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Developing an automatized optimization problem in FEniCS for parameter determination of metamaterials

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FEniCS 2021, Cambridge

26 Mar. 2021

Introduction

What are metamaterials?

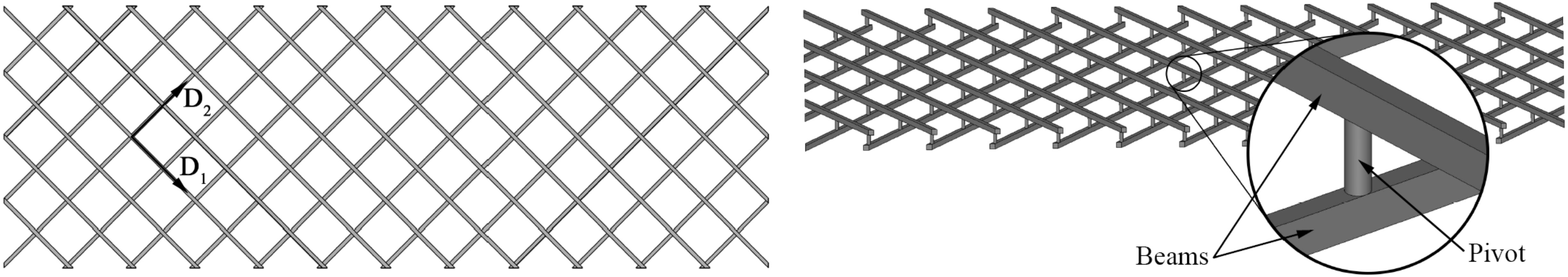
- engineered materials, with properties not found in natural materials
- usually arranged in repeating patterns
- at scales smaller than the wavelengths of the phenomena they influence
- derive their properties from their designed structures

We need to identify the parameters of metamaterials’ models

Introduction

An example of metamaterials:

Pantographic structures



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Introduction

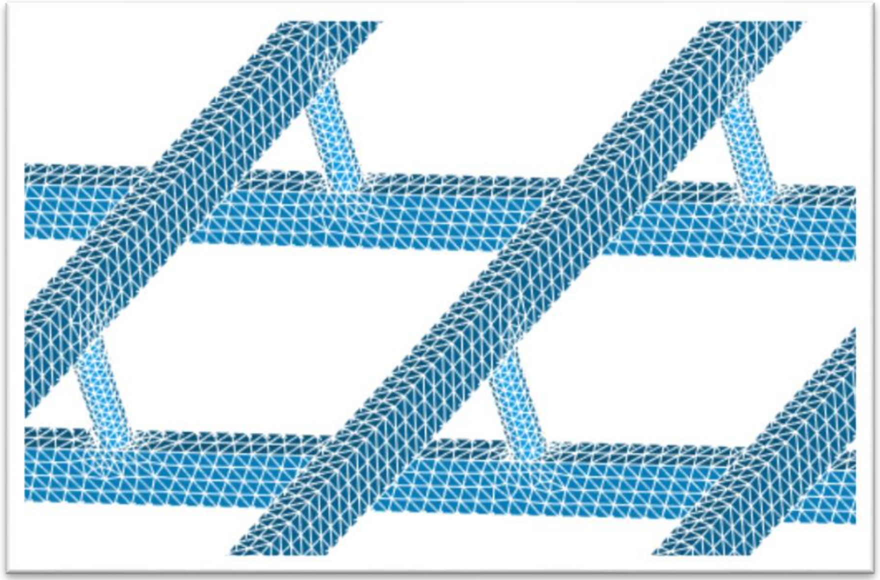
Pantographic Structures

- **Properties**:
  - Large deformation in the elastic region
  - High toughness: absorbing large amount of energy in the elastic and plastic regimes
  - Extraordinarily high specific strength
- **Main Deformation Energy Mechanisms:**
  - Shear deformation of the elastic pivots
  - Bending of beams
  - Stretching of beams

Introduction

Modeling Pantographic Structures

- **Micro-scale Model**
  - Using Cauchy first-gradient continuum theory



- **Macro-scale Model**
  - Using a strain-gradient energy model

Micro-scale Model

- **Nonlinear Elasticity**
  - Deformation of a body $x_i = X_i + u_i$
  - Deformation gradient $F_{ij} = \dfrac{\partial x_i}{\partial X_j}$
  - Green-Lagrange strain tensor $E_{ij} = \dfrac{1}{2}(F_{ki}F_{kj} - \delta_{ij}) = \dfrac{1}{2}(u_{k,i}u_{k,j} + u_{i,j} + u_{j,i})$
  - Strain energy density: $W_\mathrm{m}(\boldsymbol{E}) = \dfrac{\lambda}{2}E_{kk}^2 + \mu E_{ij}E_{ij}$
  - Elasticity action functional: $\mathcal{A} = \int_{\mathcal{B}_0} \left(\dfrac{1}{2}\rho_0 \dot{u}_i \dot{u}_i - W_\mathrm{m} + \rho_0 f_i u_i\right) \mathrm{d}V + \int_{\partial\mathcal{B}_0^N} \hat{t}_i u_i \,\mathrm{d}A$
  - Weak form:

$$-\int_{\mathcal{B}_0} \frac{\partial W_\mathrm{m}}{\partial u_{i,j}} \delta u_{i,j} \,\mathrm{d}V + \int_{\partial\mathcal{B}_0^N} \hat{t}_i \delta u_i \,\mathrm{d}A = 0$$

Abali, B. E., Müller, W. H., & dell'Isola, F. (2017). *Archive of Applied Mechanics*, *87*(9), 1495-1510.

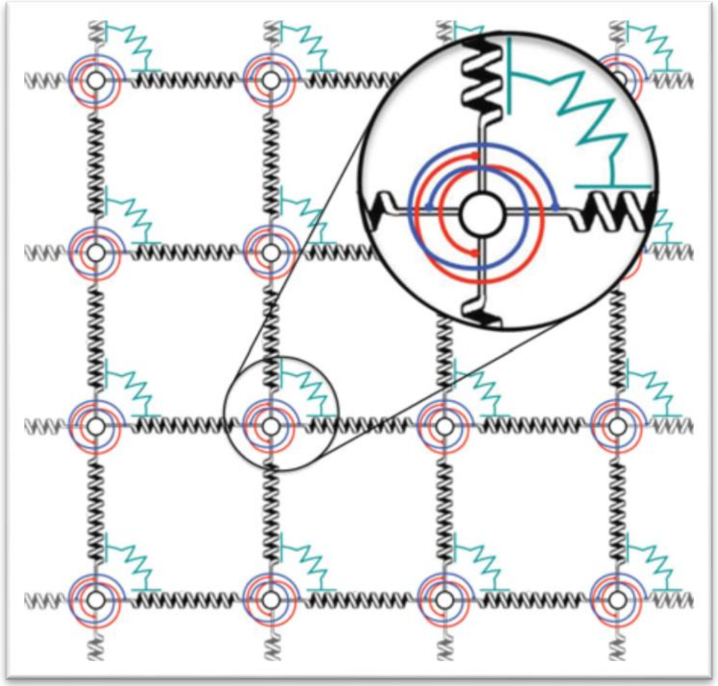
Macro-scale Model

A macro-scale model for planar pantographic structures

- A homogenized model with strain-gradient terms

$$W_M(\boldsymbol{\varepsilon},\boldsymbol{\kappa},\gamma)=\frac{1}{2}K_{\mathrm{e}}(\varepsilon_1^2+\varepsilon_2^2)+\frac{1}{2}K_{\mathrm{g}}(\kappa_1^2+\kappa_2^2)+\frac{1}{2}K_{\mathrm{s}}\gamma^2$$

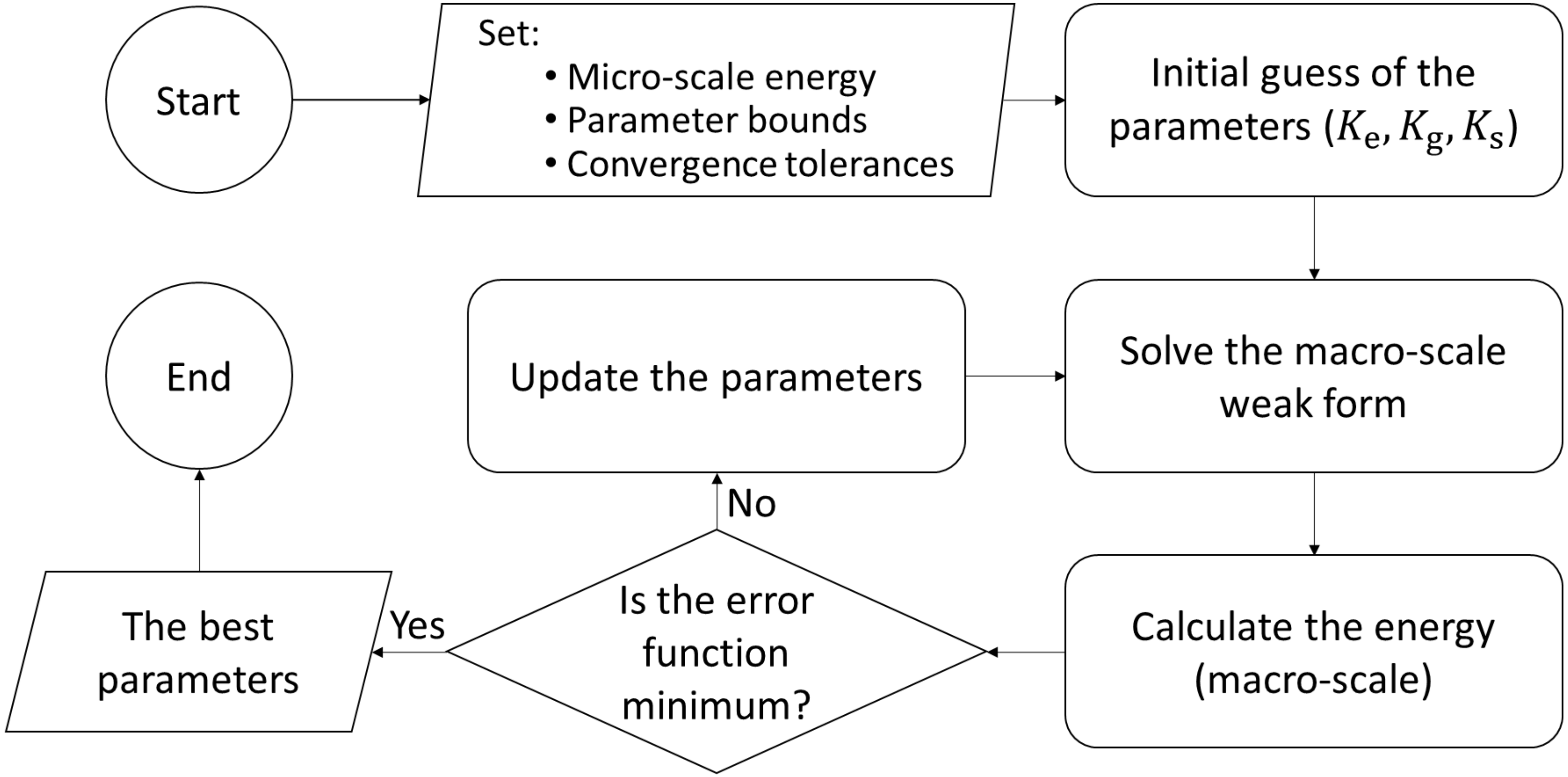
$$-\int_{\mathcal{B}_0}\frac{\partial W_{\mathrm{M}}(\boldsymbol{\varepsilon},\boldsymbol{\kappa},\gamma)}{\partial u_{i,j}}\delta u_{i,j}\,\mathrm{d}V+\int_{\partial\mathcal{B}_0^N}\hat{t}_i\delta u_i\,\mathrm{d}A=0$$



dell'Isola, F., Giorgio, I., Pawlikowski, M., & Rizzi, N. L. (2016). Large deformations of planar extensible beams and pantographic lattices: heuristic homogenization, experimental and numerical examples of equilibrium. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 472(2185), 20150790.

Optimization problem

Numerical Identification



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Optimization

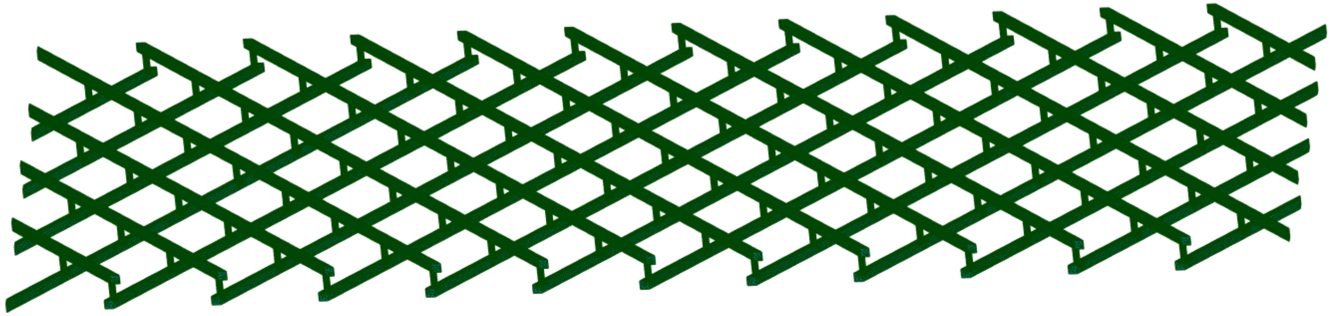
Numerical Identification

- Optimization function: *scipy.optimize.least_squares* (from Python)
- Optimization method: Trust Region Reflective (*trf*) algorithm

https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.least_squares.html

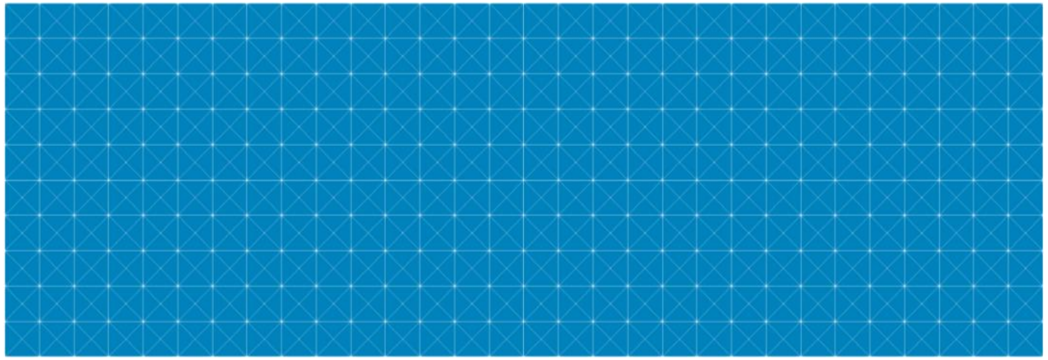
Modeling

- Creating 3D CAD model and meshing in SALOME
- 230k degrees of freedom



Netgen

- Creating 2D homogenized model in FEniCS
- 5k degrees of freedom

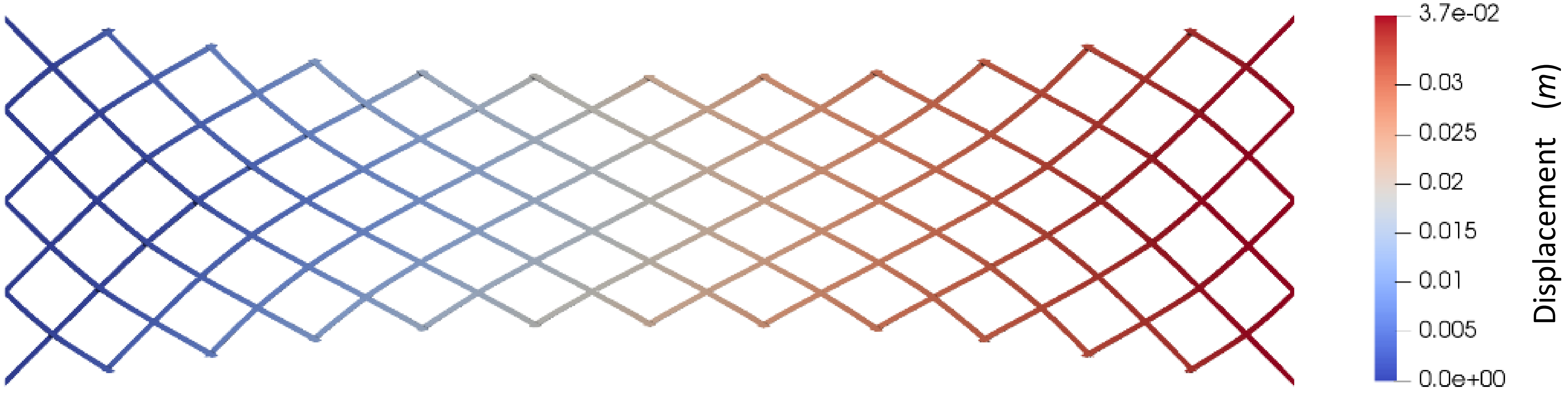


- Simulate a tensile test

Abali, B. E. (2017). Computational Reality. Springer, Singapore.

Results

- Micro-scale model results:
  - Plot of displacement (17.6 % normal strain)



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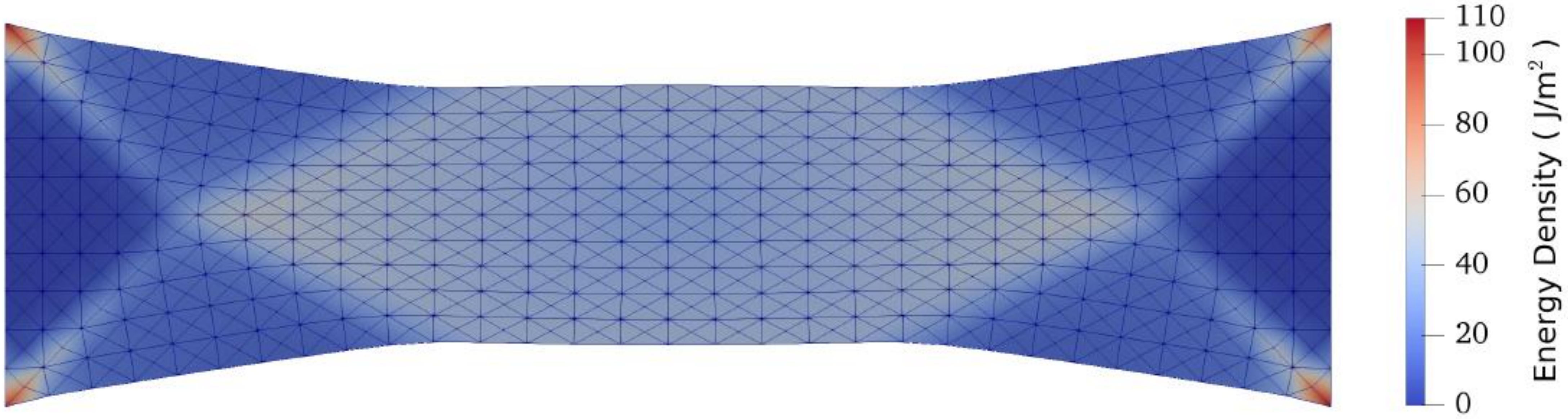
Results

- Macro-scale model results:
  - Plot of energy



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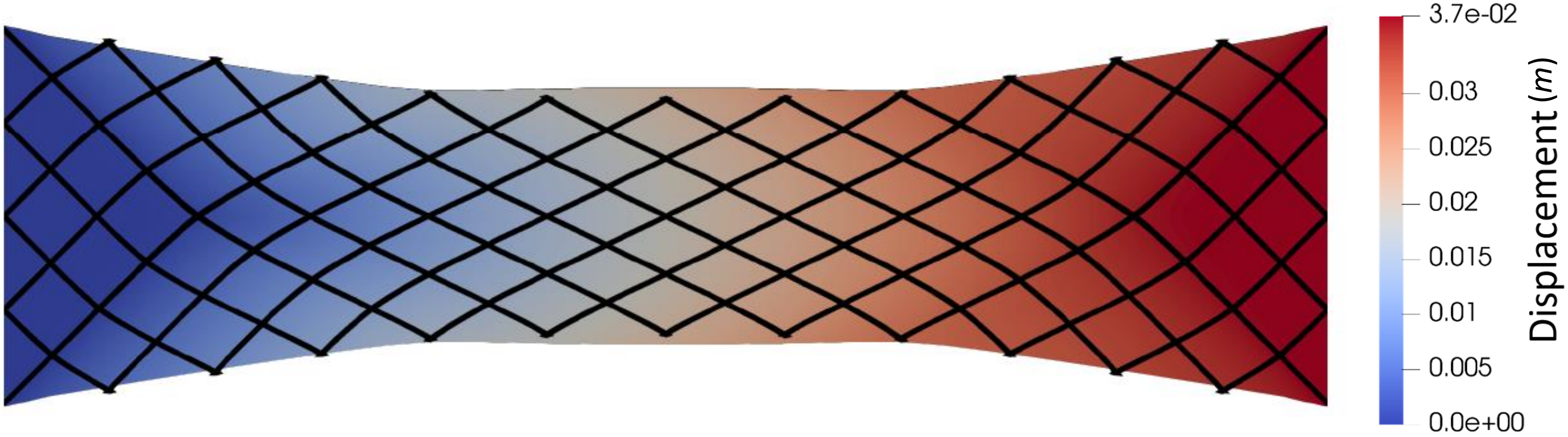
Results

- Comparing the models:
  - Displacement plot: micro-scale (in black), macro-scale (in color)



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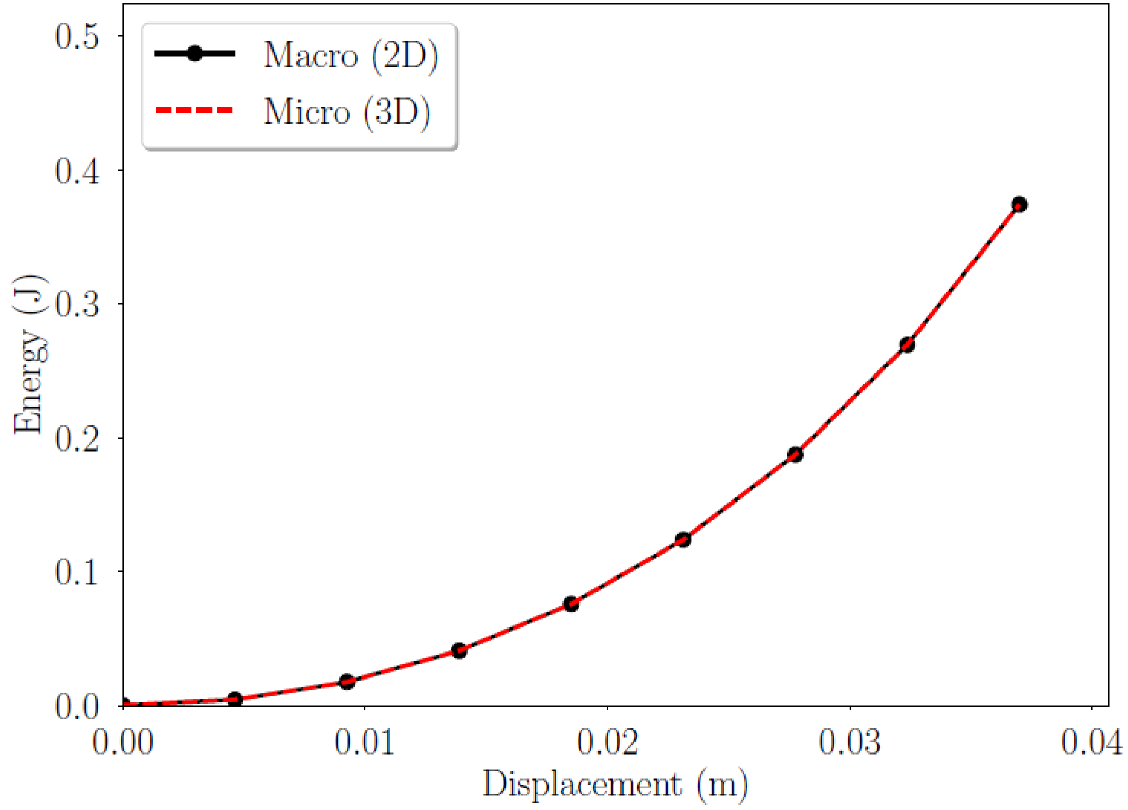
Results

- Numerical identification results:



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Results

- Numerical identification results:

Constitutive Parameters

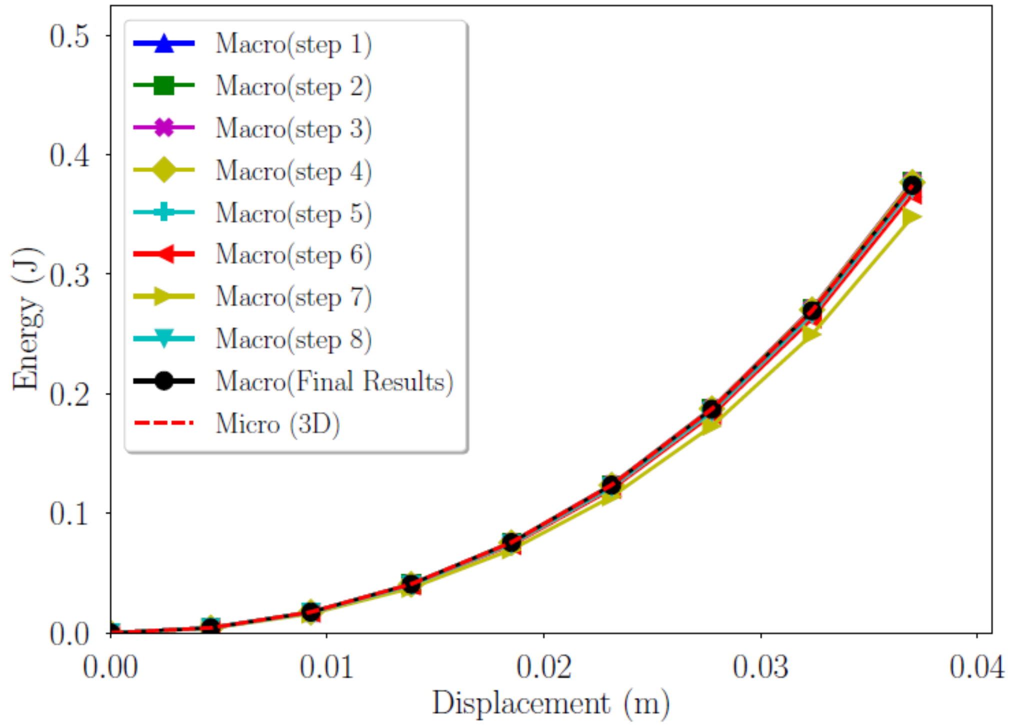
Parameter	Initial Guess	Final Results
K_e (N/m)	$K_e^0 = \frac{E w_b h_b}{p_b} = 2.107 \times 10^5$	1.406×10^5
K_g (Nm)	$K_g^0 = \frac{E I_z}{p_b} = 1.756 \times 10^{-2}$	2.699×10^{-2}
K_s (N/m)	$K_s^0 = \frac{G \pi d_p^4}{32 h_p p_b^2} = 1.364 \times 10^2$	2.138×10^2

Results

- Numerical identification results:
  - Sensitivity analysis

Table 2: Sensitivity analysis

Parameter	Displacement (mm)							
	4.6	9.2	13.9	18.5	23.1	27.7	32.4	37.0
K_e/K_e^0	1.011	1.021	1.029	1.042	1.065	1.100	1.094	1.097
K_g/K_g^0	1.026	1.035	1.037	1.036	1.032	1.025	1.018	1.032
K_s/K_s^0	1.550	1.573	1.572	1.568	1.555	1.519	1.440	1.543



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Results

- Macro-scale model results:
  - Mesh convergence

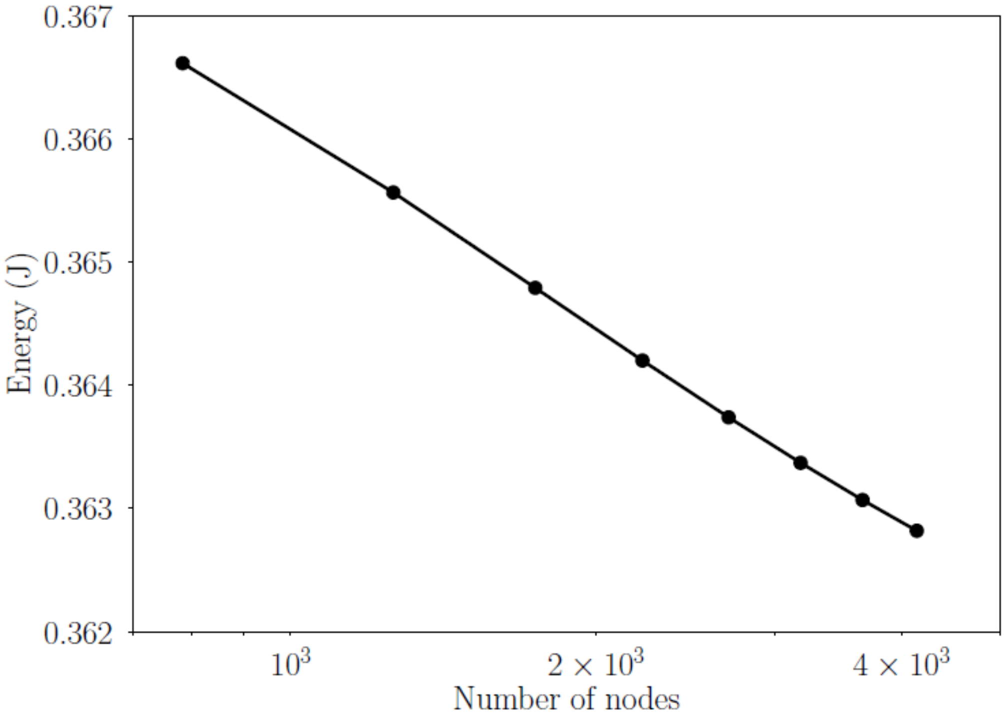

Table 3: Convergence results

	Number of nodes							
	783	1097	1469	1899	2379	2909	3497	4143
Energy (J)	0.3666	0.3655	0.3647	0.3641	0.3637	0.3633	0.3630	0.3628
Error (%)		0.29	0.21	0.16	0.13	0.10	0.08	0.07

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Conclusion

- Implementing a novel optimization procedure for the numerical identification of the parameters
- Consistency of the micro-scale and the macro-scale models in terms of deformation and energy
- Efficiency and robustness of the Trust Region Reflective Algorithm
- Robustness of the developed code by checking the sensitivity

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