

June 7, 2023

MICROSTRUCTURE-BASED ESTIMATION OF THE EFFECTIVE STIFFNESS OF CROSSLINKED, EMBEDDED FIBER NETWORKS

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Sotirios Kakaletsis^{*1}, Emma Lejeune², Manuel K. Rausch¹

¹Aerospace Engineering and Engineering Mechanics, The University of Texas at Austin

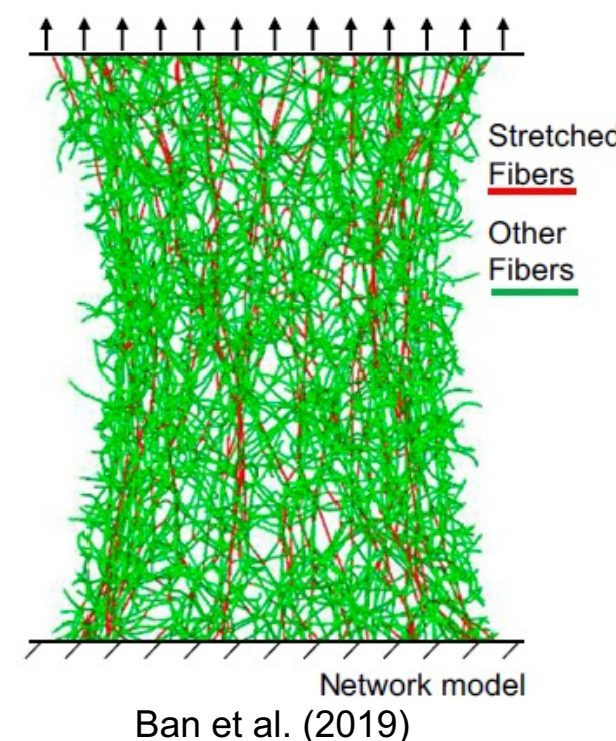
²Mechanical Engineering, Boston University

Introduction

- Semi-flexible biopolymers are ubiquitous building blocks of life, often organized in **fibrous networks**
 - Collagen networks in myocardium, skin, blood vessels, ligaments, tendons etc.
 - Fibrin networks in blood clots

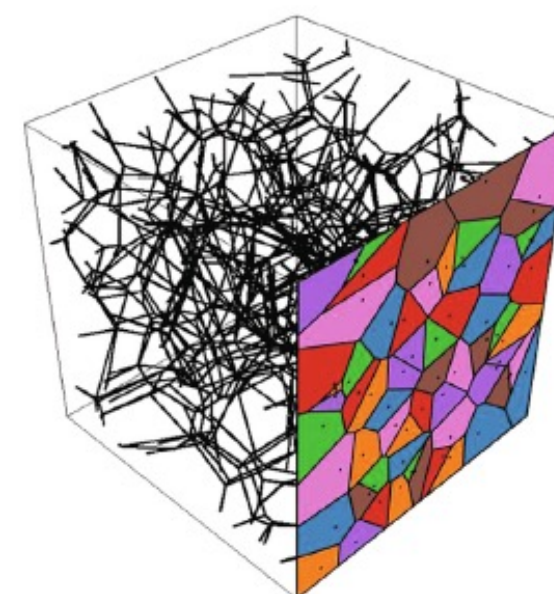
- They exhibit **complex mechanical phenomena**

- Strong nonlinearities
- Strain stiffening
- Anomalous Poisson's effect
- Negative Poynting effect



- Previous efforts have modeled fiber networks in **isolation**:

- No embedding matrix
- Elastic behavior
- Discrete elements



Merson & Picu (2020)

- Why in isolation? – **Discretization**

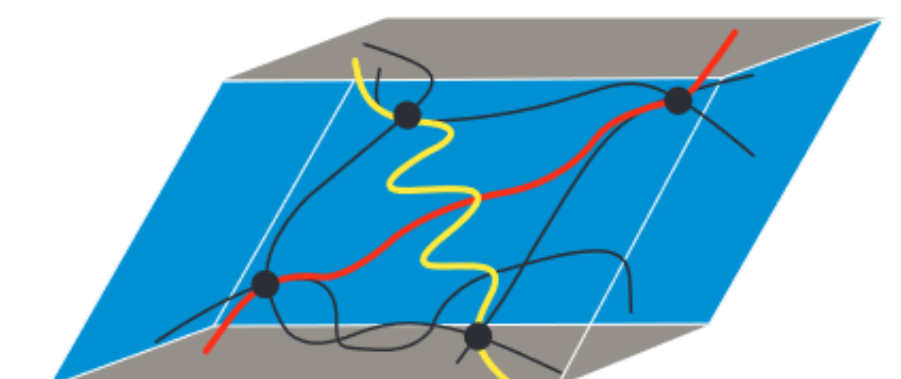
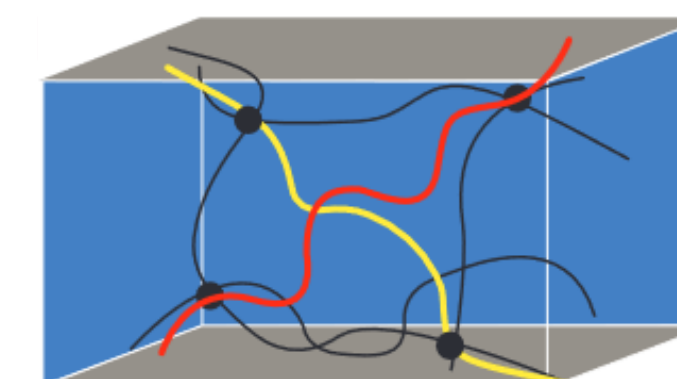
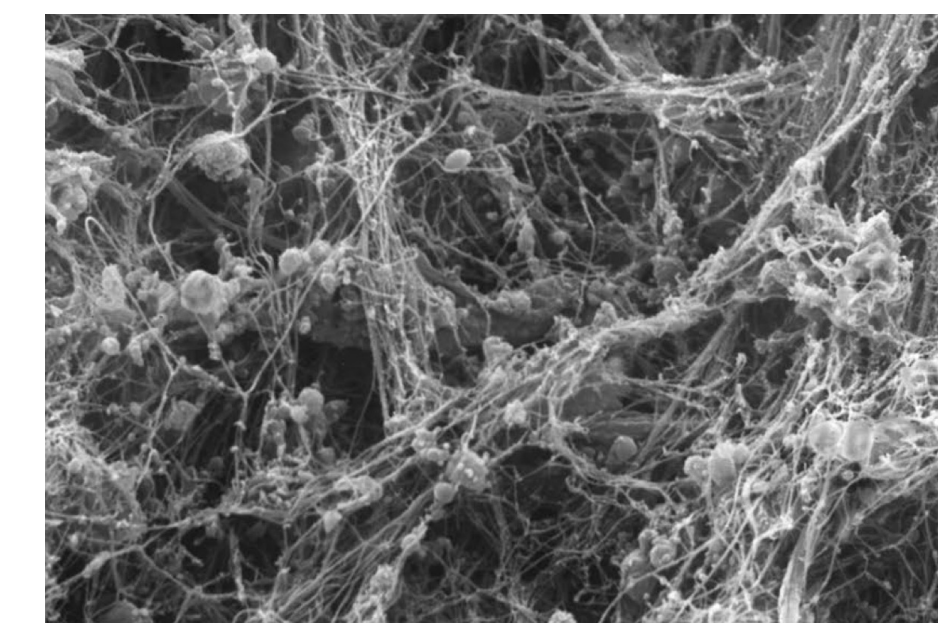
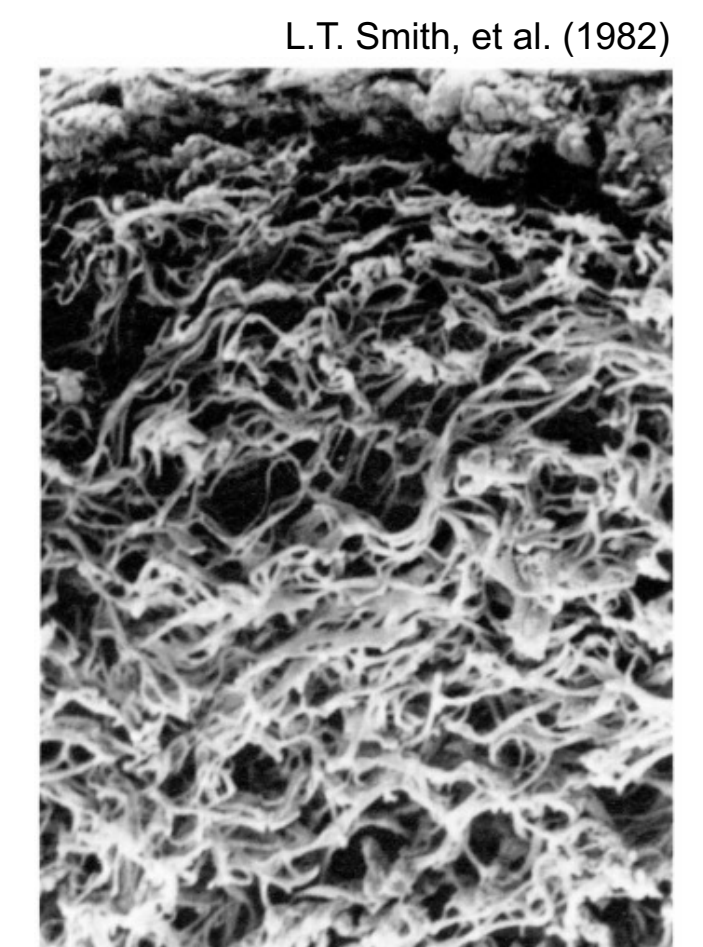
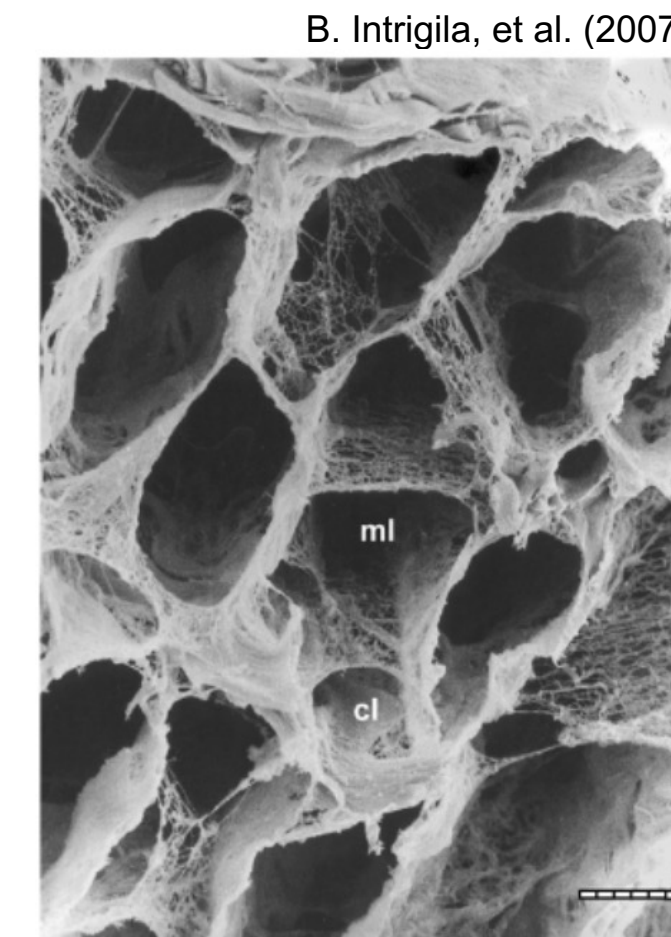
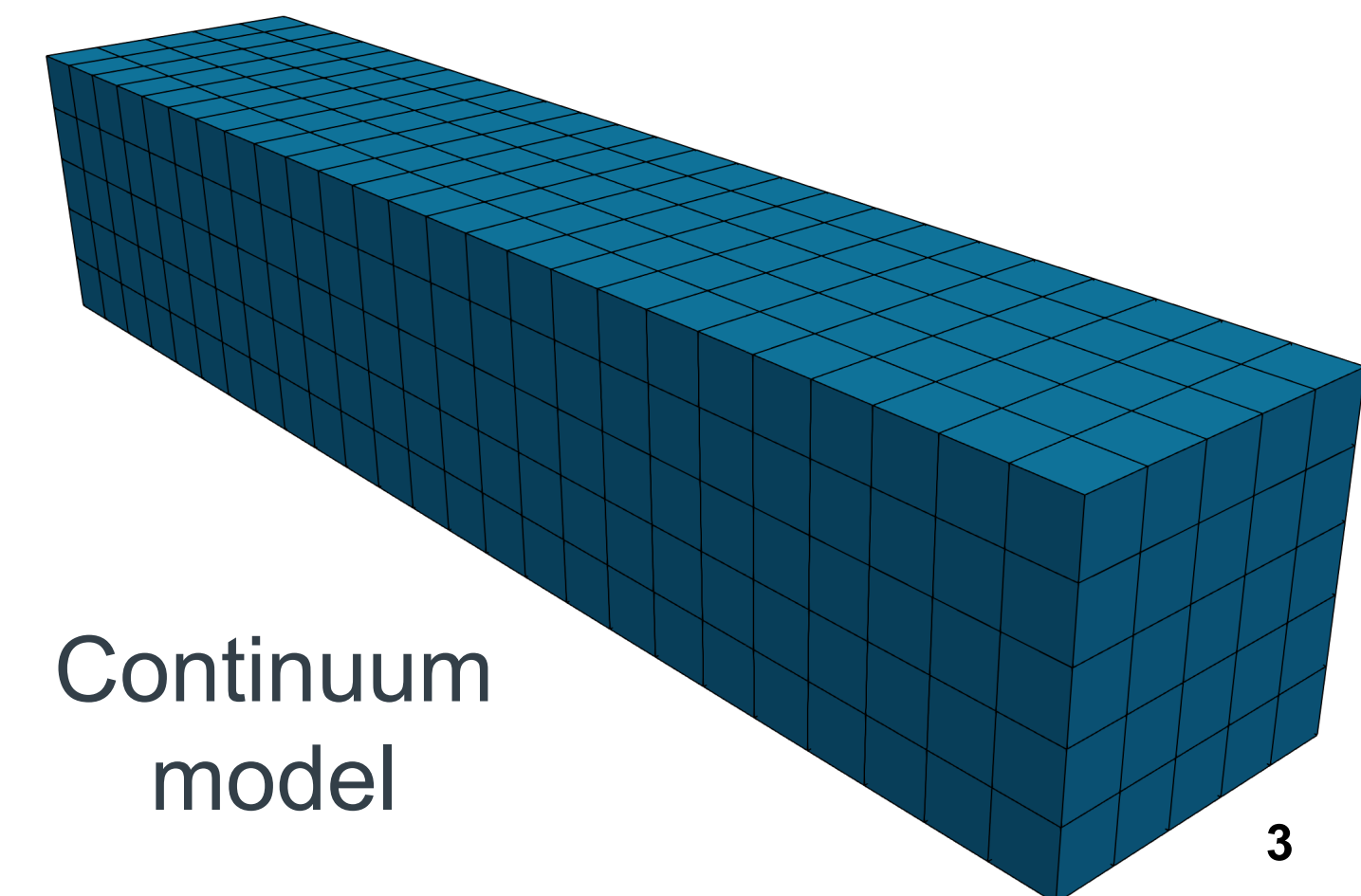
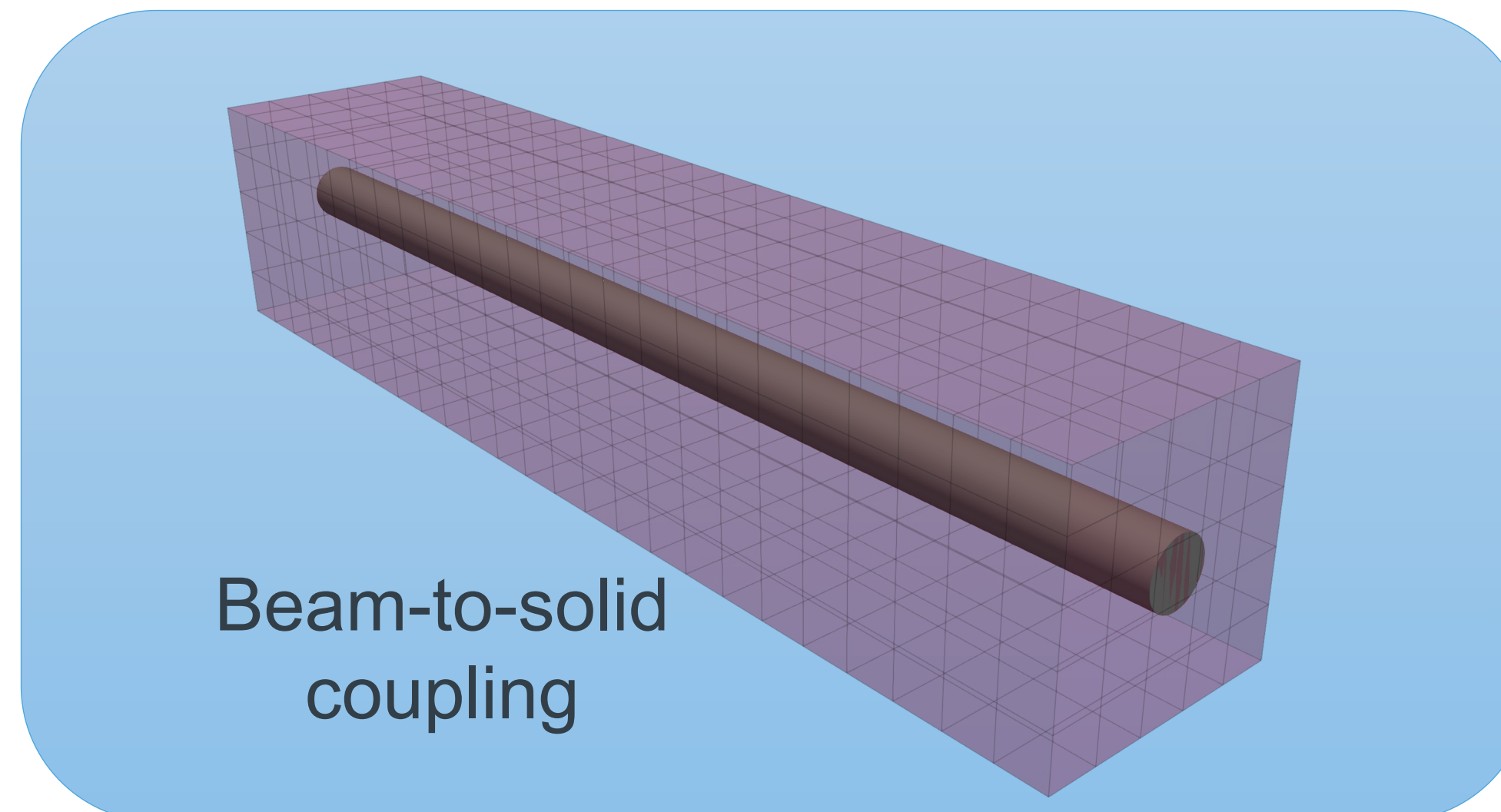
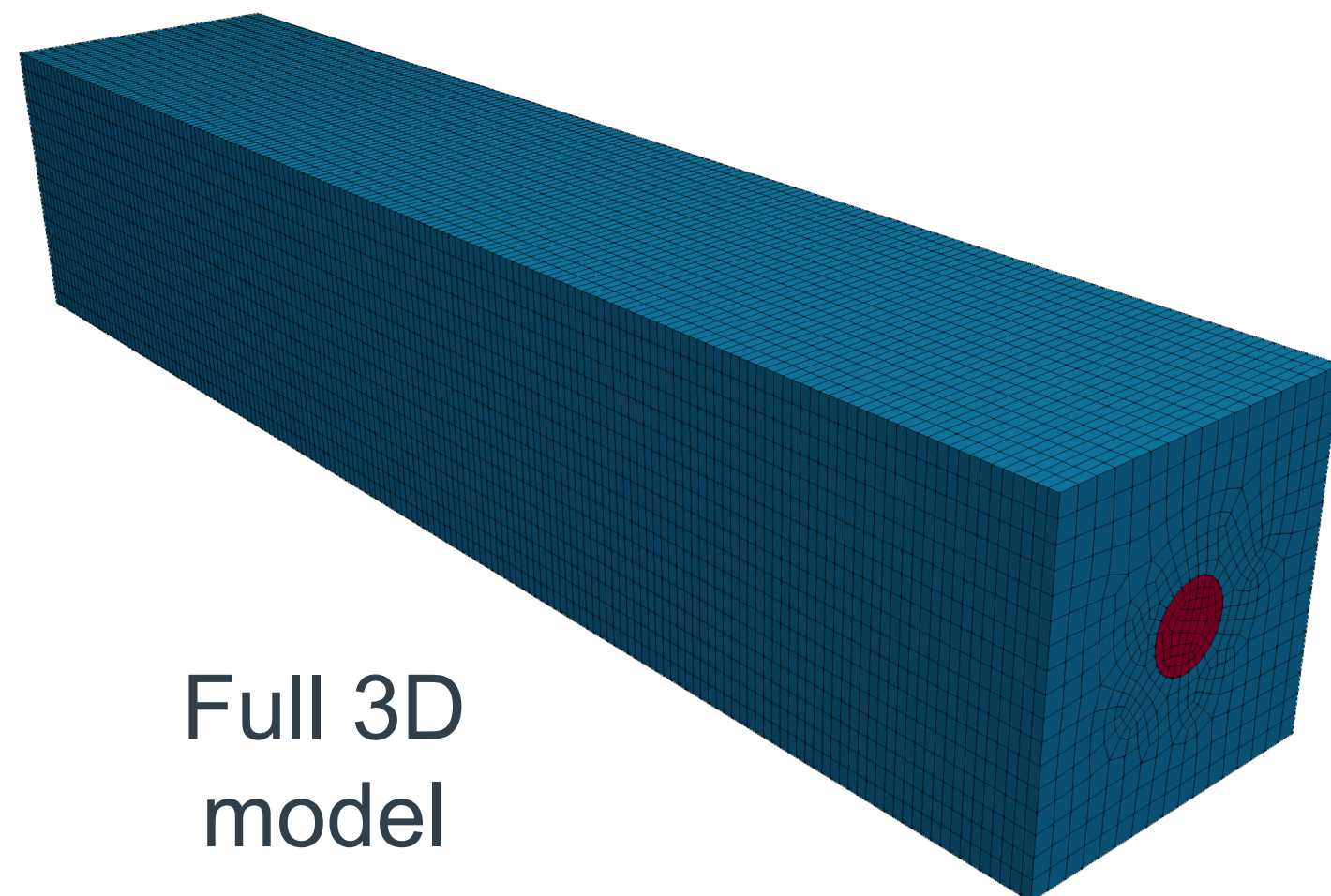


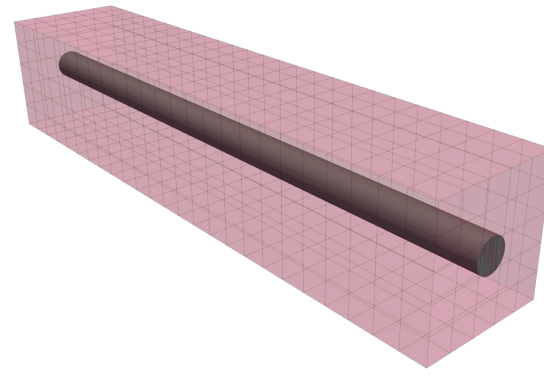
Figure adapted from Janmey P. A., et al. (2016)

Introduction

- **Motivation:** Delineate contributions of each constituent: **matrix** and **fibers**
 - How does network architecture affect the mechanics/ apparent stiffness?
 - Mean fiber length?
 - Fiber undulations?
- **Objective:** Develop a computationally efficient model of the elastic behavior of embedded fiber networks under large deformation.
- Modeling approaches for embedded elastic fibers:



Theory



- Based on previous work by Steinbrecher, Ivo, et al. "**A mortar-type finite element approach for embedding 1D beams into 3D solid volumes.**" *Computational Mechanics* (2020).

- Coupling Constraint:

$$\underline{\mathbf{u}}^B - \underline{\mathbf{u}}^S = \underline{\mathbf{0}} \text{ on } \Gamma_c^{1D-3D} = \Omega^B \text{ (beam centerline)}$$

- Principle of virtual work:

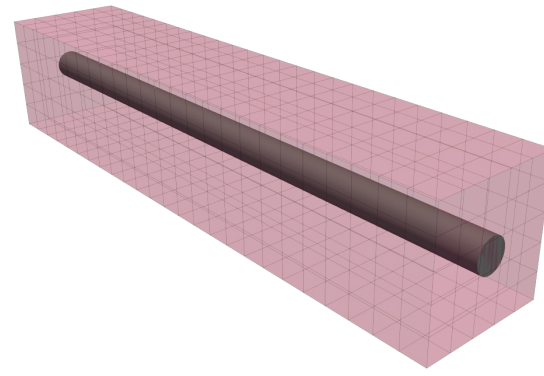
$$\begin{array}{ccc} \text{Solid} & \text{Beam} & \text{Coupling} \\ \delta W^S + \delta W^B + \delta W^C = 0 \end{array}$$

$$\delta W^C = -\delta W_c + \delta W_\lambda = \int_{\Gamma_c^{1D-3D}} \underline{\lambda} (\delta \underline{\mathbf{u}}^B - \delta \underline{\mathbf{u}}^S) ds + \int_{\Gamma_c^{1D-3D}} \delta \underline{\lambda} (\underline{\mathbf{u}}^B - \underline{\mathbf{u}}^S) ds$$

where

$\underline{\lambda} \in \mathbb{R}^3$: Lagrange multiplier field (interface line load)

Theory



- Linearized system:

$$\begin{bmatrix} K_{SS} & \mathbf{0} & -M^T \\ \mathbf{0} & K_{BB} & D^T \\ -M & D & \mathbf{0} \end{bmatrix} \begin{bmatrix} \Delta \mathbf{d}^S \\ \Delta \mathbf{d}^B \\ \lambda \end{bmatrix} = \begin{bmatrix} -f_{int}^S + f_{ext}^S \\ -f_{int}^B + f_{ext}^B \\ g_c \end{bmatrix} \quad \text{where} \quad g_c(\mathbf{d}^S, \mathbf{d}^B) = [-M \quad D] \begin{bmatrix} \mathbf{d}^S \\ \mathbf{d}^B \end{bmatrix}$$

- Enforce coupling constraint using the penalty method and setting $\lambda = \varepsilon \kappa^{-1} g_c(\mathbf{d}^S, \mathbf{d}^B)$

$$\begin{bmatrix} K_{SS} + \varepsilon M^T \kappa^{-1} M & -\varepsilon M^T \kappa^{-1} D \\ -\varepsilon D^T \kappa^{-1} M & K_{BB} + \varepsilon D^T \kappa^{-1} D \end{bmatrix} \begin{bmatrix} \Delta \mathbf{d}^S \\ \Delta \mathbf{d}^B \end{bmatrix} = \begin{bmatrix} -f_{int}^S + f_{ext}^S - f_c^S \\ -f_{int}^B + f_{ext}^B - f_c^B \end{bmatrix}$$

with

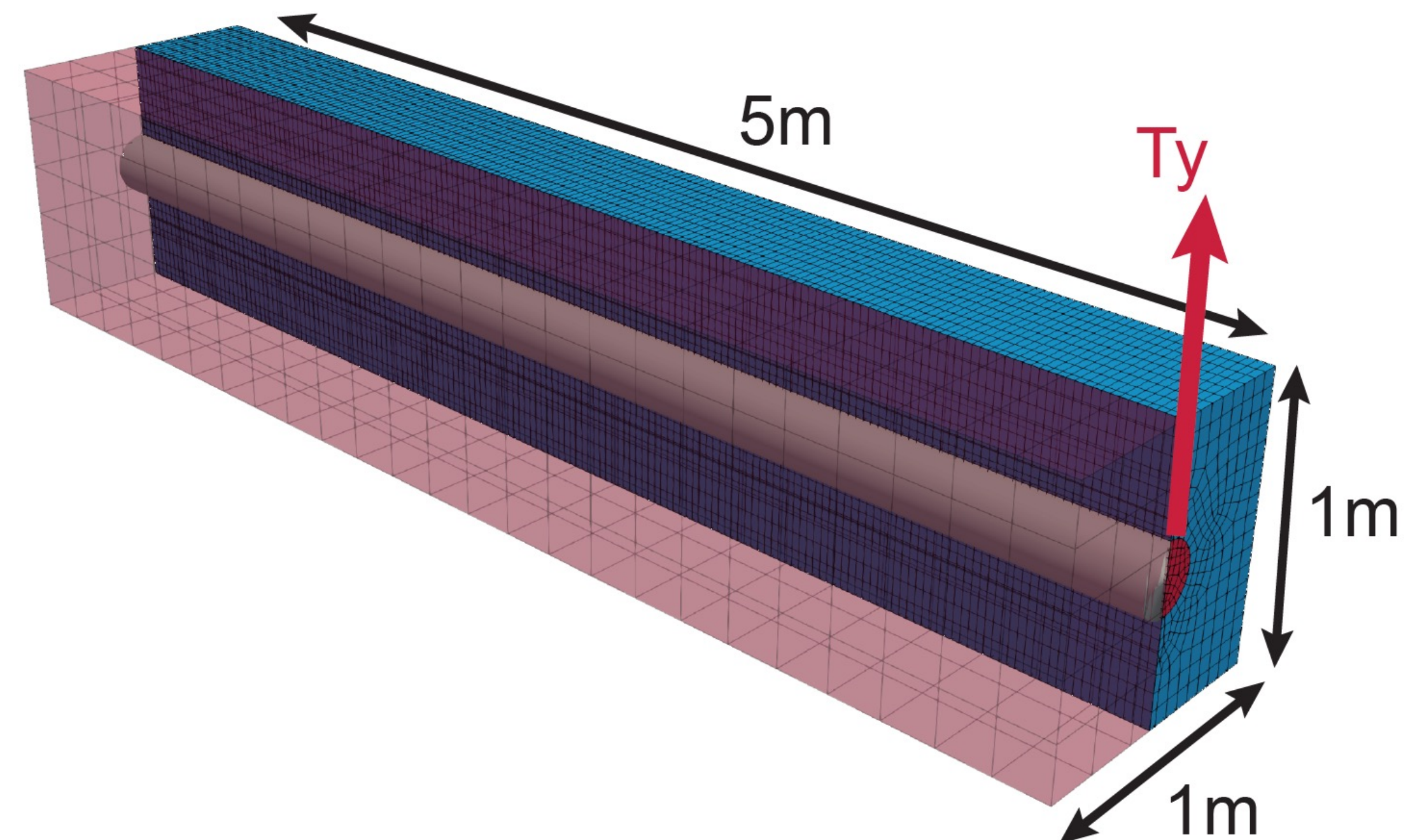
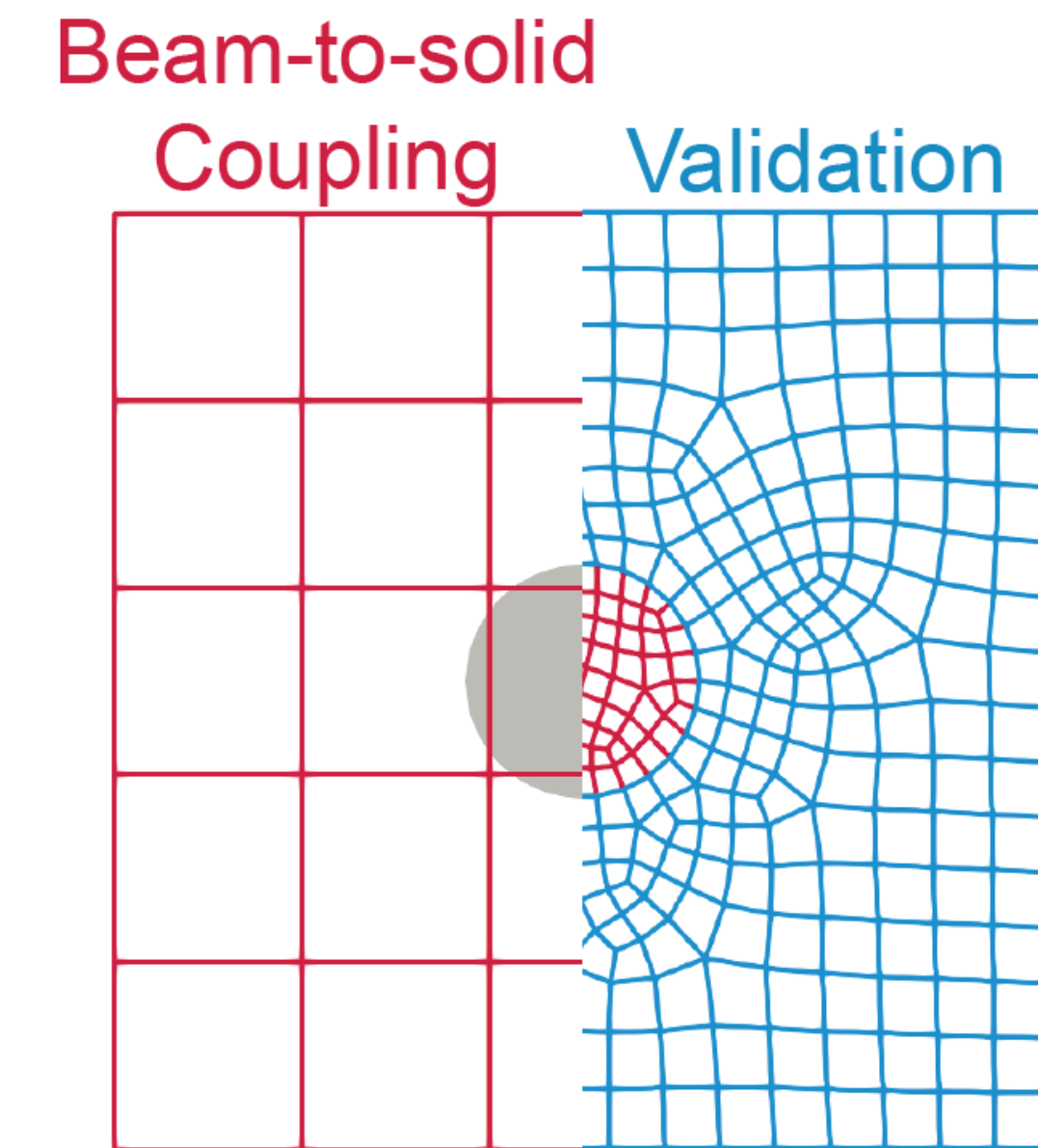
$$-f_c^S = \varepsilon M^T \kappa^{-1} [-M \quad D] \begin{bmatrix} \mathbf{d}^S \\ \mathbf{d}^B \end{bmatrix}$$

$$-f_c^B = \varepsilon D^T \kappa^{-1} [-M \quad D] \begin{bmatrix} \mathbf{d}^S \\ \mathbf{d}^B \end{bmatrix}$$

Validation

- Reinforced cantilever beam, fixed on the left end, applied distributed load on the free face (right end).
- Comparison between the full 3D model (reference solution) and our beam-to-solid coupling Abaqus implementation.
- Displacement error of the solid domain:

$$\|e\| = \sqrt{\frac{\int_{V_0} \|\underline{\mathbf{u}}^S - \underline{\mathbf{u}}_{ref}^S\|^2 dV_0}{\int_{V_0} \|\underline{\mathbf{u}}_{ref}^S\|^2 dV_0}}$$



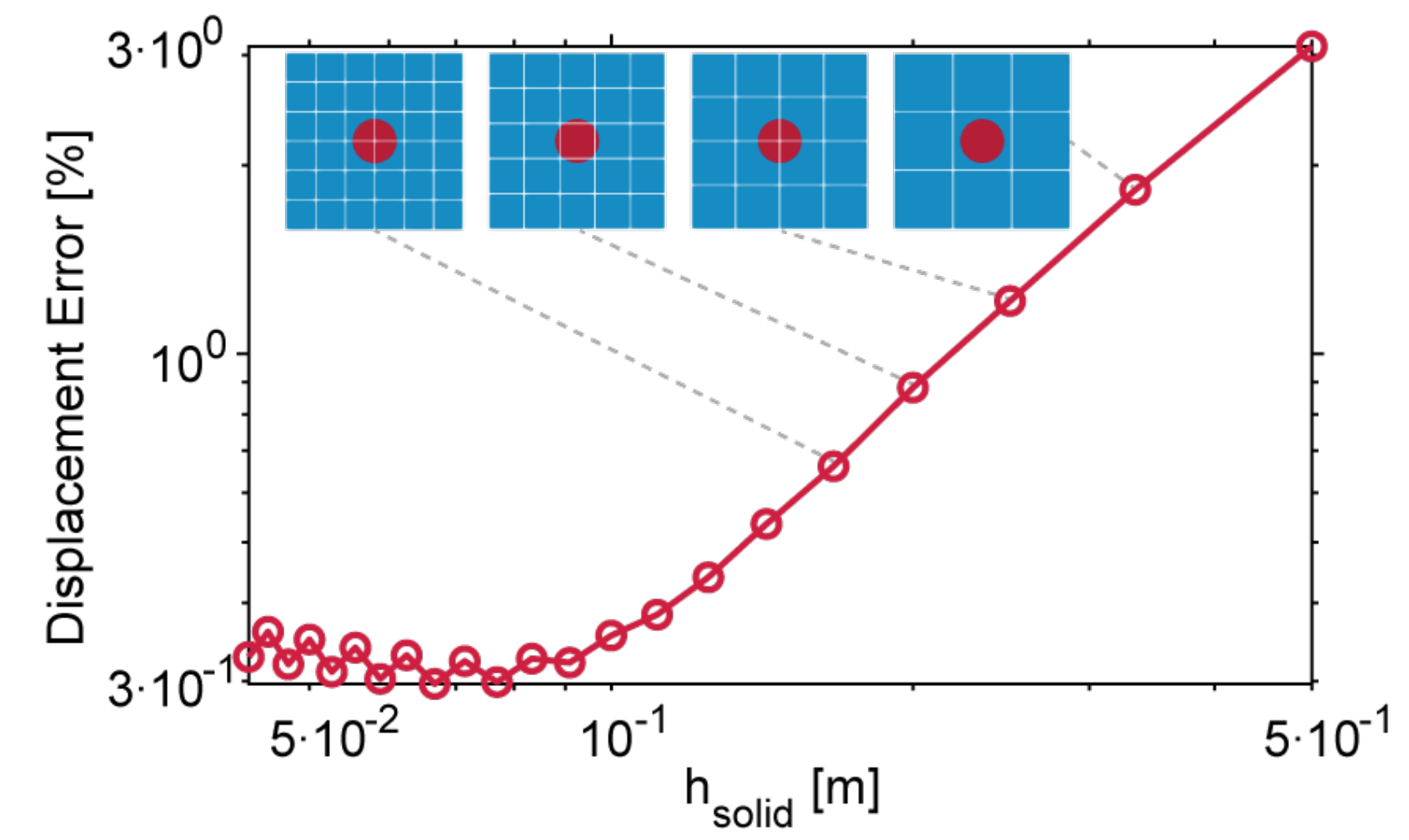
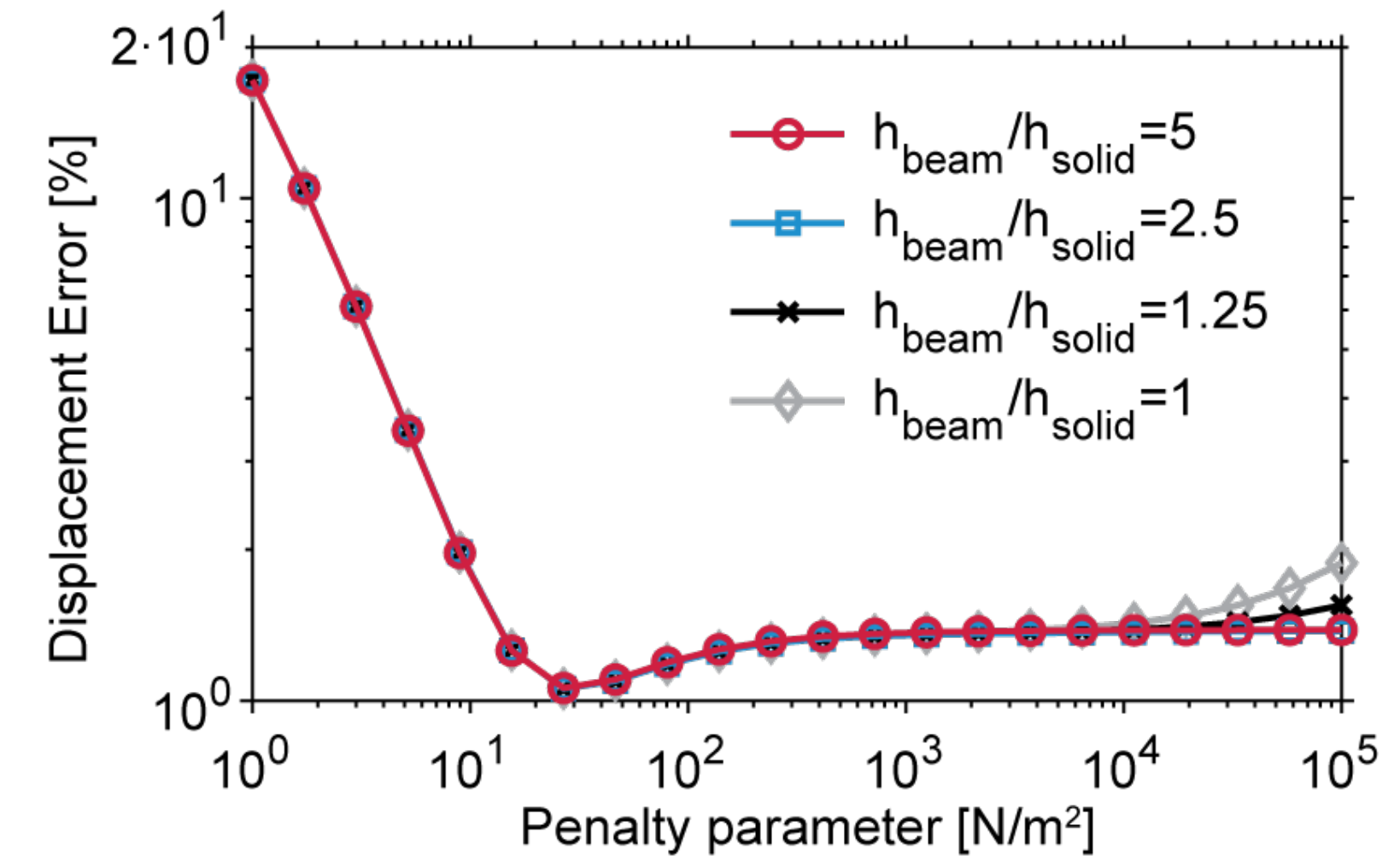
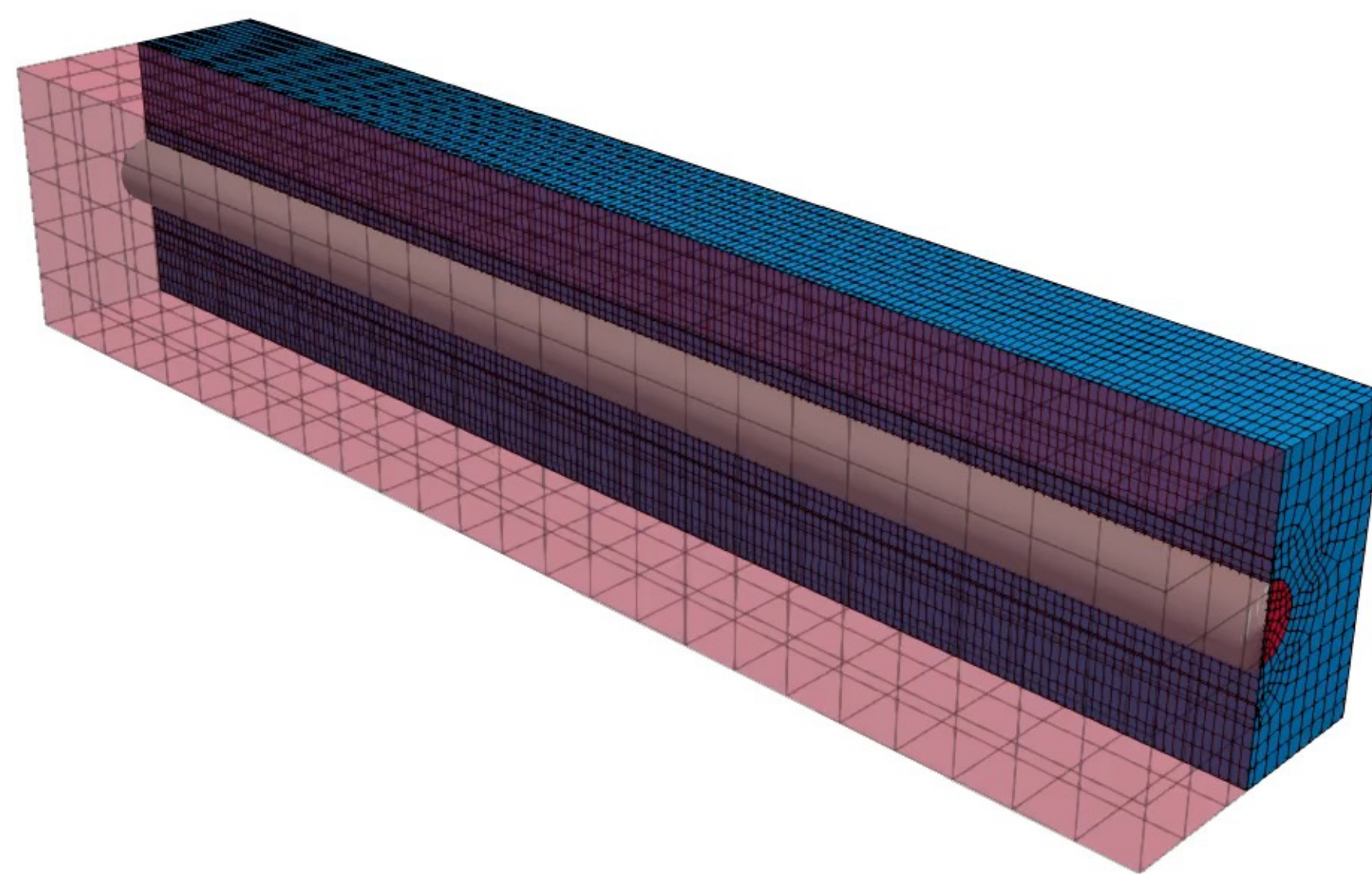
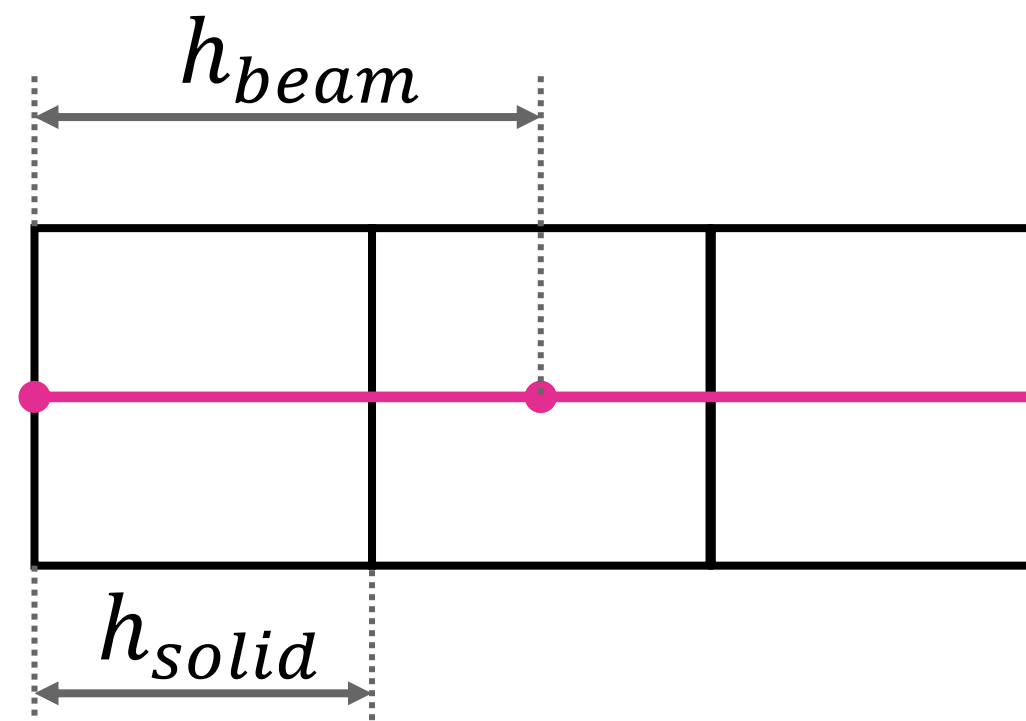
Validation – Sensitivity Studies

- Limitations
 - Beam element size > Solid element size
 - Solid element size ≈ Fiber radius

- Displacement error: < 1.0%

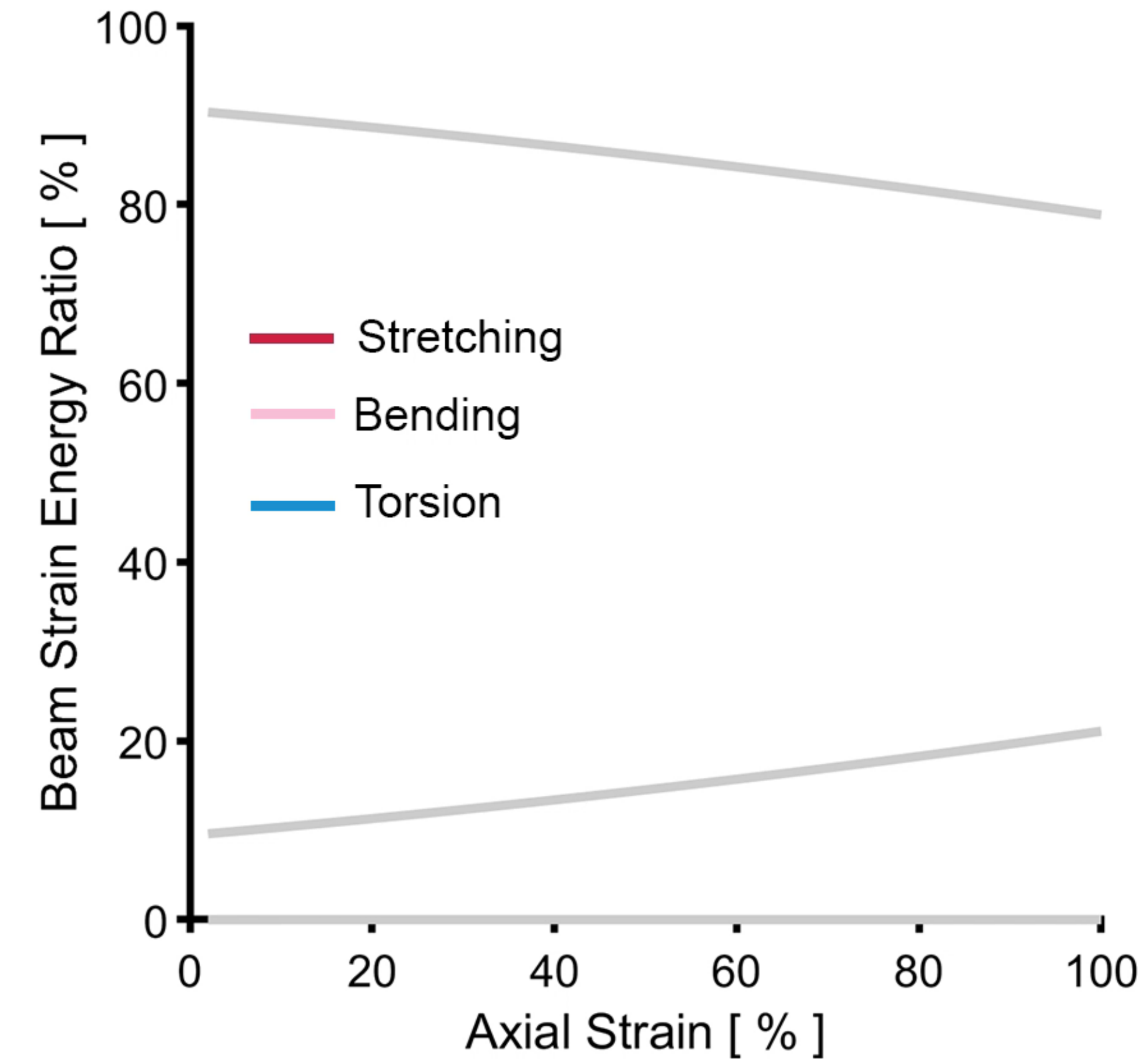
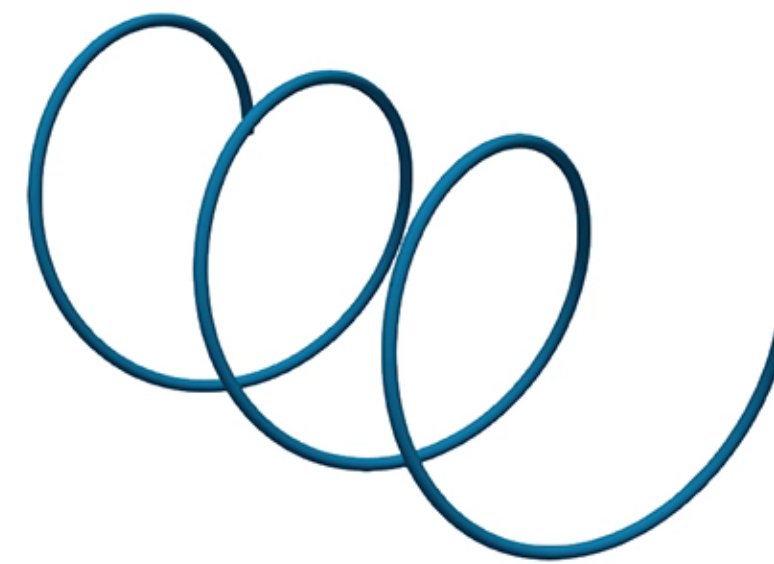
- Reference solution
 - Solid elements: 75,985
 - CPU time: 2210 sec

- Beam-to-solid coupling
 - Solid elements: 625
 - CPU time: 29 sec



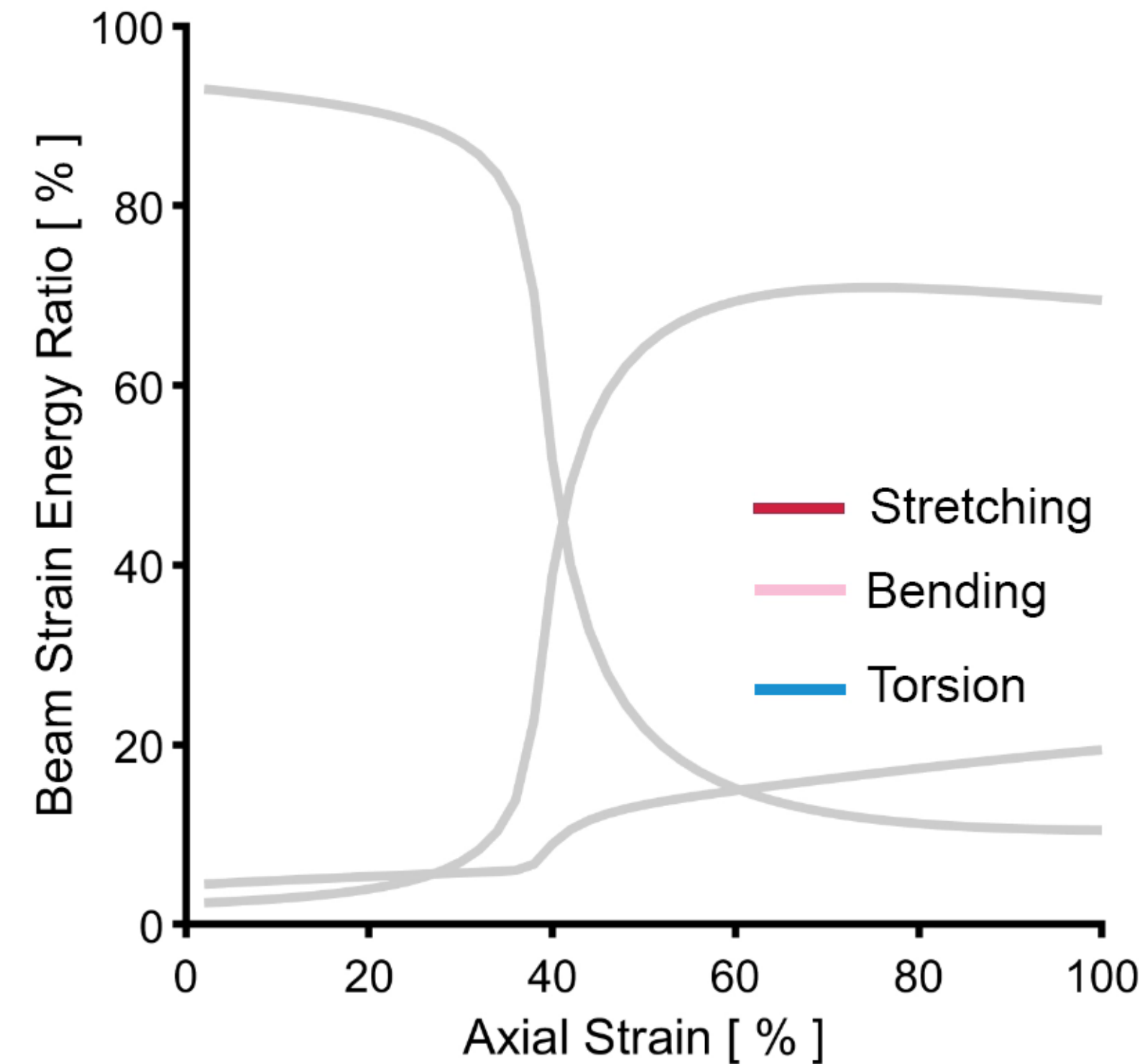
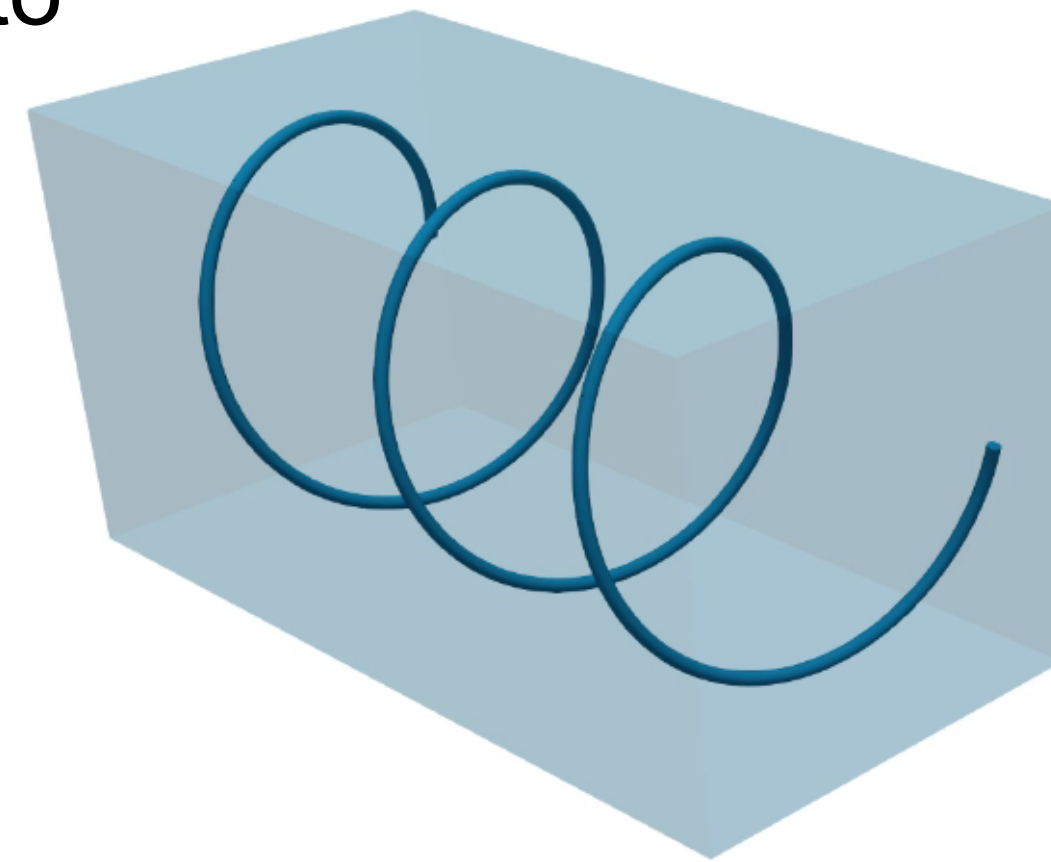
Example: Helical Beam

- Spatial Timoshenko beam.
- Linear elastic material law.
- Uniaxial extension to 100% strain.
- Strain energy components:
 - Axial stretching
 - Bending
 - Torsional



Example: Helical Beam

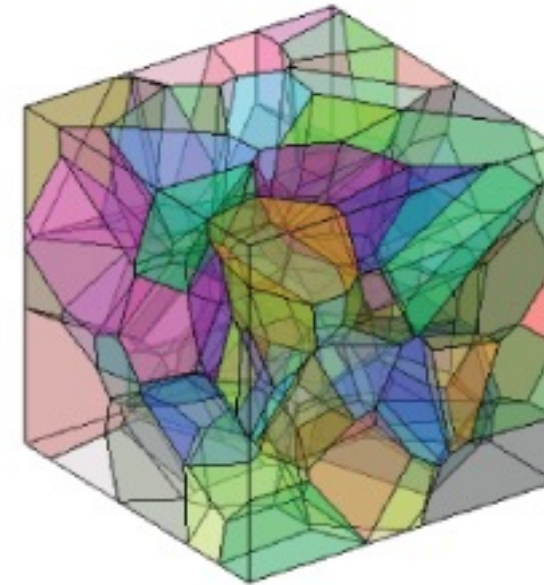
- Same beam, embedded into isotropic, incompressible Neo-hookean material.
- Our model is able to:
 - Capture beam instabilities caused by the solid-to-beam interaction forces.
 - Delineate the contribution of each strain energy component.
 - Investigate the effect of the relative stiffness between the solid matrix and the beam.



Embedded Fiber Networks

- Voronoi-based networks

- Average connectivity number $\langle z \rangle = 3.4$
- Introduce sinusoidal undulations



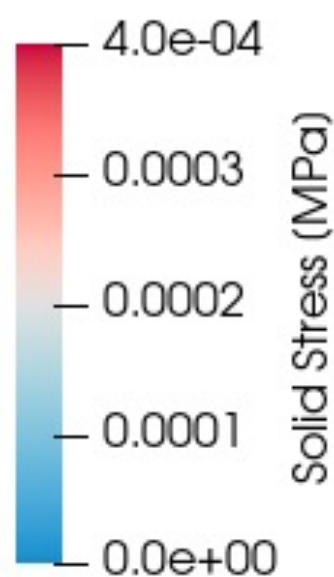
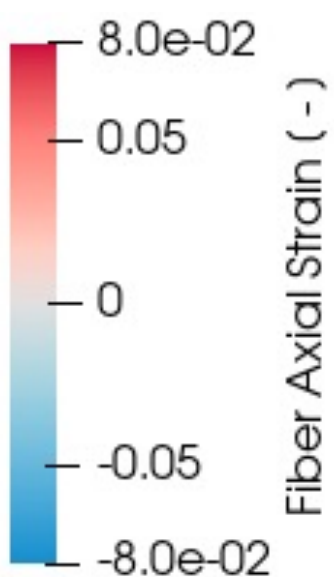
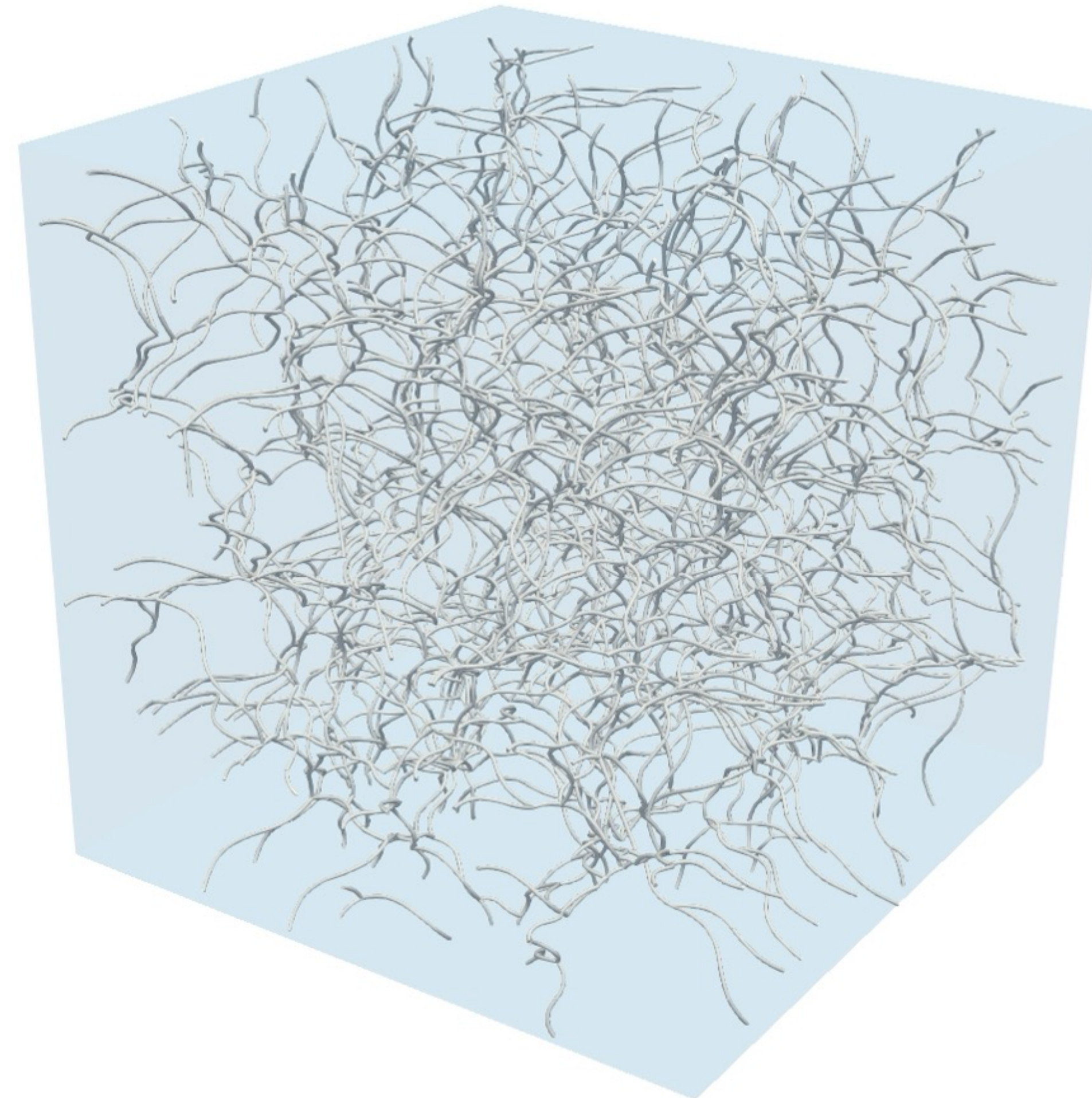
- Simple shear deformation

- Rigid displacement boundary conditions
- Cubic geometry
- Deformed up to 50% shear strain

- Effective Stiffness

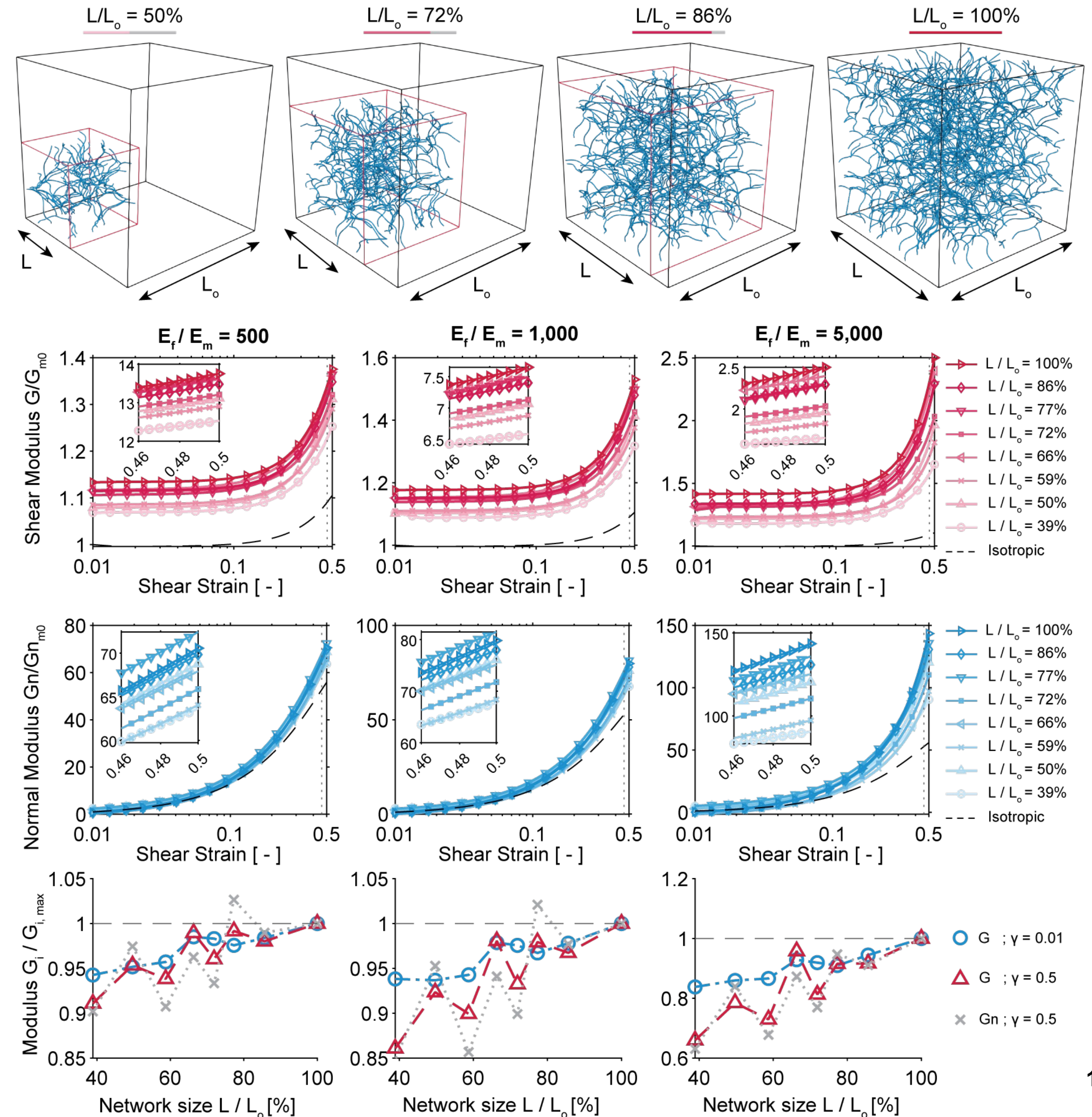
- Shear & Normal moduli

$$G = \frac{\Delta\sigma_{xy}}{\Delta\gamma}, \quad G_n = \frac{\Delta\sigma_{yy}}{\Delta\gamma}$$



Size Effect

- Investigated the size effect on the apparent stiffness
 - Varying network sizes with same density
 - Shear Modulus
 - Normal Modulus
 - At three different fiber-to-matrix stiffness ratio E_f/E_m
- The size effect is more prominent at
 - Higher fiber-to-matrix stiffness ratio
 - Shear modulus at the low-strain regime
- Highest density network converges sufficiently for both Shear and Normal moduli
 - Increasing fiber number the change in effective moduli decreases



Density Effect

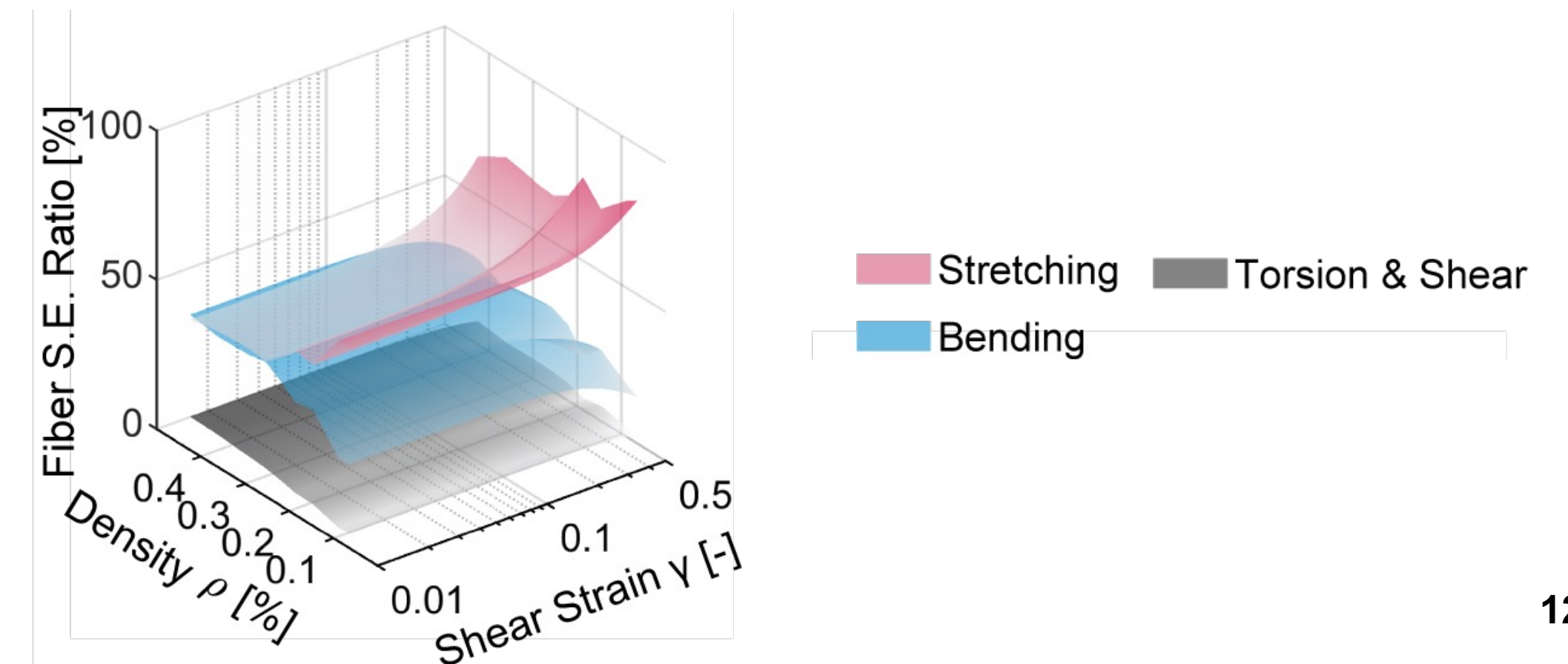
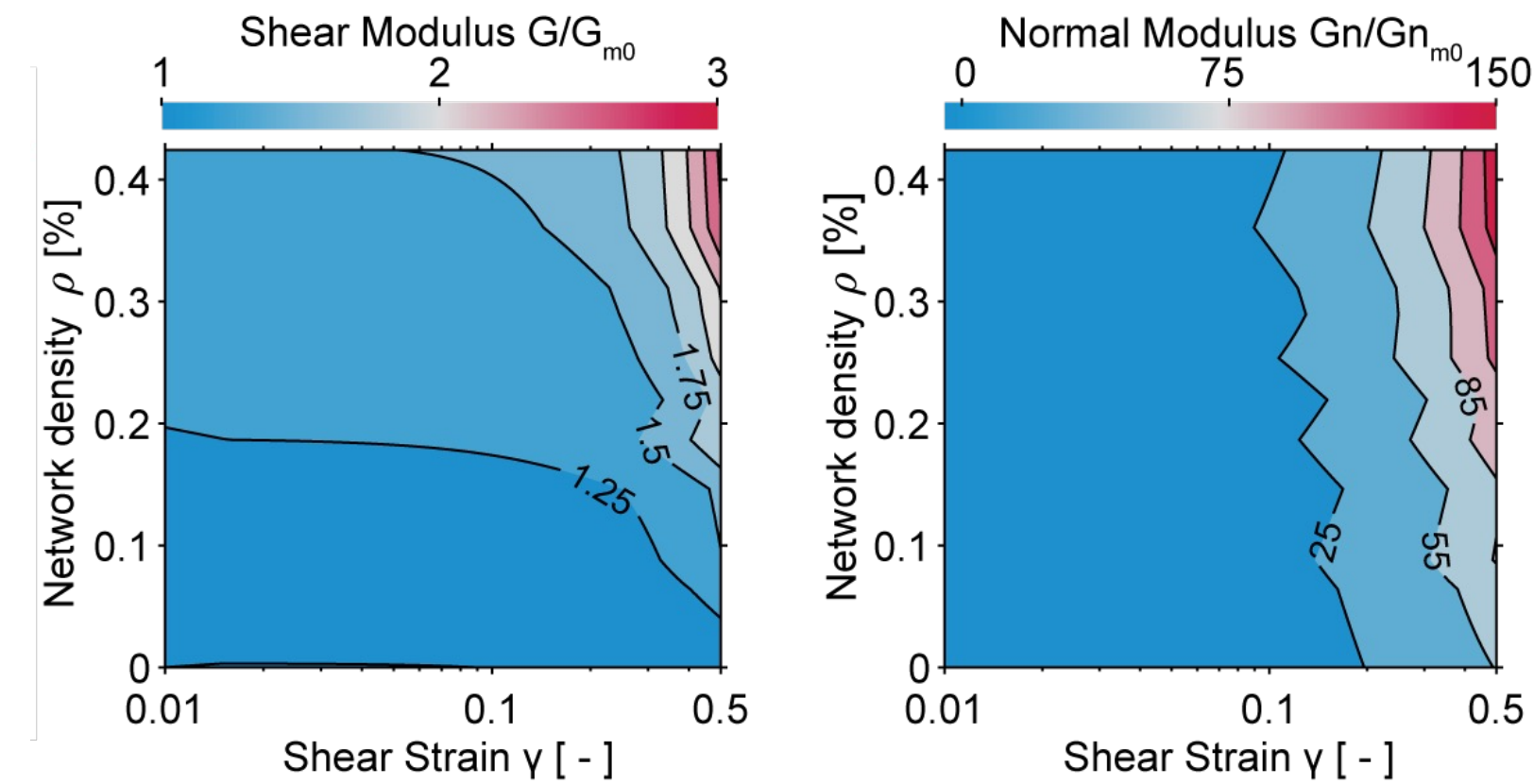
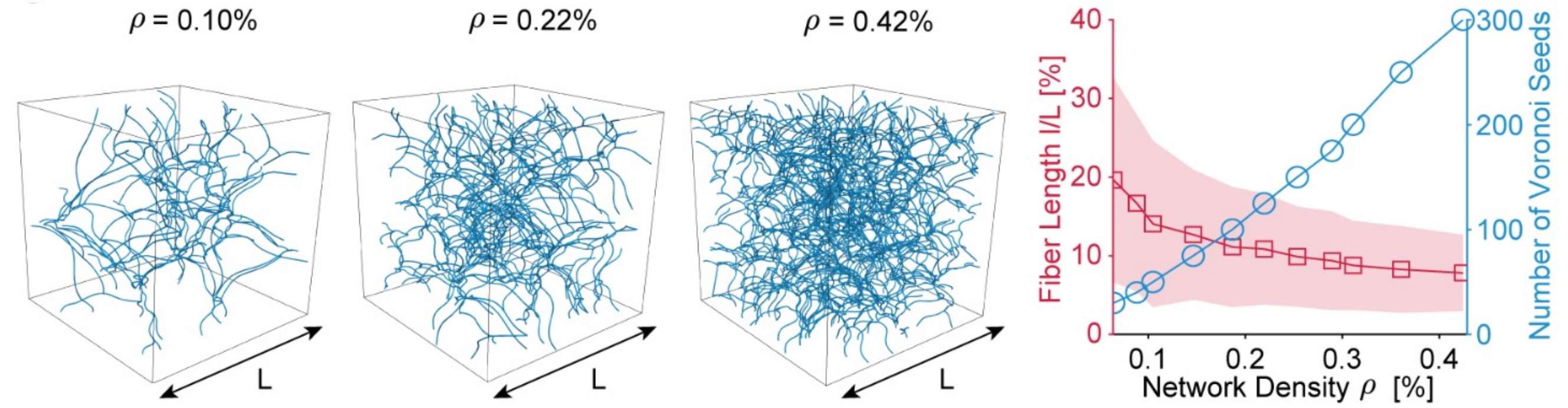
Network Density Study

- Constant network size (edge length)
- Decreasing mean fiber length
- Increasing network density
- Simple Shear deformation

Embedding fiber networks leads to

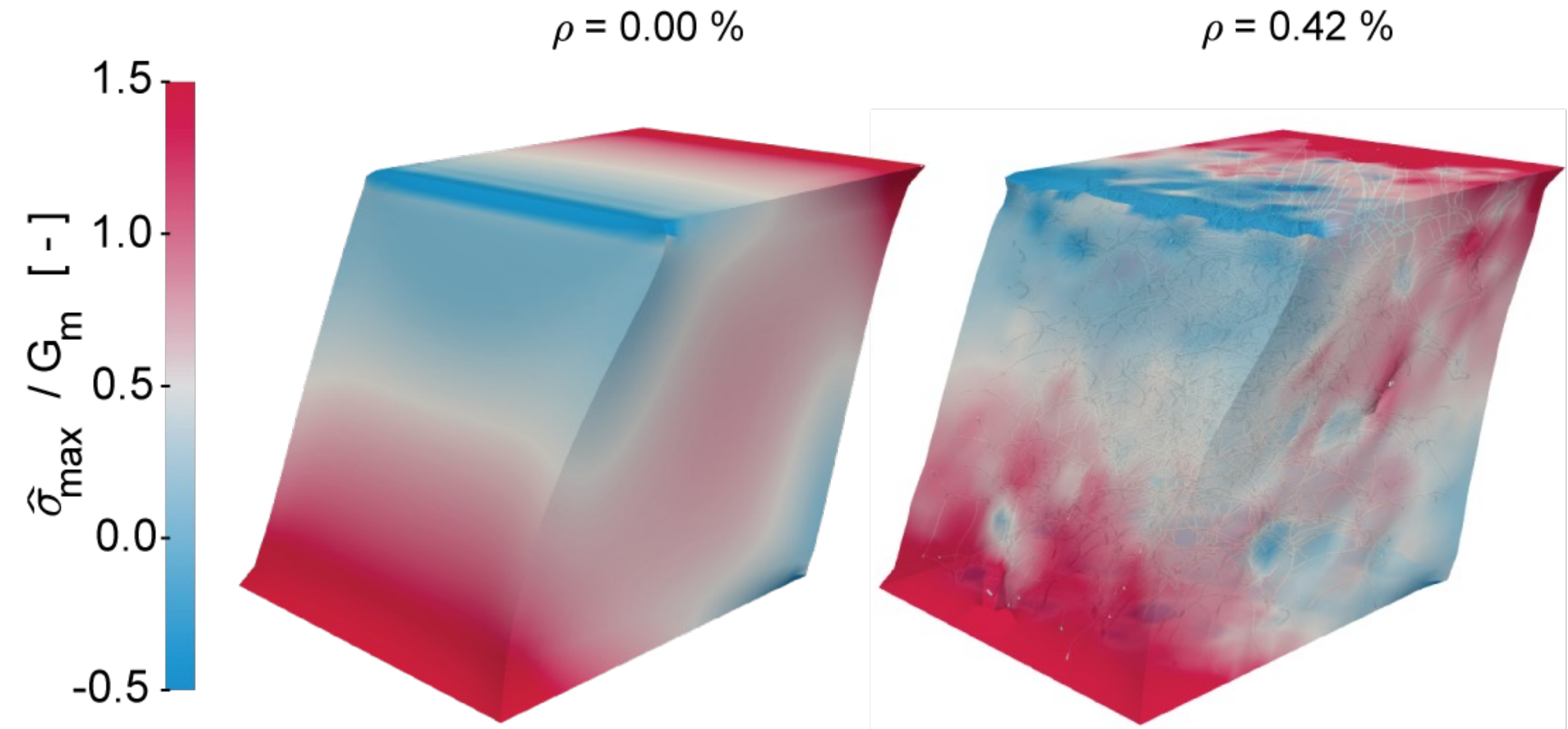
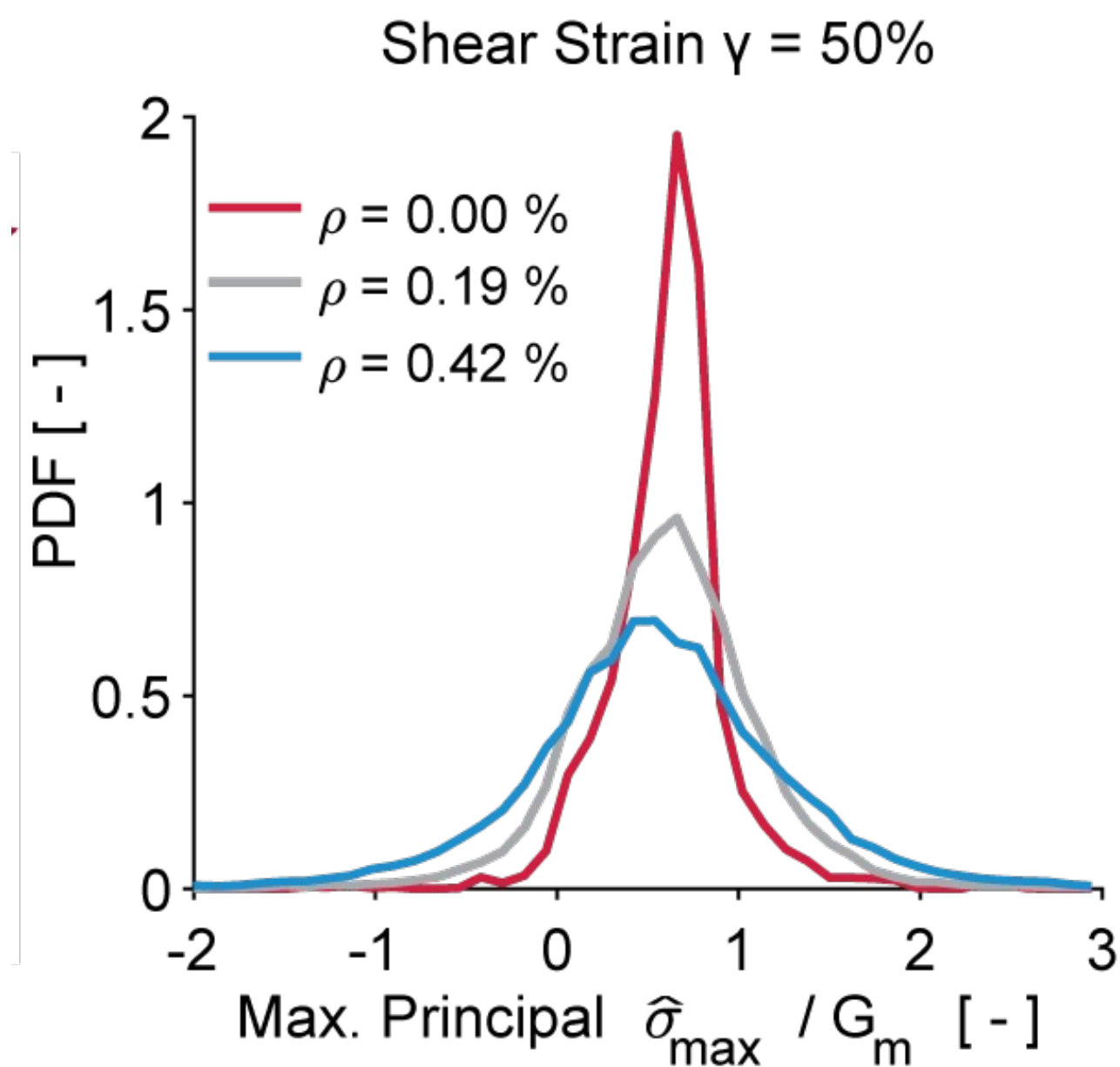
- Strain stiffening behavior
- A more pronounced negative Poynting effect

- From a strain energy perspective, these phenomena are driven primarily by fiber stretching, rather than bending or torsion



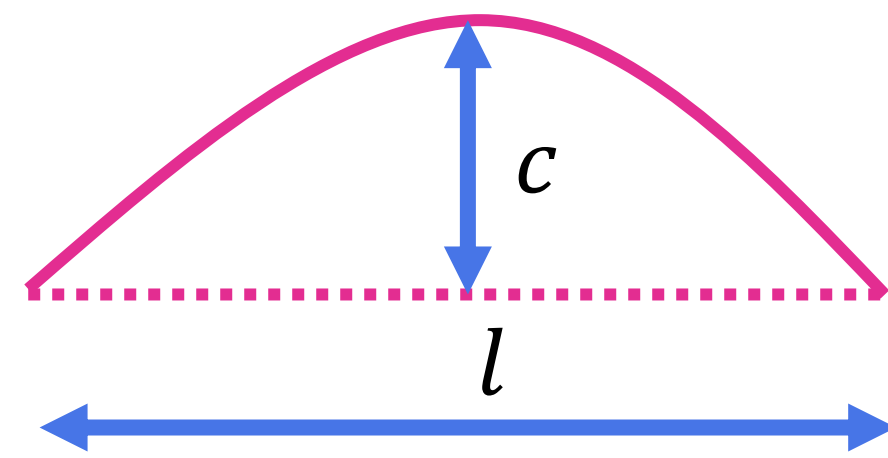
Networks and Matrix-stress Distribution

- Distribution of max. principal stress as a function of network density
- Embedding networks introduce
 - Stress heterogeneity
 - Local stress concentrations

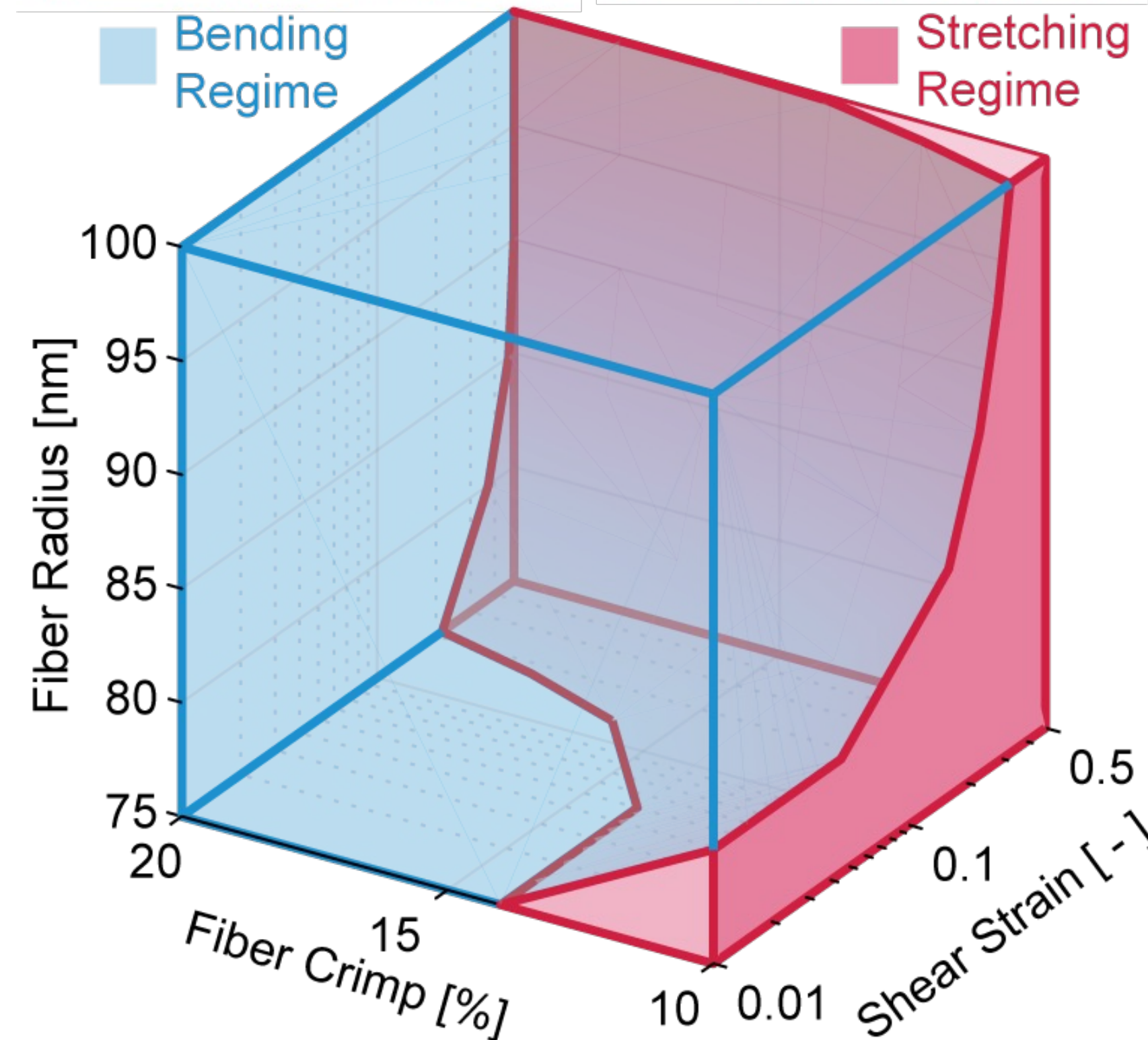
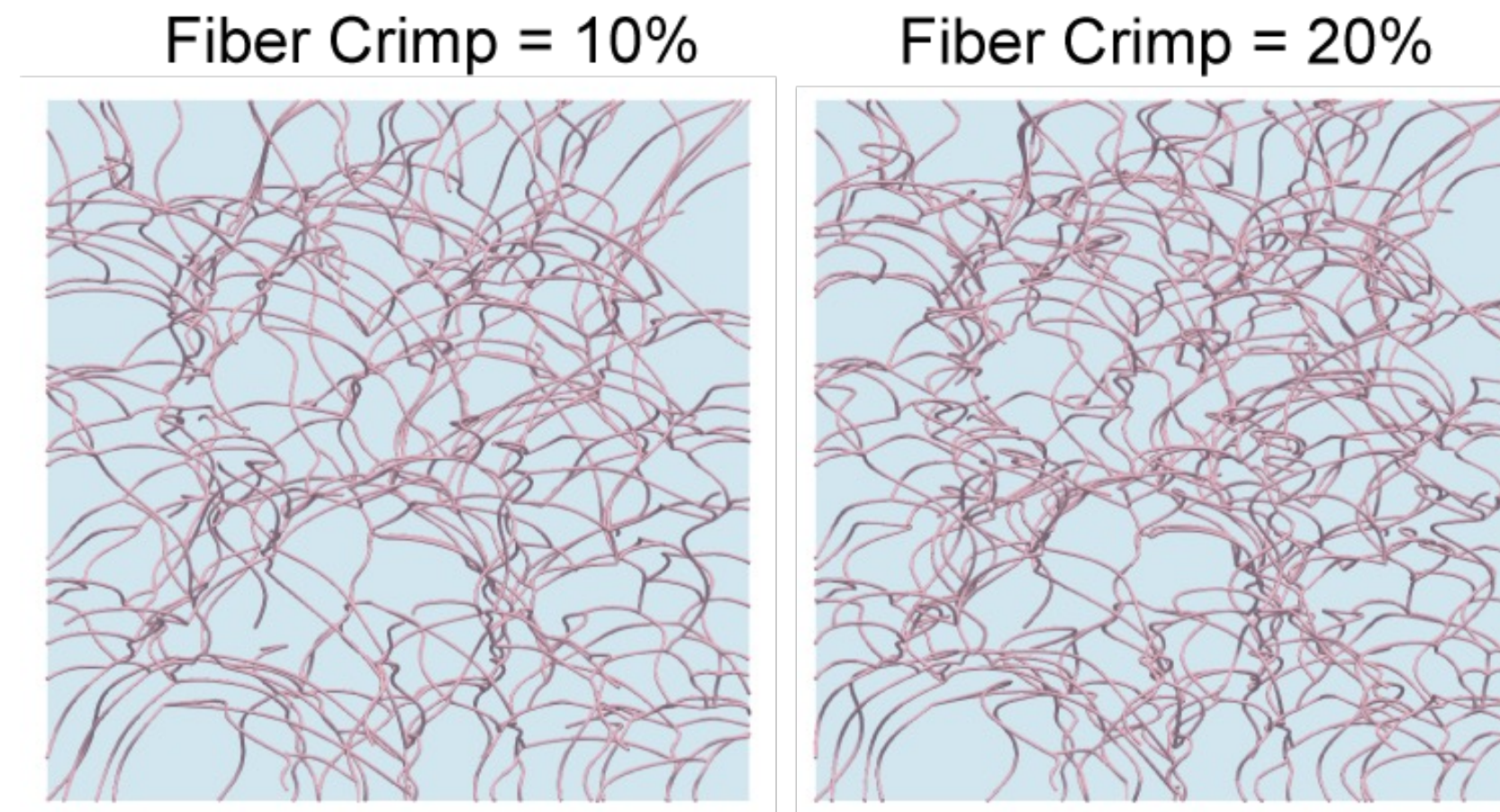


Fiber Strain Energy

- Fiber crimp c/l [%] & fiber radius

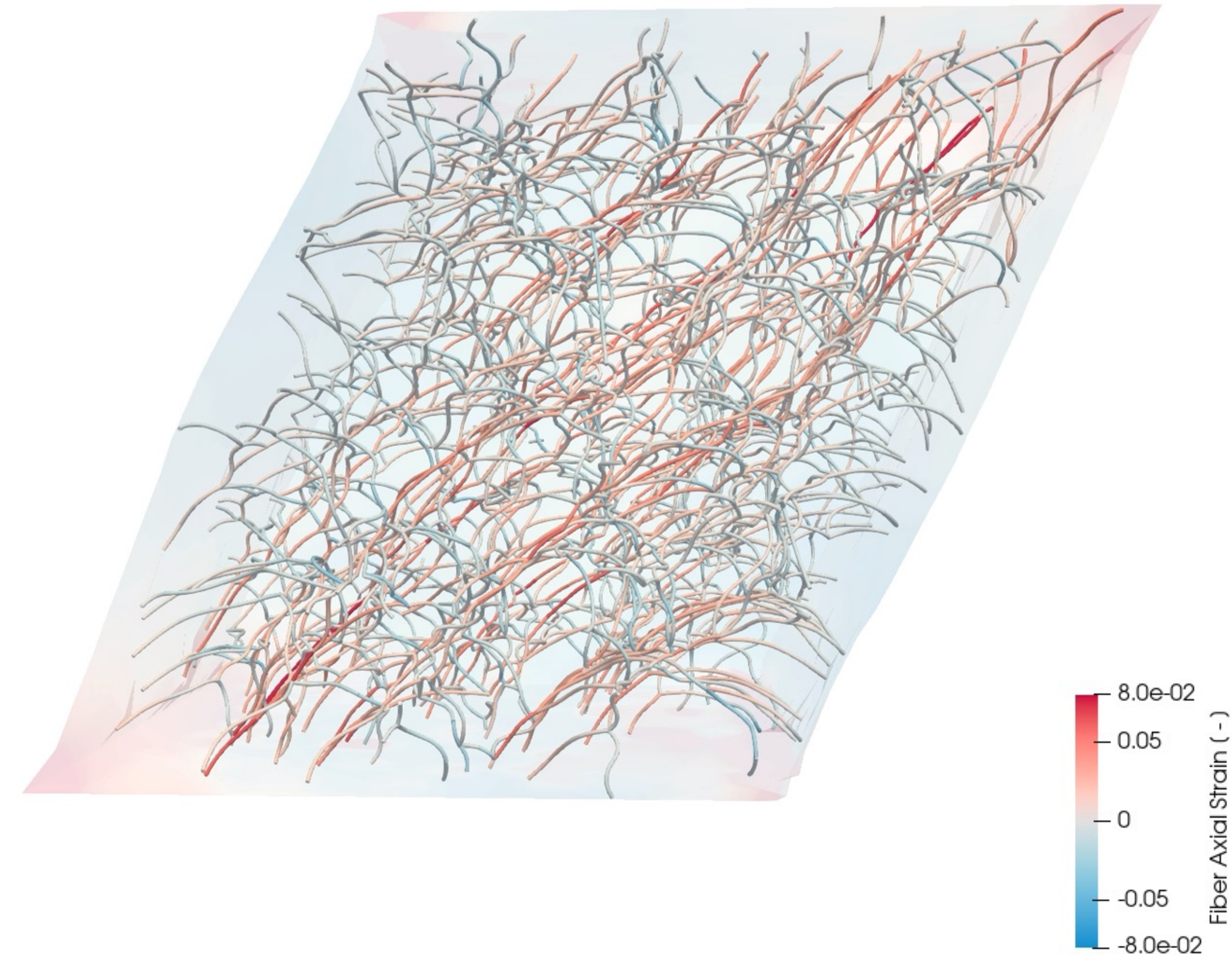


- Stretching energy dominates for
 - Large deformations
 - Fibers with small undulations
 - Fibers with small radii
- Bending energy dominates for
 - linear/small deformations
 - fibers with large undulations
 - fibers with large radii



Conclusion

- Given the limitations presented (penalty parameter, mesh size, element length ratio), the mortar-type finite element approach can provide efficient models for embedded fiber networks.
- Embedding fiber networks leads to
 - Strain stiffening behavior
 - Negative Poynting effect
 - Stress heterogeneity
- Stretching (membrane) strain energy dominates the mechanics at large deformations.
- Future work
 - Interpret experimental data (blood clot modeling).
 - Expand on viscoelastic and/or damage-failure models of the fibers.



THANK YOU.

Dr. Manuel Rausch

**SOFT TISSUE
BIOMECHANICS
LABORATORY**



The University of Texas at Austin
Aerospace Engineering
and Engineering Mechanics
Cockrell School of Engineering



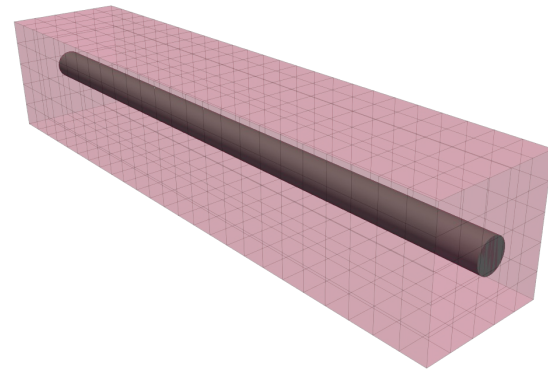


The University of Texas at Austin

**Aerospace Engineering
and Engineering Mechanics**

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Theory



- Discretization of the solid, beam displacement and the Lagrange multiplier (LM) fields:

$$\underline{\mathbf{u}}_h^S = \sum_{k=1}^{n_S} N_k(\xi, \zeta, \eta) \mathbf{d}_k^S$$

$$\underline{\mathbf{u}}_h^B = \sum_{l=1}^{n_B} H_l(\xi^B) \mathbf{I}^{3 \times 3} \mathbf{d}_l^B$$

$$\underline{\boldsymbol{\lambda}}_h = \sum_{j=1}^{n_\lambda} \Phi_j(\xi^B) \boldsymbol{\lambda}_j$$

- Coupling matrices from δW^c (integration on the beam centerline):

$$\mathbf{D}^{(j,l)} = \int_{\Gamma_{c,h}^B} \Phi_j H_l(\xi^B) ds \mathbf{I}^{3 \times 3}$$

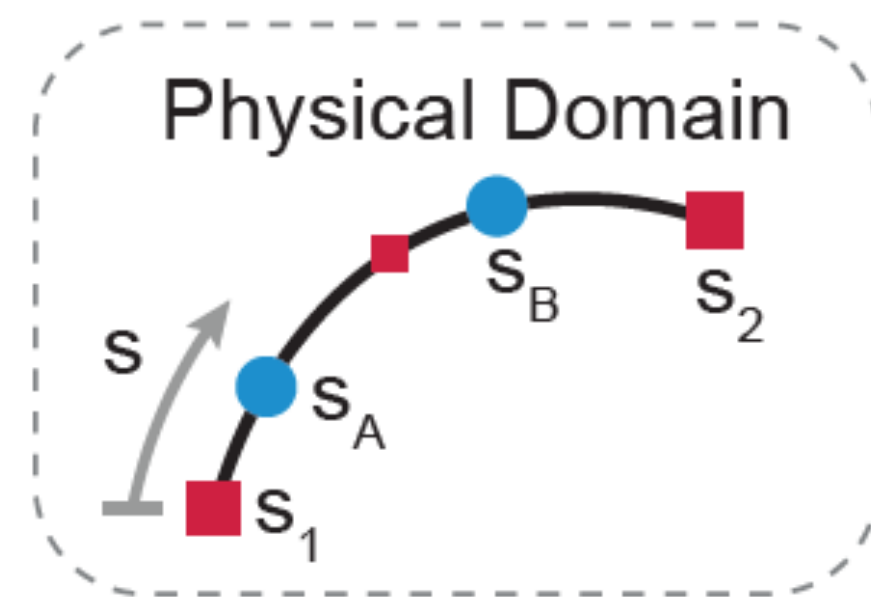
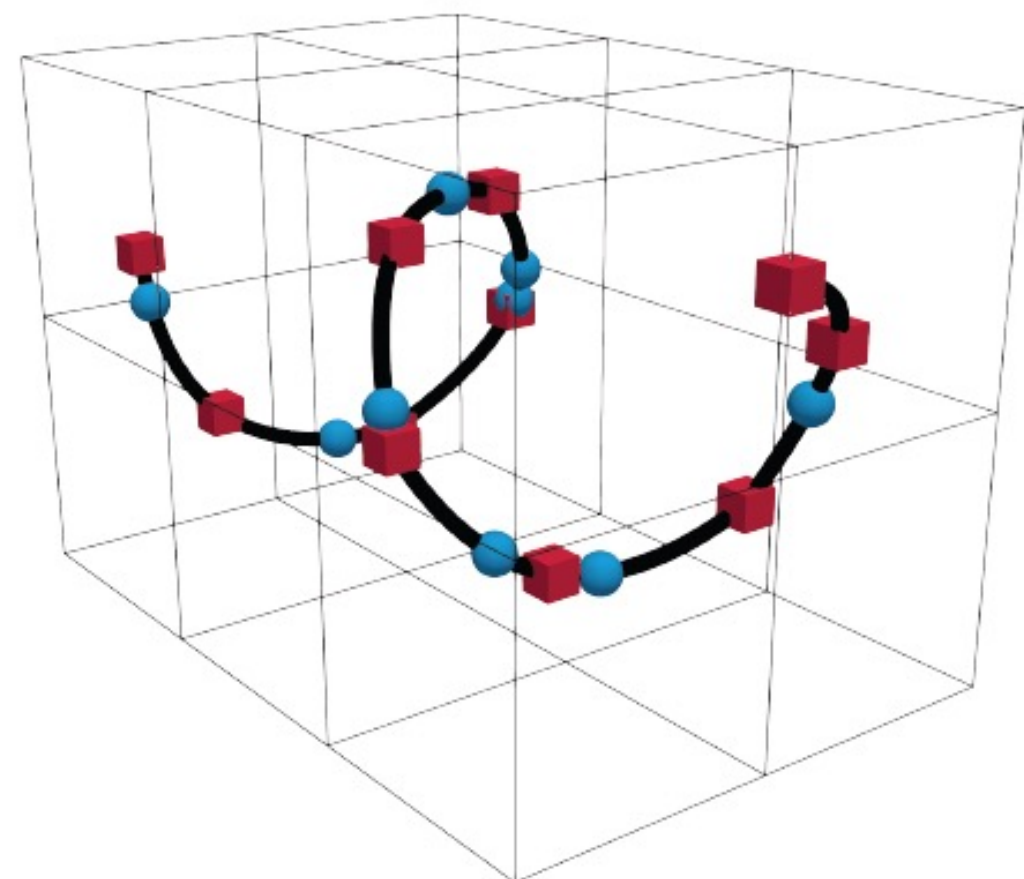
LM node $j \leftrightarrow$ Beam node l .

$$\mathbf{M}^{(j,k)} = \int_{\Gamma_{c,h}^B} \Phi_j N_k ds \mathbf{I}^{3 \times 3}$$

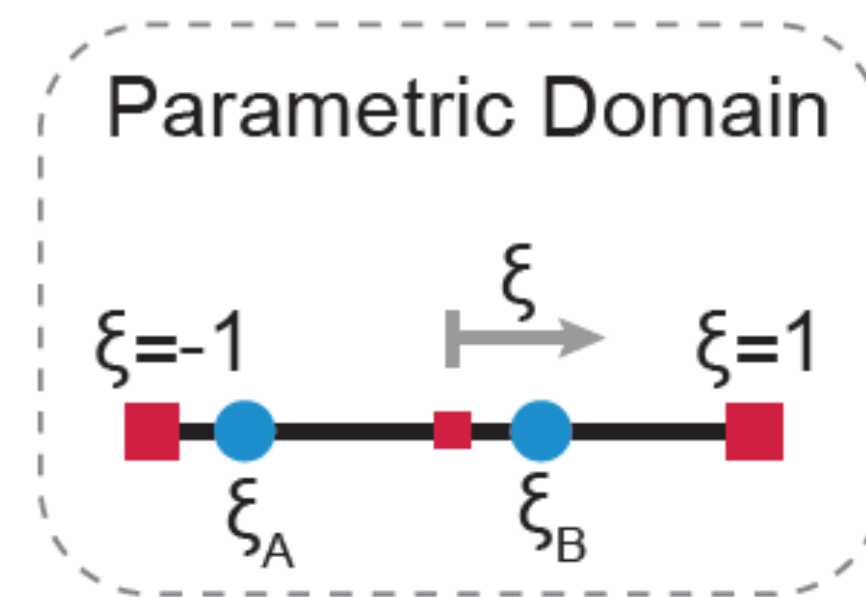
LM node $j \leftrightarrow$ Solid node k
Projection to solid domain to evaluate N_k

$$\boldsymbol{\kappa}^{(j,j)} = \int_{\Gamma_{c,h}^B} \Phi_j ds \mathbf{I}^{3 \times 3}$$

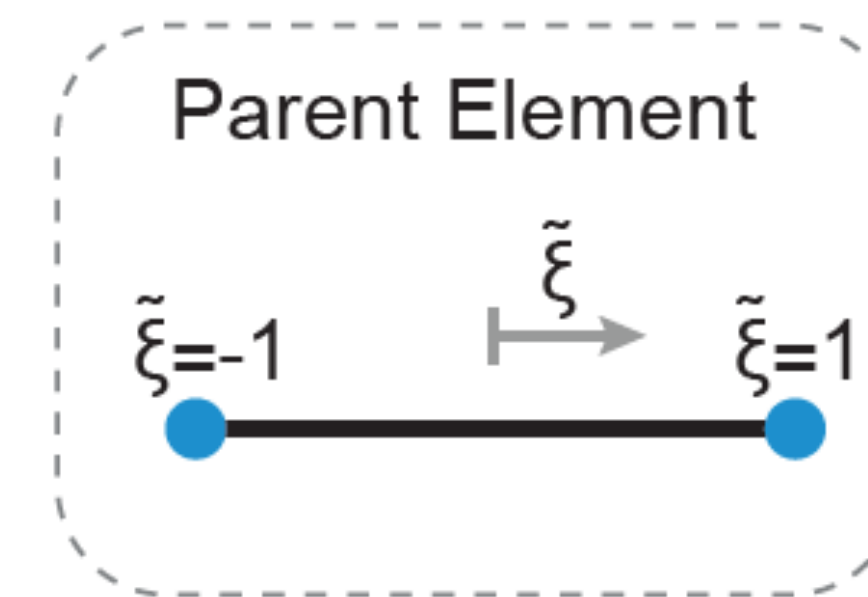
Scaling matrix: LM node j



$$ds = J_A d\xi$$



$$d\xi = J_B d\tilde{\xi}$$

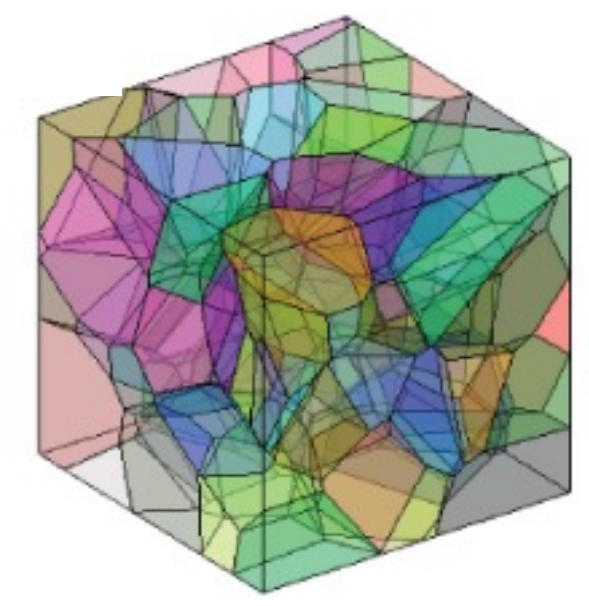


■ Element Node

● Segment End Point

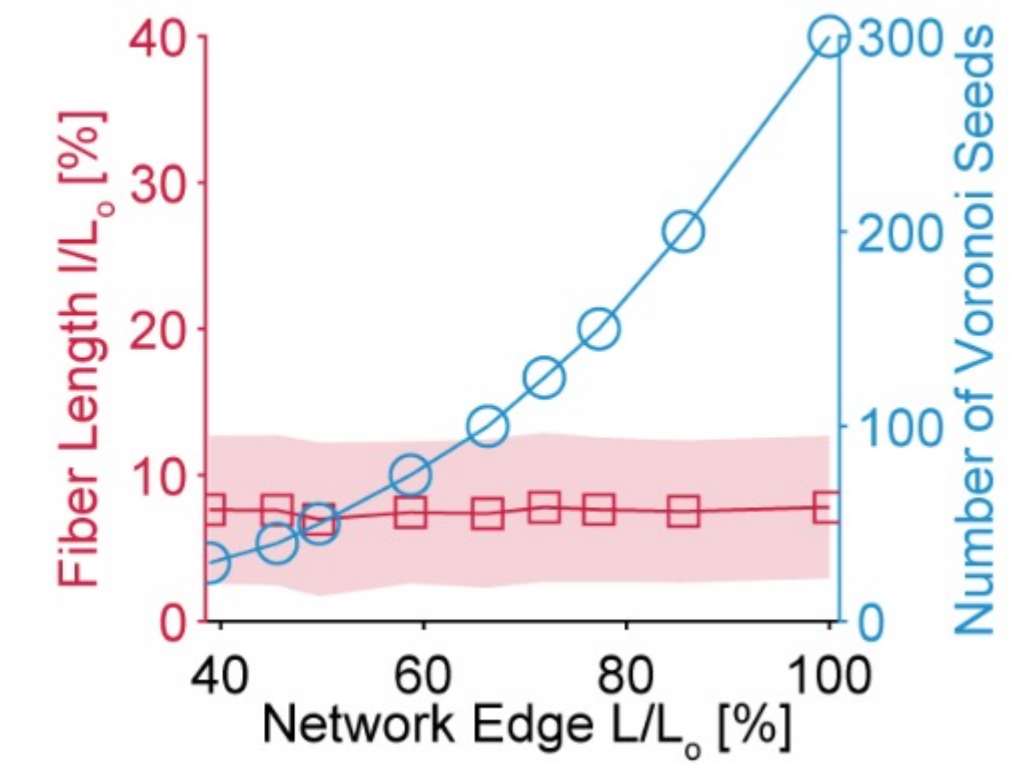
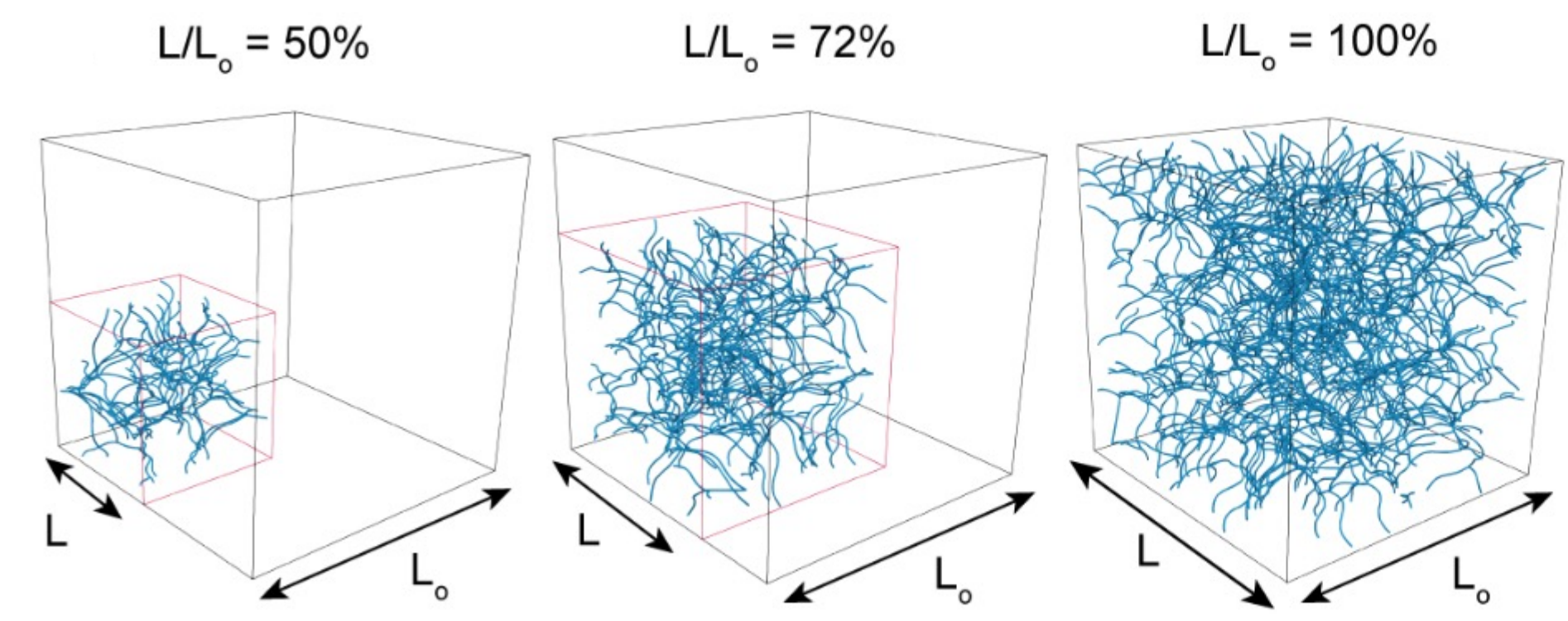
— Beam Domain

Embedded Fiber Networks



- Voronoi-based networks
 - Average connectivity number $\langle z \rangle = 3.4$
 - Introduce sinusoidal undulations

Size Effect Study



Density Effect study

