{g}) = \boldsymbol{f}_{ij}^{\mathrm{FEM}}(\boldsymbol{g}),$$

  where $\boldsymbol{K}_{ij}(\boldsymbol{g})$ and $\boldsymbol{f}_{ij}^{\mathrm{FEM}}(\boldsymbol{g})$ are known functions of geometrical parameters $\boldsymbol{g}$.

- Differentiation of the above system with respect to $\boldsymbol{g}$ yields the derivative FEM system

$$\delta_{\boldsymbol{g}}\boldsymbol{K}_{ij}(\boldsymbol{g})\boldsymbol{q}_{ij}(\boldsymbol{g}) + \boldsymbol{K}_{ij}(\boldsymbol{g})\delta_{\boldsymbol{g}}\boldsymbol{q}_{ij}(\boldsymbol{g}) = \delta_{\boldsymbol{g}}\boldsymbol{f}_{ij}^{\mathrm{FEM}}(\boldsymbol{g}).$$

  $\delta_{\boldsymbol{g}}\boldsymbol{K}_{ij}(\boldsymbol{g})$ and $\delta_{\boldsymbol{g}}\boldsymbol{f}_{ij}^{\mathrm{FEM}}(\boldsymbol{g})$ can be obtained with automatic symbolic differentiation. Isolate $\delta_{\boldsymbol{g}}\boldsymbol{q}_{ij}(\boldsymbol{g})$:

$$\boldsymbol{K}_{ij}(\boldsymbol{g})\delta_{\boldsymbol{g}}\boldsymbol{q}_{ij}(\boldsymbol{g}) = \delta_{\boldsymbol{g}}\boldsymbol{f}_{ij}^{\mathrm{FEM}}(\boldsymbol{g}) - \delta_{\boldsymbol{g}}\boldsymbol{K}_{ij}(\boldsymbol{g})\boldsymbol{q}_{ij}(\boldsymbol{g}).$$

At this point we are able to compute the derivatives of the effective tensor $\delta_{\boldsymbol{g}}\boldsymbol{A}^{\mathrm{hom}}$ by the chain rule.

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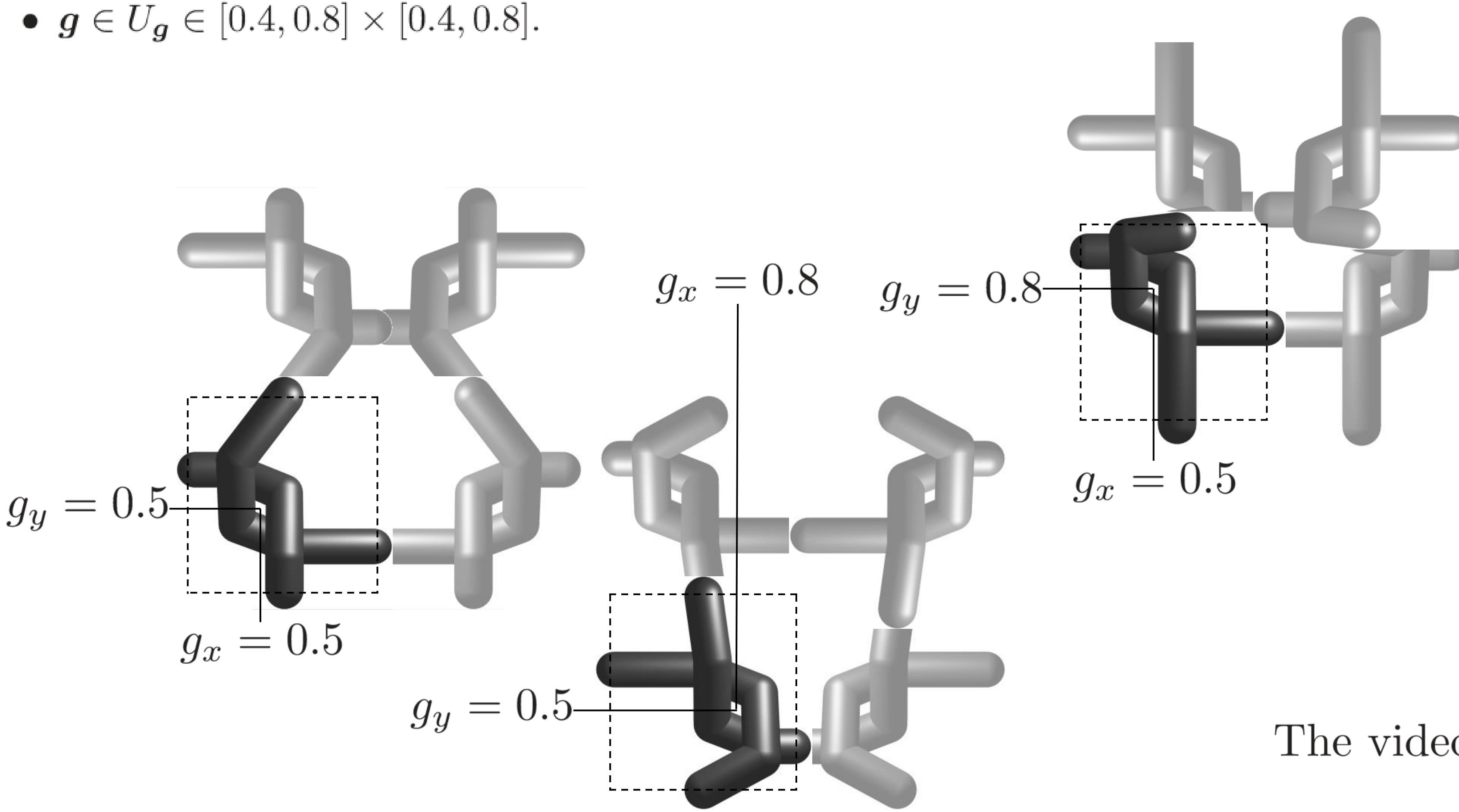
DESIGN SPACE

Design space

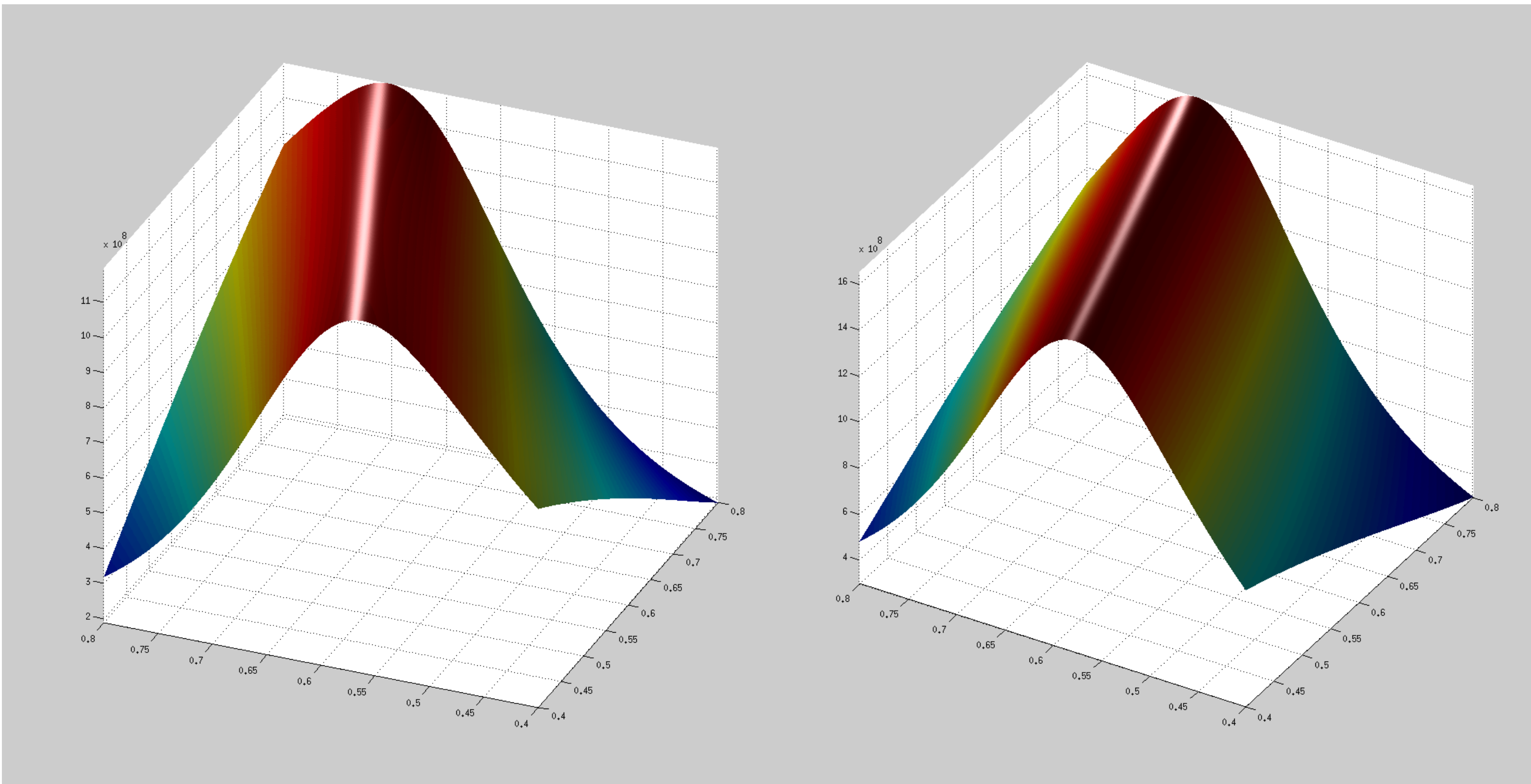
- the microgeometry at a point $\boldsymbol{x}$ is parametrized by two numbers $\boldsymbol{g}(\boldsymbol{x}) = (g_x(\boldsymbol{x}), g_y(\boldsymbol{x}))$,
- $\boldsymbol{g} \in U_{\boldsymbol{g}} \in [0.4, 0.8] \times [0.4, 0.8]$.



The video.

The homogenized coefficients as functions of the params

- no convexity of the homogenized properties with respect to the geometrical parameters



A^{hom}_{1111} A^{hom}_{1122}

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STRESS PROFILE OPTIMIZATION

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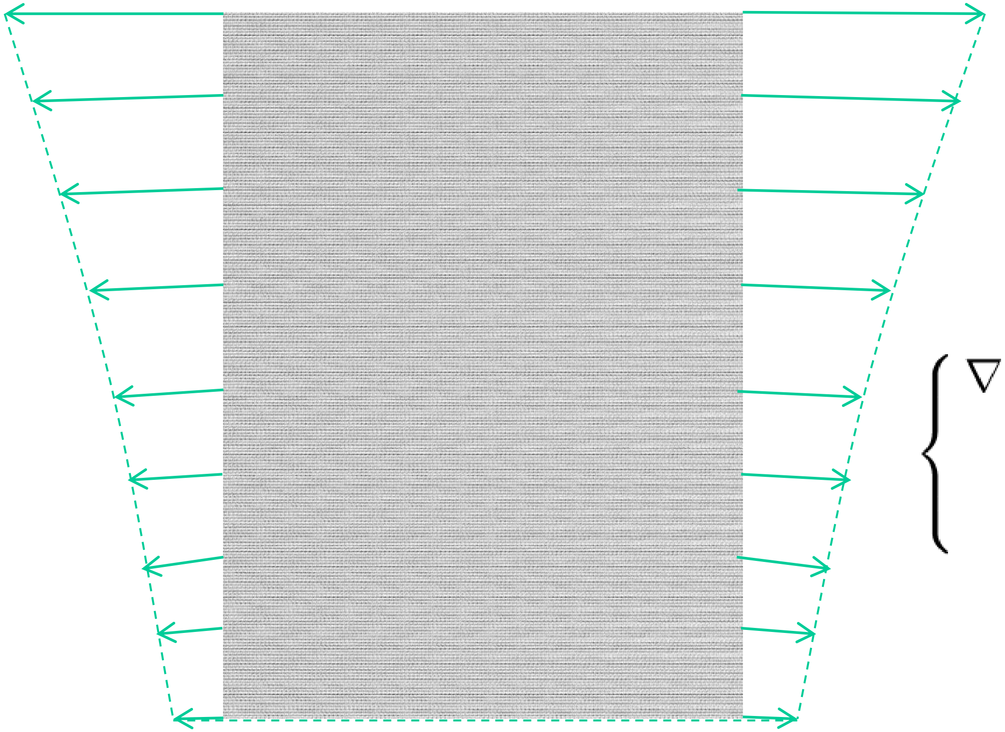
Stress profile optimization

Consider the following optimization problem.

$$J(\boldsymbol{g}) = \int_\Omega (\boldsymbol{A}^{\mathrm{hom}}(\boldsymbol{g})e(\boldsymbol{u}(\boldsymbol{g})) - \boldsymbol{\sigma}_d) : (\boldsymbol{A}^{\mathrm{hom}}(\boldsymbol{g})e(\boldsymbol{u}(\boldsymbol{g})) - \boldsymbol{\sigma}_d)\, d\boldsymbol{x} \to \min_{\boldsymbol{g}},$$



$$\begin{cases} \nabla \cdot (\boldsymbol{A}^{\mathrm{hom}}(\boldsymbol{g})e(\boldsymbol{u})) = 0 \text{ in } \Omega, \\ \boldsymbol{u} = \boldsymbol{l} \text{ on } \partial\Omega_D, \\ \boldsymbol{A}^{\mathrm{hom}}(\boldsymbol{g})e(\boldsymbol{u})\boldsymbol{n} = 0 \text{ on } \partial\Omega_N. \end{cases}$$

This is a PDE-constrained optimization problem.

Adjoint approach for the homogenized equation

Theorem. *The minimizer exists in any bounded set in the space of Lipschitz functions.*

Standard procedure of the objective functional's gradient computation leads to

$$\delta_{\boldsymbol{g}} J = 2 \int_\Omega (\boldsymbol{A}^{\mathrm{hom}} e(\boldsymbol{u}) - \boldsymbol{\sigma}^\star) : (\delta_{\boldsymbol{g}} \boldsymbol{A}^{\mathrm{hom}} e(\boldsymbol{u}))\, d\boldsymbol{x} - 2 \int_\Omega \delta_{\boldsymbol{g}} \boldsymbol{A}^{\mathrm{hom}} e(\boldsymbol{u}) : e(\boldsymbol{p})\, d\boldsymbol{x},$$

$$\boldsymbol{h}(\boldsymbol{g}) = \boldsymbol{A}^{\mathrm{hom}}(\boldsymbol{g})(\boldsymbol{A}^{\mathrm{hom}}(\boldsymbol{g}) e(\boldsymbol{u}(\boldsymbol{g})) - \boldsymbol{\sigma}^\star),$$

where $\boldsymbol{p}$ is the solution of the adjoint problem

$$\begin{cases} \nabla \cdot (\boldsymbol{A}^{\mathrm{hom}}(\boldsymbol{g}) e(\boldsymbol{p})) = -\nabla \cdot \boldsymbol{h} \text{ in } \Omega, \\ \boldsymbol{p} = 0 \text{ on } \partial\Omega_D, \\ \boldsymbol{A}^{\mathrm{hom}}(\boldsymbol{g}) e(\boldsymbol{p}) \boldsymbol{n} = -\boldsymbol{h}\boldsymbol{n} \text{ on } \partial\Omega_N. \end{cases}$$

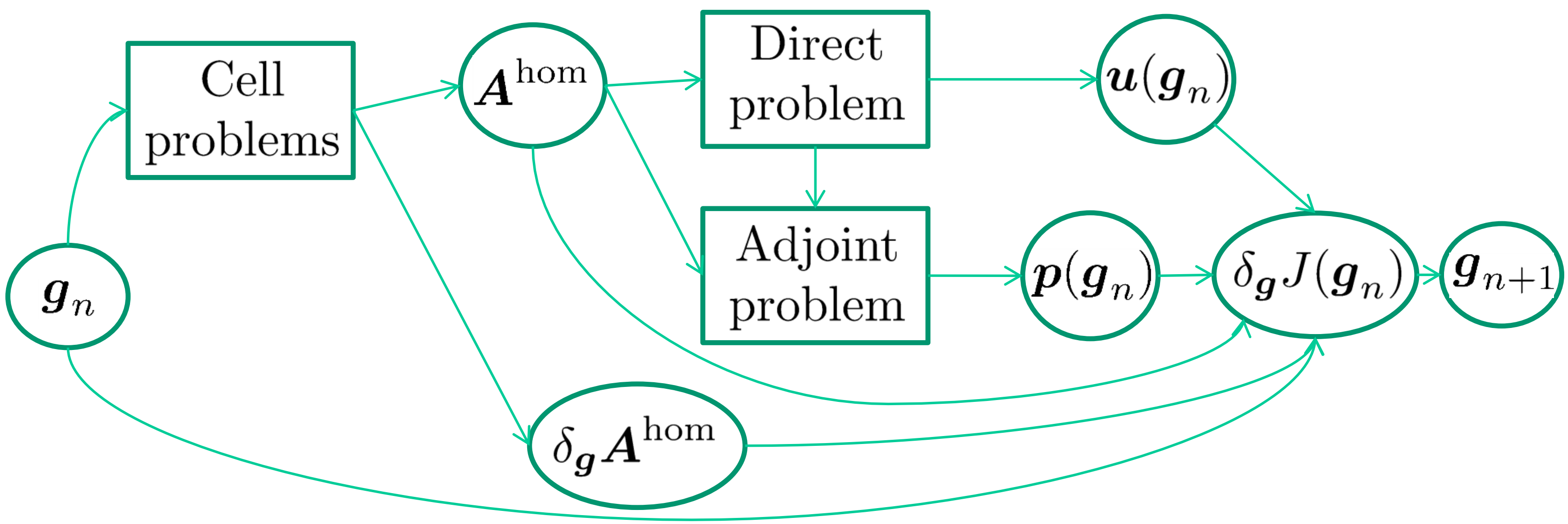
Allaire, G. *Shape optimization by the Homogenization Method*, Springer, 2001.

Hinze, M., Pinnau, R., Ulbrich, M. and Ulbrich, S. *Optimization with PDE Constraints*, Springer, 2010.

Optimization loop scheme

With $\boldsymbol{A}^{\text{hom}}$ and $\delta_{\boldsymbol{g}} \boldsymbol{A}^{\text{hom}}$ obtained from the cell problems, we are ready to close the projected gradient method's optimization loop:

$$\boldsymbol{g}^{n+1} = \Pr_{U_{\boldsymbol{g}}} \left(\boldsymbol{g}^n - \alpha \nabla_{\boldsymbol{g}} J(\boldsymbol{g}^n) \right).$$



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POISSON'S RATIO OPTIMIZATION

Poisson's ratio optimization

Homogenization often yields orthotropic effective tensors.
Hooke's law of a 2D orthotropic material has the following form:

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} pE_1 & pE_1\nu_{21} & 0 \\ pE_2\nu_{12} & pE_2 & 0 \\ 0 & 0 & G_{12} \end{pmatrix} \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \end{pmatrix},$$

where $p = (1 - \nu_{12}\nu_{21})^{-1}$. Anisotropic Poisson's ratios can be computed as

$$\nu_{12} = \frac{A_{1122}}{A_{2222}}, \quad \nu_{21} = \frac{A_{1122}}{A_{1111}}.$$

ν_{ij} characterizes contraction of the structure in the j-th direction when stretched in the i-th direction. In the textile industry this effect is usually to be reduced.

A study on properties of homogenized tensors is available in Bakhvalov N., Panasenko G.: *Homogenization: Averaging processes in periodic media.* Springer, 1989.

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Poisson's ratio optimization

Assume that $\boldsymbol{A}^{\text{hom}}$ and its increments $\delta_{\boldsymbol{g}}\boldsymbol{A}^{\text{hom}}$ are available, then

$$\delta_{\boldsymbol{g}}\nu_{12} = \frac{\delta_{\boldsymbol{g}}A^{\text{hom}}{}_{1122}}{A^{\text{hom}}{}_{2222}} - \frac{A^{\text{hom}}{}_{1122}}{A^{\text{hom}}{}^2_{2222}}\delta_{\boldsymbol{g}}A^{\text{hom}}{}_{2222},$$

$$\delta_{\boldsymbol{g}}\nu_{21} = \frac{\delta_{\boldsymbol{g}}A^{\text{hom}}{}_{1122}}{A^{\text{hom}}{}_{1111}} - \frac{A^{\text{hom}}{}_{1122}}{A^{\text{hom}}{}^2_{1111}}\delta_{\boldsymbol{g}}A^{\text{hom}}{}_{1111}.$$

Projected gradient descent procedure with respect to $\boldsymbol{g}$:

$$\boldsymbol{g}^{k+1} = \mathrm{Pr}_{U_{\boldsymbol{g}}}\left(\boldsymbol{g}^k - \alpha\nabla_{\boldsymbol{g}}\nu_{12}(\boldsymbol{g}^k)\right),$$

$$\boldsymbol{g}^{k+1} = \mathrm{Pr}_{U_{\boldsymbol{g}}}\left(\boldsymbol{g}^k - \alpha\nabla_{\boldsymbol{g}}\nu_{21}(\boldsymbol{g}^k)\right).$$

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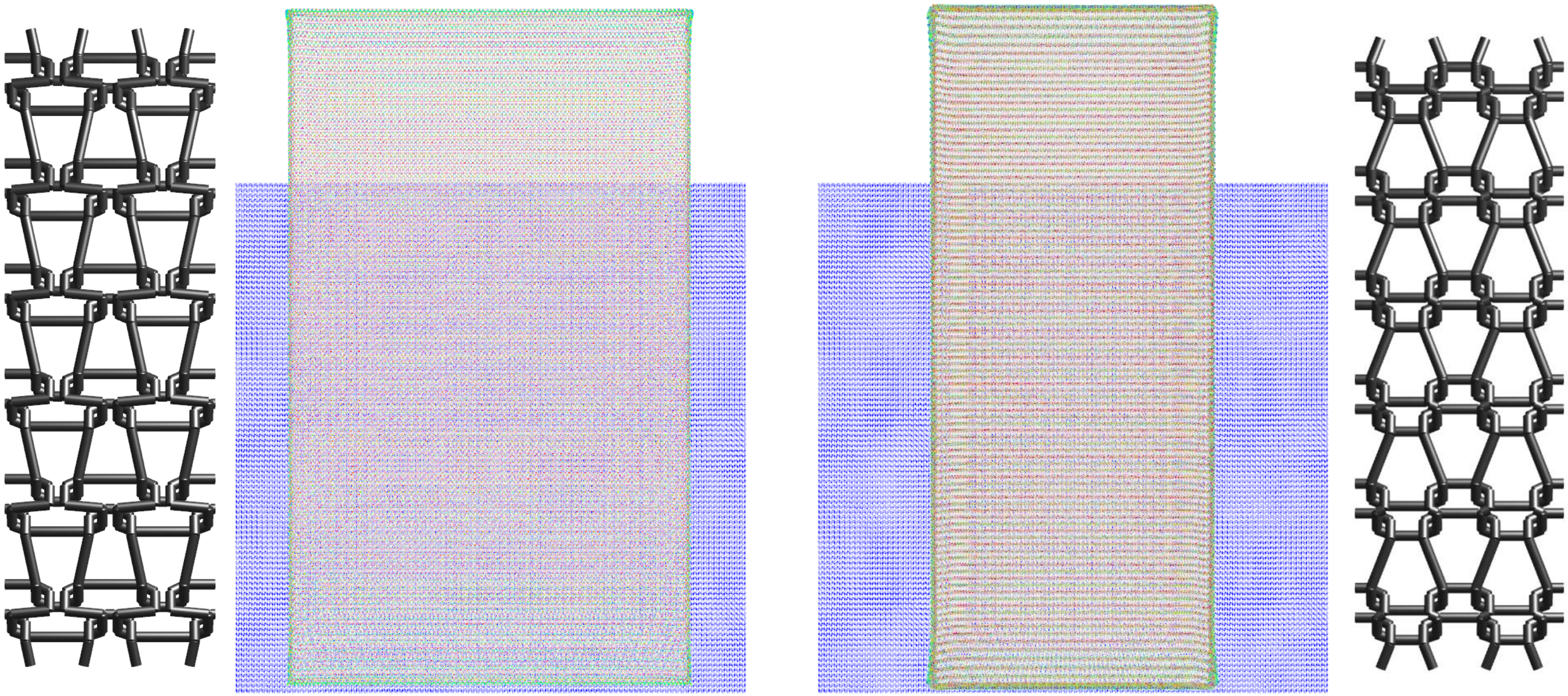
Poisson's ratios optimization: numerical example

Two initially square fabrics of different microstructure undergo the same vertical strain. The left one is optimized for the minimum Poisson's ratio. The right one is optimized for the maximum Poisson's ratio.



$\nu_{21} = 0.2671$ $\qquad$ $\nu_{21} = 0.8639$