Computational Design of Metamaterials

Pengbin Tang

Computational Design Lab

ETH zürich

SGP 2025 Graduate School

Outline Today

- Introduction to Computational Design of Metamaterials
- Computational Models
  - Rigid Body, Finite Element Method, Discrete Elastic Rods
- Numerical Homogenization
- Case Study1: Mechanical Characterization
  - Discrete Interlocking Materials
- Numerical Methods in Inverse Design
- Case Study2: Metamaterials Design with Desired Behaviors
  - Inverse Design of Structured Surfaces and Discrete Interlocking Materials

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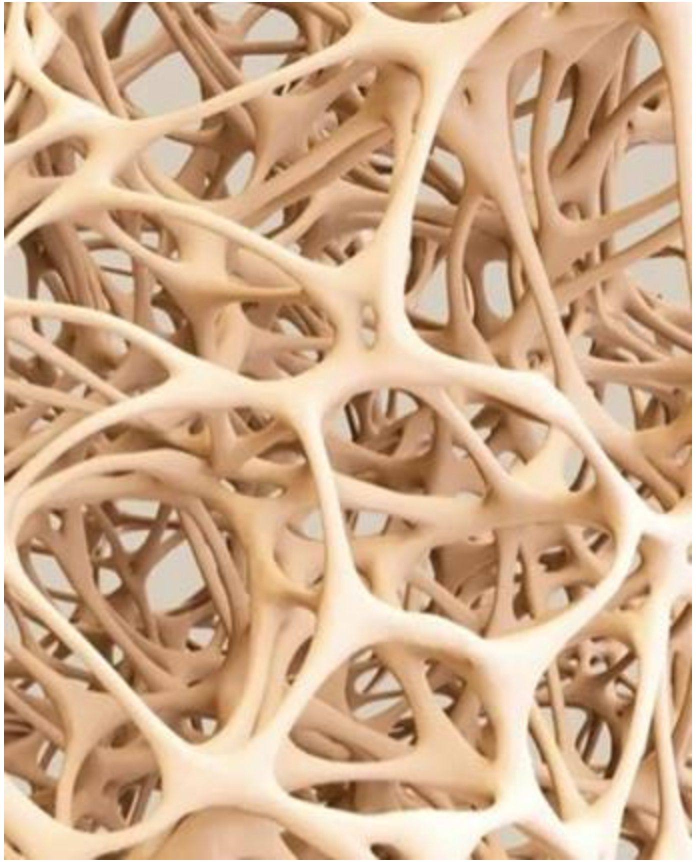
Nature materials



Trabecular structure of bone

Venation pattern of dragonfly wing

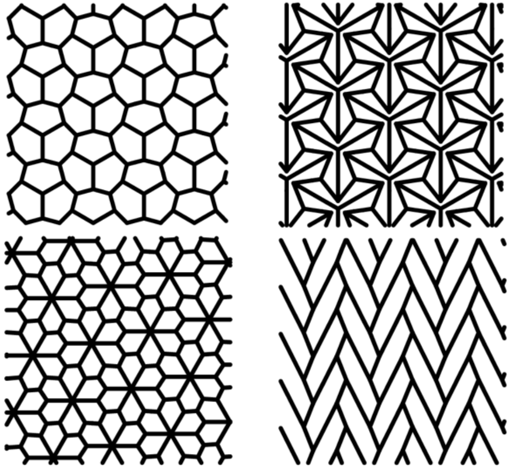
Scale skin of Pangolin

What is metamaterials?

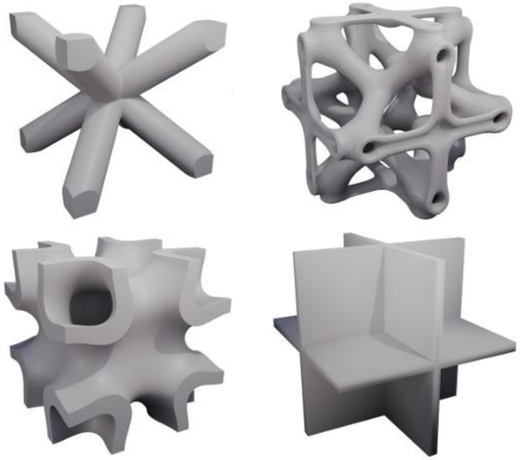
- Materials with tailored small-scale structures are metamaterials.

Mechanical Metamaterials

- Carefully designed microstructures allow for various macroscopic material properties with a single material
  - High stiffness-to-weight ratio
  - High durability
  - High energy absorption
  - Negative Poisson's ratio …



[Schumacher et al. 2028]



[Xue et al. 2025]

Application - Soft Robotics

[Pascali et al. 2022]

[Jeong et al. 2018]

[Gao et al. 2023]

Application - Wearables

[Tang et al. 2023]

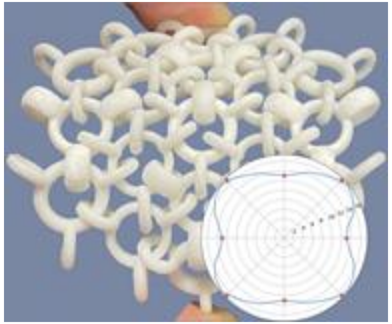
[Luo et al. 2022]

[Deng et al. 2022]

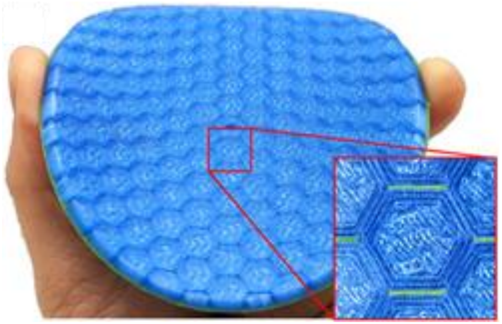
Design Challenges

- Forward prediction and characterization.

Large deformation/
Nonlinearity



Strong anisotropy



Contact

- Inverse design.
  - Nonlinear effect
  - High-dimensional design space

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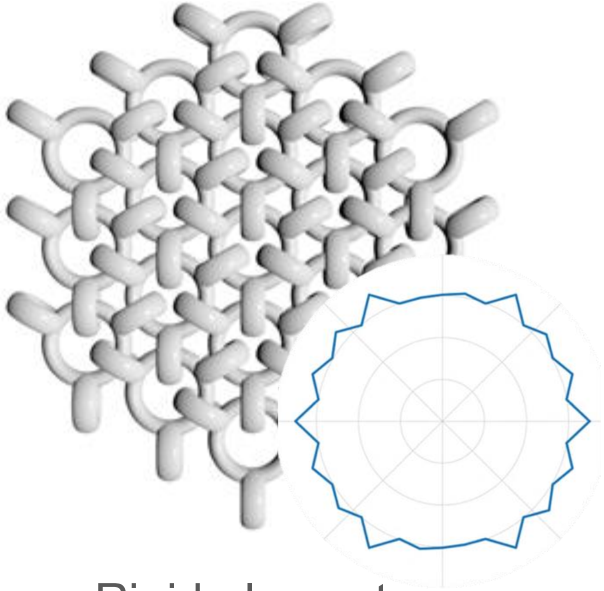
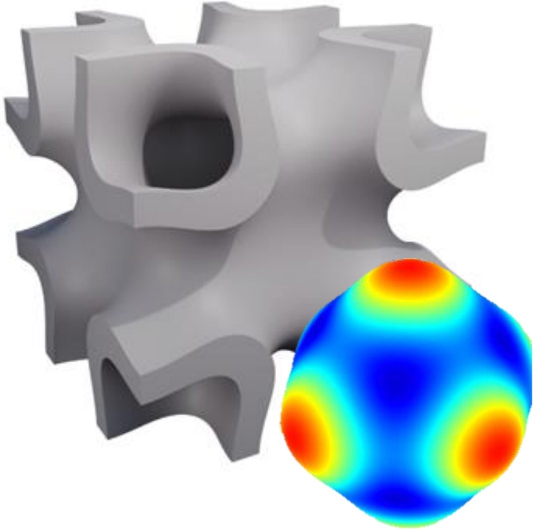
Computational Model

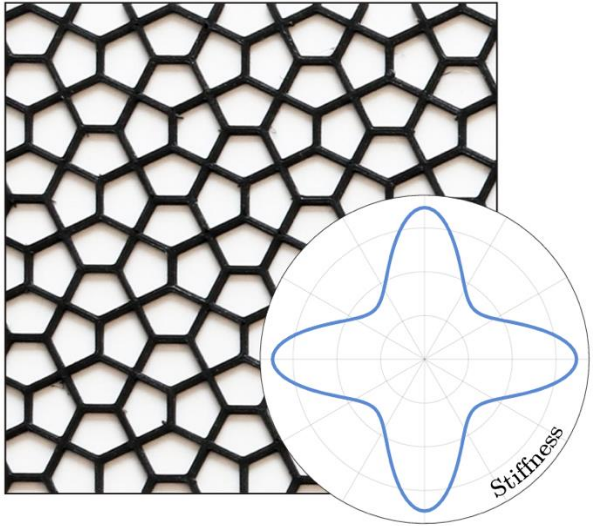
- Material characterization under static equilibrium.



Rigid elements



Continuum media



Elastic rods network

Rigid body

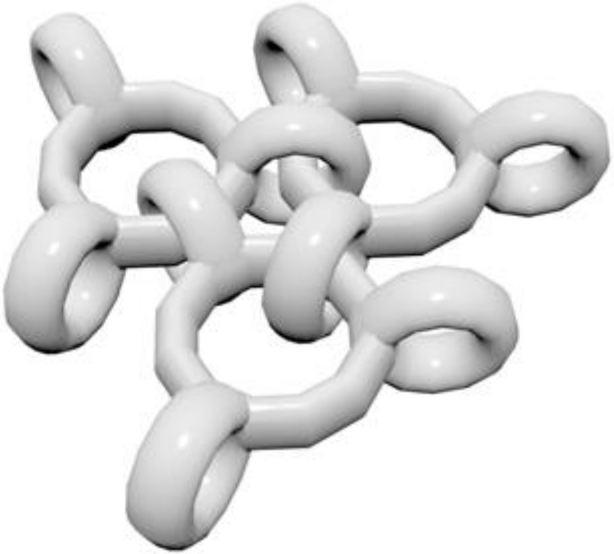
Finite Element Method

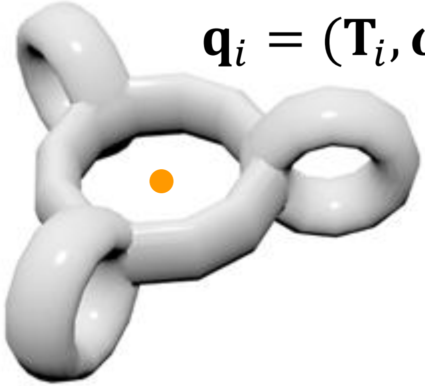
Discrete elastic rods

Rigid Body

Compute static equilibrium state of rigid bodies with contact by an unconstrained minimization problem

$$\arg\min_{\mathbf{q}} E = E_{\mathrm{Ext}}(\mathbf{q}) + E_{\mathrm{Coll}}(\mathbf{q})$$





$$\mathbf{q}_i = (\mathbf{T}_i, \boldsymbol{\omega}_i)$$

Rigid Body

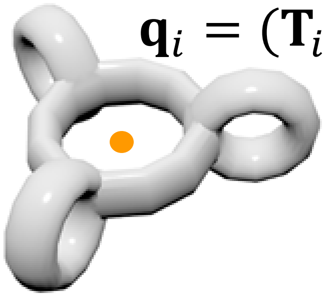
Vertex position of a rigid body

$$\mathbf{x} = \mathbf{T}_i + \mathbf{R}(\boldsymbol{\omega}_i)\mathbf{V}$$

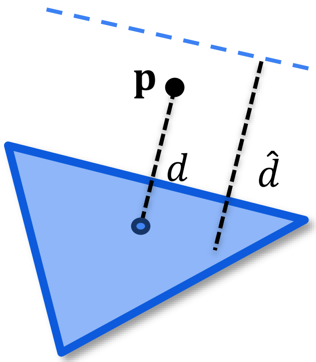
- The rotation matrix is computed by the Rodrigues' Rotation Formula

$$R(\omega) = \mathbf{I} + \mathrm{sinc}(\|\boldsymbol{\omega}\|)[\boldsymbol{\omega}] + 2\mathrm{sinc}^2\left(\frac{\|\boldsymbol{\omega}\|}{2}\right)[\boldsymbol{\omega}]^2$$

$$\mathbf{q}_i = (\mathbf{T}_i, \boldsymbol{\omega}_i)$$



Rigid Body

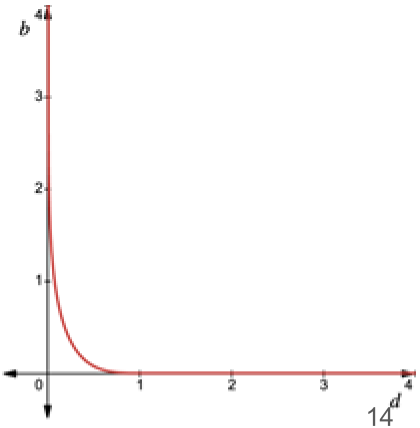


We use incremental potential contact (IPC) [Li et al. 2020] to compute contact energy

$$E_{Coll} = \kappa \sum_{k \in C} b(d_k(\mathbf{x}), \hat{d})$$

- b is the barrier potential

$$b(d, \hat{d}) = \begin{cases} -(d - \hat{d})^2 \ln(d/\hat{d}) & 0 < d \\ 0 & d \geq \hat{d} \end{cases}$$



Rigid Body

Solve the unconstrained minimization problem via Newton's method

$$\arg\min_{\mathbf{q}} E = E_{\text{Ext}}(\mathbf{q}) + E_{\text{Coll}}(\mathbf{q})$$

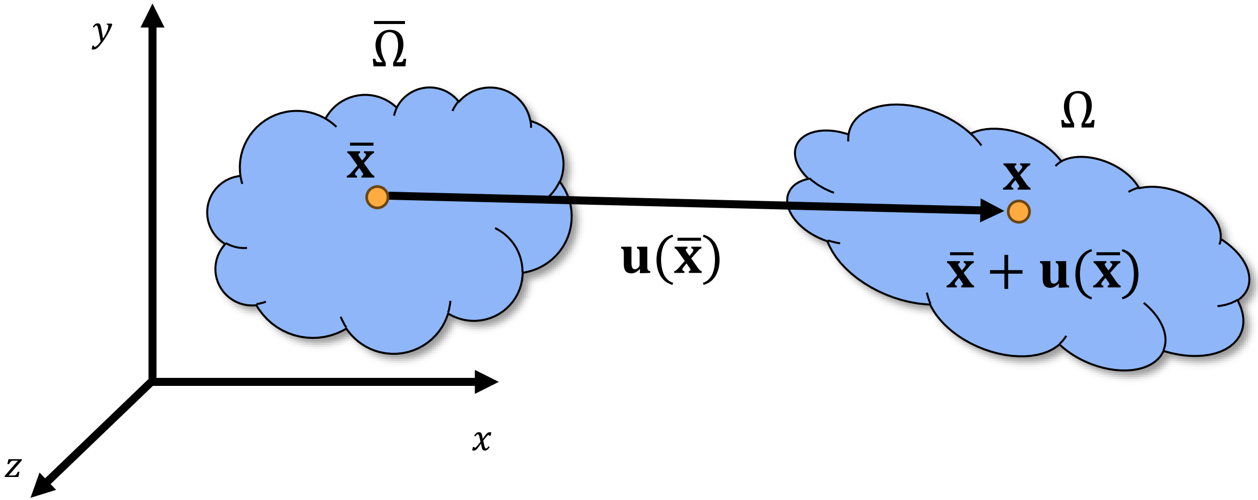
Newton's method:

- Start from initial guess $\mathbf{q}_0$
- For each iteration (until convergence)
  - Compute gradient $\nabla_{\mathbf{q}_i}\mathrm{E}$, Hessian$\nabla^2_{\mathbf{q}_i}\mathrm{E}$
  - Compute search direction $\Delta\mathbf{q}_i = \left(\nabla^2_{\mathbf{q}_i}\mathrm{E}\right)^{-1}\nabla_{\mathbf{q}_i}\mathrm{E}$
  - Compute largest intersection-free step size α_m via Continuous Collision Detection (CCD)
  - Back tracking line search α with maximum step size α_m
  - $\mathbf{q}_{i+1} = \mathbf{q}_i + \boldsymbol{\alpha} \cdot \Delta\mathbf{q}_i$

Finite Element Method

- For a deformable body, identify the
  - Undeformed state $\overline{\Omega} \subset \mathbf{R}^3$ describe by positions $\bar{\mathbf{x}}$
  - Deformed state $\Omega \subset \mathbf{R}^3$ describe by positions $\mathbf{x}$
- Displacement filed $\mathbf{u}$ describe Ω in terms of $\overline{\Omega}$:

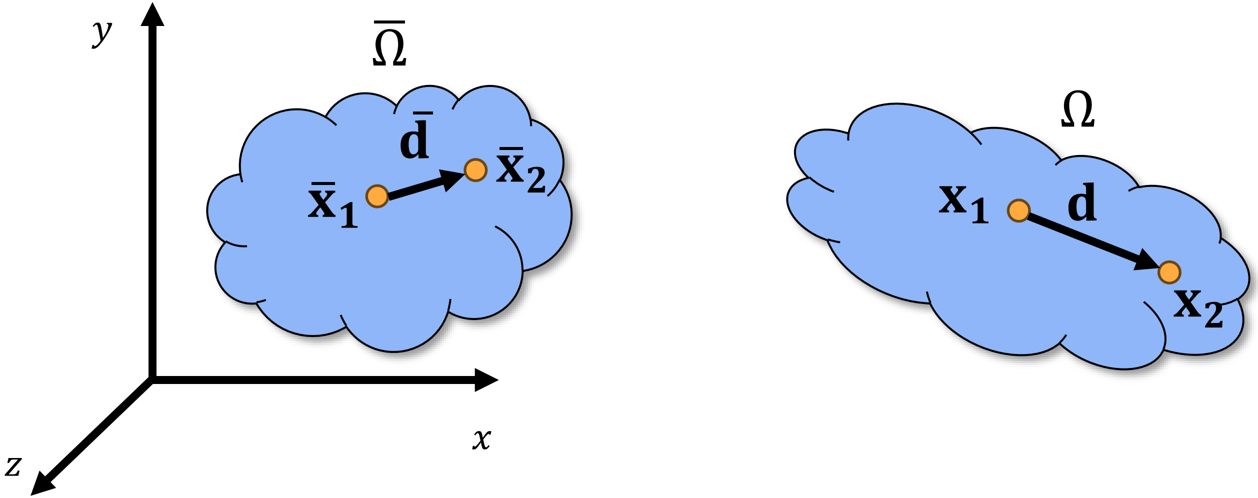
$$\mathbf{u}(\bar{\mathbf{x}}): \overline{\Omega} \to \Omega \qquad \mathbf{x}(\bar{\mathbf{x}}) = \bar{\mathbf{x}} + \mathbf{u}(\bar{\mathbf{x}})$$



Finite Element Method

- Consider material points $\bar{\mathbf{x}}_1$ and $\bar{\mathbf{x}}_2$ and $\bar{\mathbf{d}} = \bar{\mathbf{x}}_2 - \bar{\mathbf{x}}_1$ such that $|\bar{\mathbf{d}}|$ is infinitesimal
- The deformed vector

$$\begin{aligned}
\mathbf{d} = \mathbf{x}_2 - \mathbf{x}_1 &= \bar{\mathbf{x}}_2 + \mathbf{u}(\bar{\mathbf{x}}_2) - \bar{\mathbf{x}}_1 - \mathbf{u}(\bar{\mathbf{x}}_1) \\
&= \bar{\mathbf{d}} + \mathbf{u}\left(\bar{\mathbf{x}}_1 + \bar{\mathbf{d}}\right) - \mathbf{u}(\bar{\mathbf{x}}_1) \\
&\approx \bar{\mathbf{d}} + \boxed{\mathbf{u}(\bar{\mathbf{x}}_1) + \nabla\mathbf{u}\,\bar{\mathbf{d}}} - \mathbf{u}(\bar{\mathbf{x}}_1) = \overbrace{(\mathbf{I} + \nabla\mathbf{u})}^{\text{Deformation gradient } \mathbf{F}}\bar{\mathbf{d}}
\end{aligned}$$



Finite Element Method

- Deformation gradient $\mathbf{F} = \mathbf{I} + \nabla\mathbf{u}$ maps undeformed vectors to deformed vectors as $\mathbf{d} = \mathbf{F}\bar{\mathbf{d}}$
- Alternatively, we can write

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \bar{\mathbf{x}}} = \frac{\partial}{\partial \bar{\mathbf{x}}}\left(\bar{\mathbf{x}} + \mathbf{u}(\bar{\mathbf{x}})\right) = \mathbf{I} + \nabla\mathbf{u}$$

- Measure change in length squared in arbitrary directions,

$$\mathbf{d}^T\mathbf{d} - \bar{\mathbf{d}}^T\bar{\mathbf{d}} = \bar{\mathbf{d}}^T(\mathbf{F}^{\mathrm{T}}\mathbf{F} - \mathbf{I})\bar{\mathbf{d}}$$

- Green strain

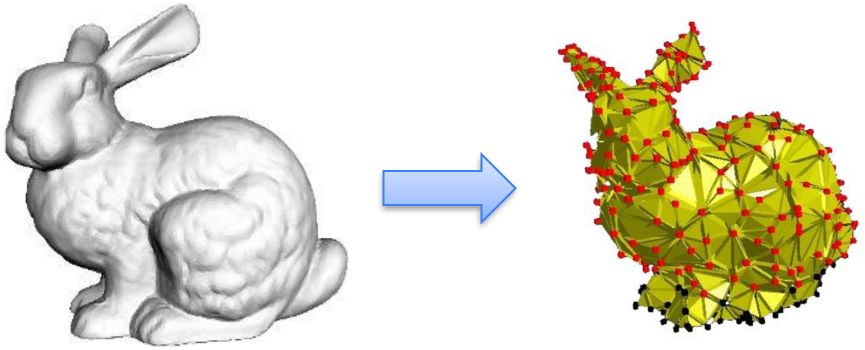
$$\mathbf{E} = \frac{1}{2}\left(\mathbf{F}^{\mathrm{T}}\mathbf{F} - \mathbf{I}\right) = \frac{1}{2}(\nabla\boldsymbol{u} + \nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T\nabla\boldsymbol{u})$$

- Neglecting quadratic terms leads to the linear Cauchy strain

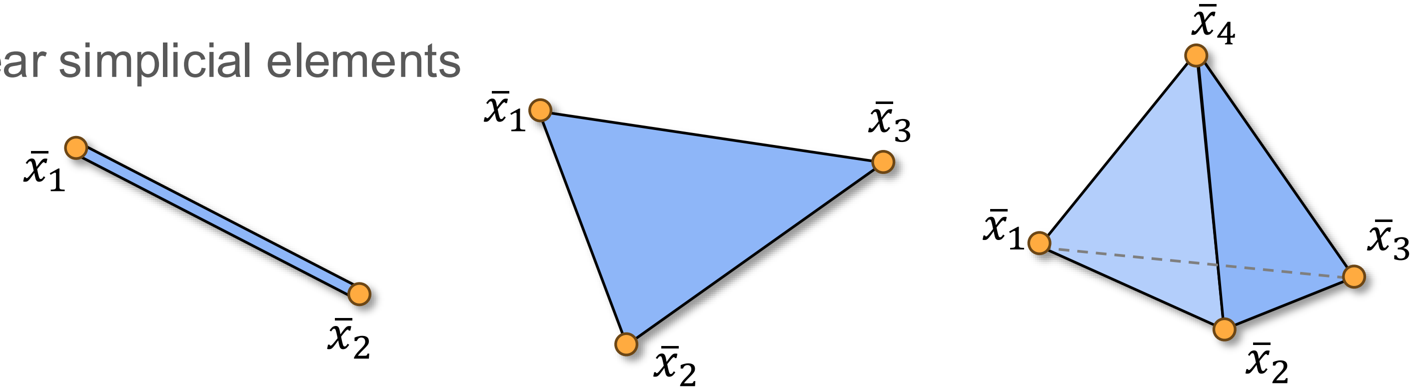
$$\boldsymbol{\varepsilon} = \frac{\mathbf{1}}{\mathbf{2}}(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}) = \frac{\mathbf{1}}{\mathbf{2}}\left(\mathbf{F} + \mathbf{F}^{\mathrm{T}}\right) - \mathbf{I}$$

Finite Element Method

- Divide input solid model into elements



- Linear simplicial elements



1D: **Line segment** 2D: **Triangle** 3D: **Tetrahedron**

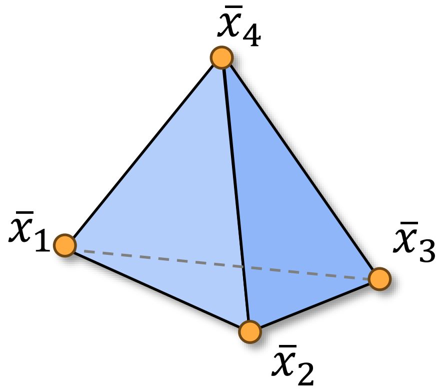
Finite Element Method

- 4-node tetrahedron has 4 linear basis functions
- Basis function are linear

$$N_i(\bar{x}, \bar{y}, \bar{z}) = a_i\bar{x} + b_i\bar{y} + c_i\bar{z} + d_i$$

- From $N_i(\bar{\mathbf{x}}_j) = \delta_{ij}$, we obtain coefficient by solving

$$\begin{pmatrix} \bar{x}_1 & \bar{y}_1 & \bar{z}_1 & 1 \\ \bar{x}_2 & \bar{y}_2 & \bar{z}_2 & 1 \\ \bar{x}_3 & \bar{y}_3 & \bar{z}_3 & 1 \\ \bar{x}_4 & \bar{y}_4 & \bar{z}_4 & 1 \end{pmatrix} \begin{pmatrix} a_i \\ b_i \\ c_i \\ d_i \end{pmatrix} = \begin{pmatrix} \delta_{1i} \\ \delta_{2i} \\ \delta_{3i} \\ \delta_{4i} \end{pmatrix}$$

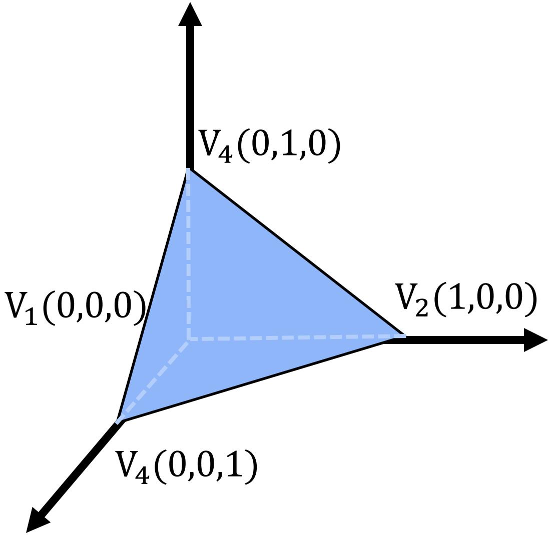


Finite Element Method

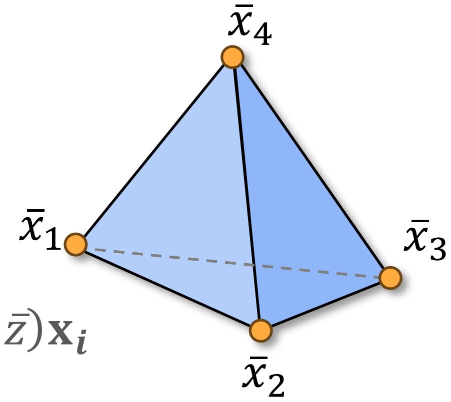
- Solve for coefficients of N_1

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ b_1 \\ c_1 \\ d_1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

- $N_1(\bar{x}, \bar{y}, \bar{z}) = -\bar{x} - \bar{y} - \bar{z} + 1$
- $N_2(\bar{x}, \bar{y}, \bar{z}) = \bar{x}$
- $N_3(\bar{x}, \bar{y}, \bar{z}) = \bar{y}$
- $N_4(\bar{x}, \bar{y}, \bar{z}) = \bar{z}$



Finite Element Method



- Interpolate using basis functions

$$\bar{\mathbf{x}}(\bar{x},\bar{y},\bar{z}) = \sum_{\boldsymbol{i=1}}^{\boldsymbol{n_e}} N_i(\bar{x},\bar{y},\bar{z})\bar{\mathbf{x}}_{\boldsymbol{i}} \qquad \mathbf{x}(\bar{x},\bar{y},\bar{z}) = \sum_{\boldsymbol{i=1}}^{\boldsymbol{n_e}} N_i(\bar{x},\bar{y},\bar{z})\mathbf{x}_{\boldsymbol{i}}$$

- Deformation gradient

$$\mathbf{F} = \frac{\partial \mathbf{x}(\bar{\mathbf{x}})}{\partial \bar{\mathbf{x}}} = \sum_{i=0}^{4} \mathbf{x}_i \left(\frac{\partial N_i}{\partial \bar{\mathbf{x}}}\right)^{\mathrm{T}}$$

- N_i are linear on elements, $\mathbf{F} \in \mathbf{R}^{3\times3}$ is constant within a linear tetrahedral element .
- Hence, element energy $E = \int_{\bar{\Omega}_e} \Psi \, dV = \Psi(\mathbf{F}) \cdot \bar{V}_e$

Finite Element Method

- Material model links strain to energy (and stress)
- Linear isotropic material (generalized Hooke's law)

- Energy density $\Psi = \frac{1}{2}\lambda \mathrm{tr}(\boldsymbol{\varepsilon})^2 + \mu \mathrm{tr}(\boldsymbol{\varepsilon}^2)$
- Cauchy stress $\sigma = \frac{\partial \Psi}{\partial \varepsilon} = \lambda \mathrm{tr}(\boldsymbol{\varepsilon})\mathbf{I} + 2\mu\boldsymbol{\varepsilon}$
- λ and μ are Lame parameters.

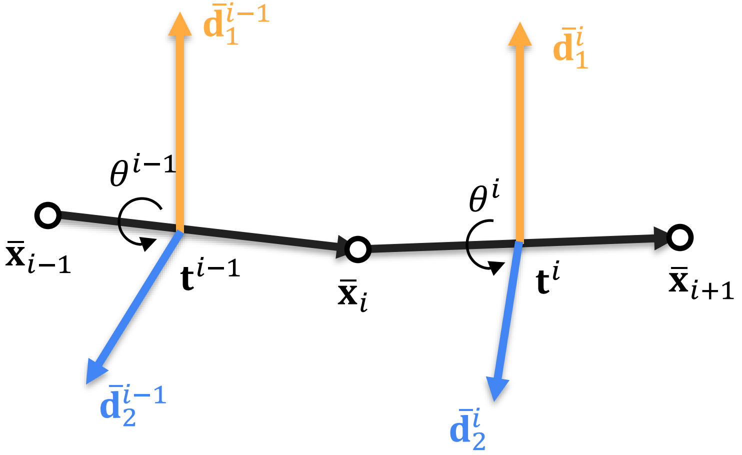
- Nonlinear elasticity, replace Cauchy strain with Green strain

- St. Venant-Kirchhoff material (StVK)
- Energy density $\Psi = \frac{1}{2}\lambda \mathrm{tr}(\mathbf{E})^2 + \mu \mathrm{tr}(\mathbf{E}^2)$

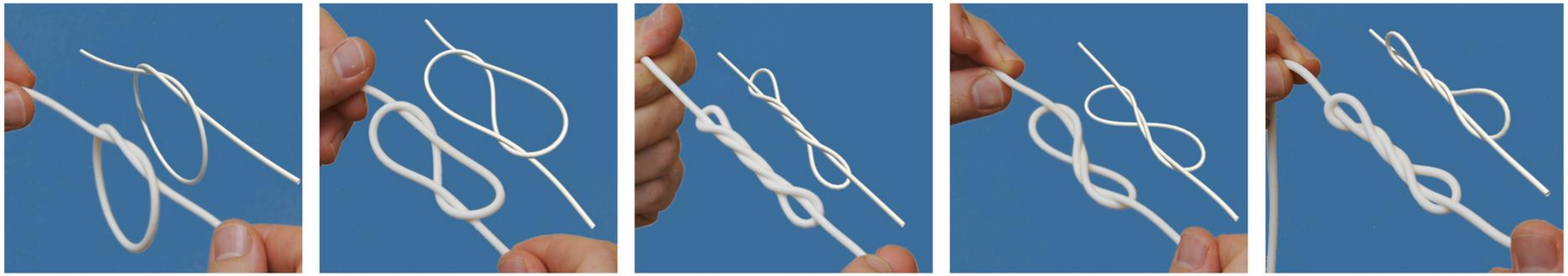
Discrete Elastic Rods

- Discrete Kirchhoff elastic rods
  - Stretching energy
  - Bending energy
  - Twisting energy

$$E_{elastic} = E_s + E_b + E_t$$



Discrete framed curve



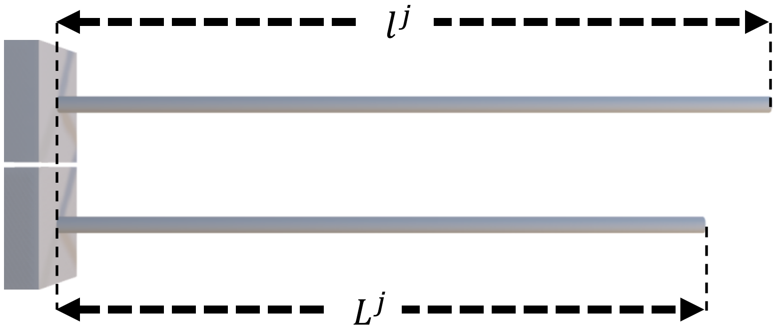
[Bergou et al. 2008]

Discrete Elastic Rods - Stretching

- Elastic stretching energy

$$E_s = \frac{1}{2}\sum_{j=0}^{n} k_s^j \left(\varepsilon^j\right)^2 L^j$$

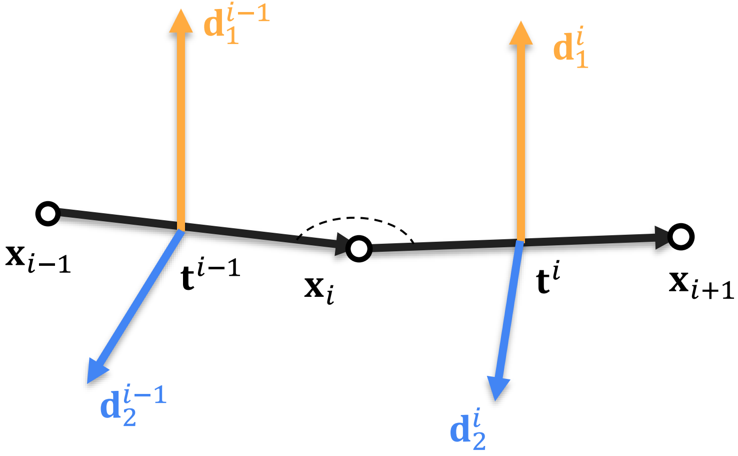
with axial strain $\varepsilon^j = \frac{l^j - L^j}{L^j}$



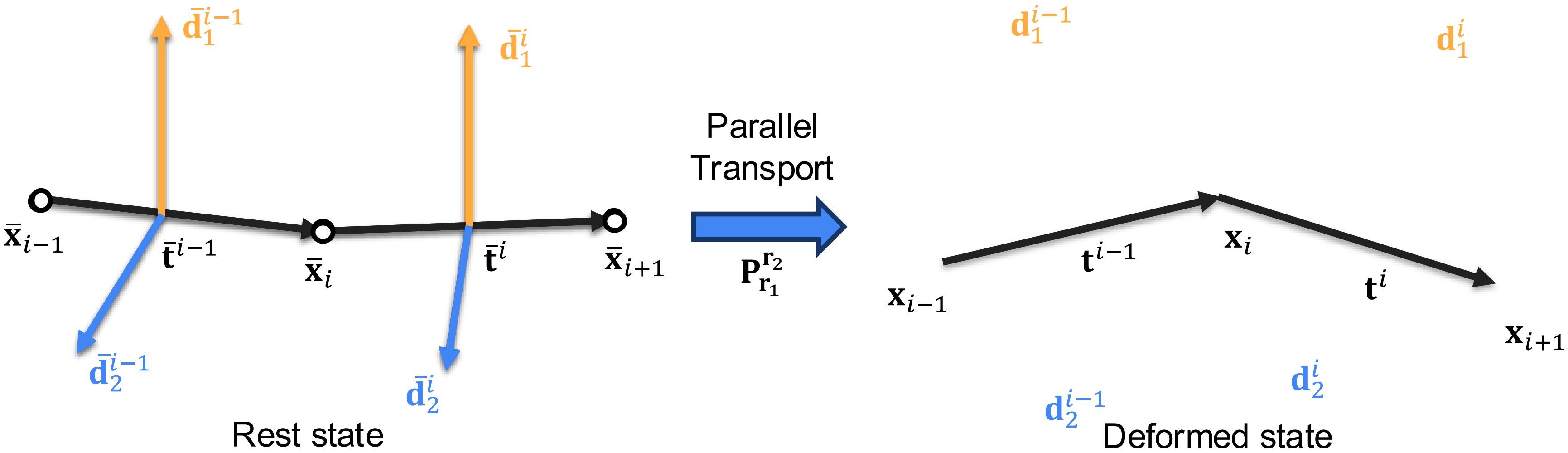
Discrete Elastic Rods - Bending

- Elastic Bending energy

$$E_b = \frac{1}{2}\sum_{i=1}^{n}\frac{1}{\bar{l}}(\kappa_i - \bar{\kappa}_i)^T B_i(\kappa_i - \bar{\kappa}_i)$$



Discrete Elastic Rods - Twisting



- Parallel transport is a minimum rotation that aligns two vectors.

$$\mathbf{P}_{\mathbf{r}_1}^{\mathbf{r}_2} = \mathbf{R}\left(\frac{\mathbf{r}_1 \times \mathbf{r}_2}{|\mathbf{r}_1 \times \mathbf{r}_2|}, \angle(\mathbf{r}_1, \mathbf{r}_2)\right)$$

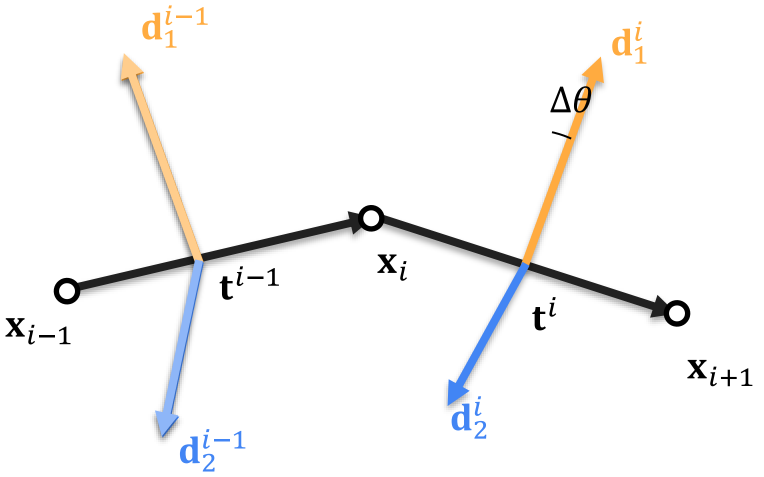
Discrete Elastic Rods - Twisting

- Measure difference between frames
  - Parallel transport frames by $\mathbf{P}_{\mathbf{t}_{i-1}}^{\mathbf{t}_i}$
  - Measure angle difference $\Delta\theta$
- Twist

$$m_i = \theta^i - \theta^{i-1} + \Delta\theta$$

- Elastic twisting energy

$$E_t = \frac{1}{2}\sum_{i=1}^{n} \frac{\beta_i (m_i - \bar{m}_i)^2}{\bar{l}_i}$$



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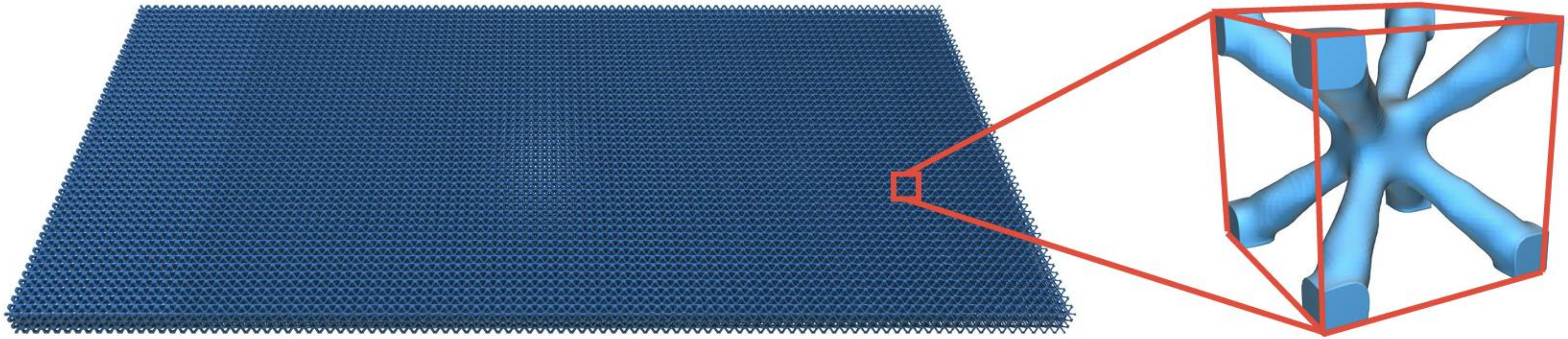
Numerical Homogenization

- Design tileable metamaterial based on ***unit cells.***



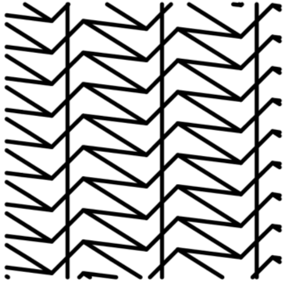
Numerical Homogenization

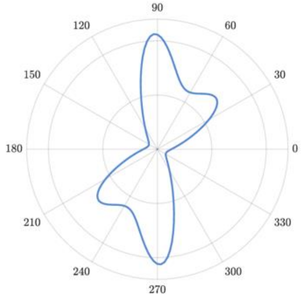
- Target: **Macroscopic** material properties from **microscopic** geometry

Microscopic structure

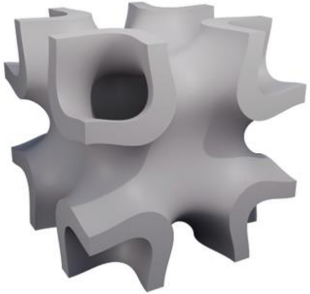
Directional stiffness / Poisson’s ratio

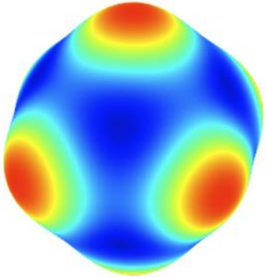
2D





3D





Macromechanical model

Anisotropic Kirchhoff plates

- Strain energy density

$$W(\boldsymbol{\epsilon}, \boldsymbol{\kappa}) = W_M + W_B = \frac{1}{2}\boldsymbol{\epsilon} : \mathbb{C} : \boldsymbol{\epsilon} + \frac{1}{2}\boldsymbol{\kappa} : \mathbb{B} : \boldsymbol{\kappa}$$

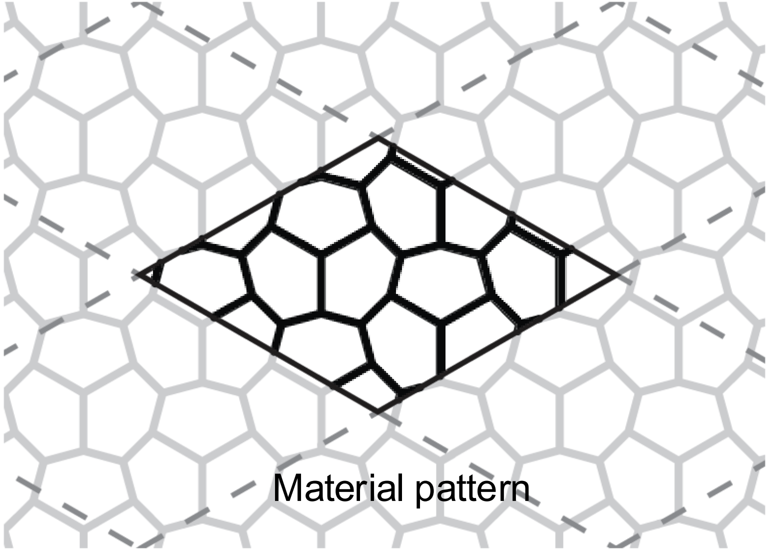
- Membrane and bending stress

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\epsilon} \qquad \mathbf{M} = \mathbb{B} : \boldsymbol{\kappa}$$

Numerical Homogenization

Problems:

- Regular simulation does not consider tiling
- How to apply directional deformations?
- Fix the positions of vertices will artificially stiffen the structure

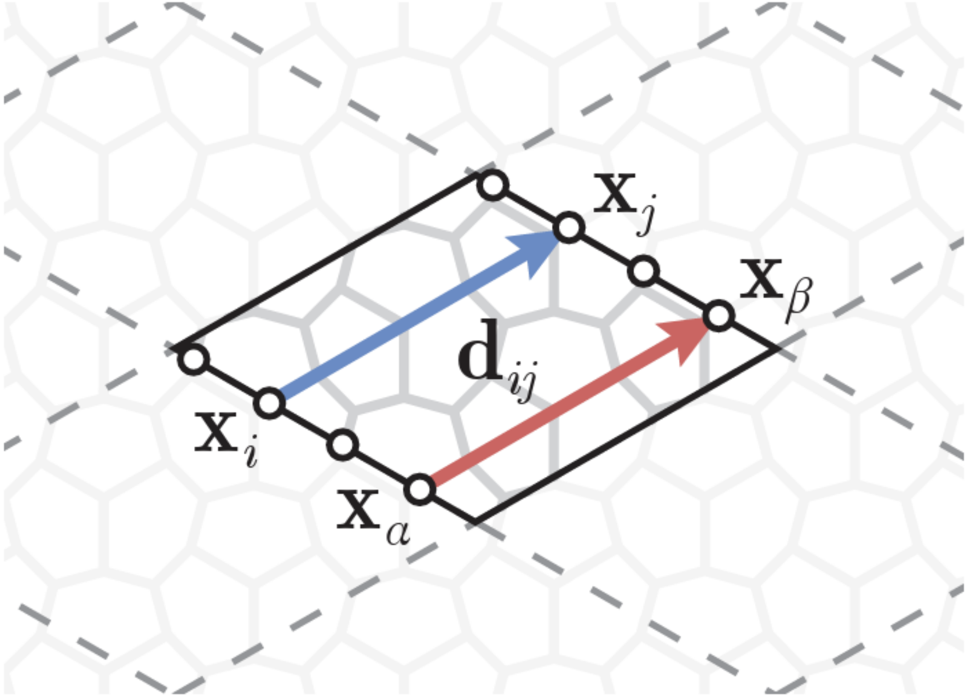


Periodic tiling

In-plane Periodic Boundary Conditions

- In-plane periodic boundary conditions

$$\mathbf{x}_j = \mathbf{x}_i + \mathbf{d}_{ij}$$



Macroscopic In-plane Deformation

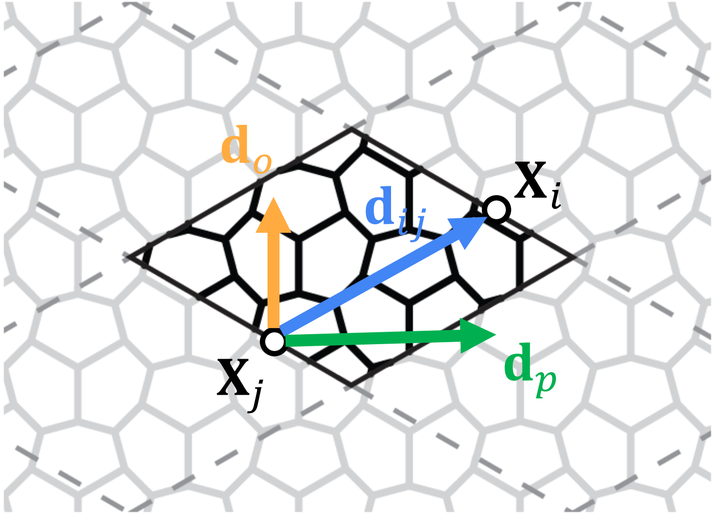
- Apply biaxial deformation

$$\mathbf{d}_{ij} = \varepsilon_p(\bar{\mathbf{d}}_{ij}^{\mathrm{T}}\mathbf{d}_p)\mathbf{d}_p + \varepsilon_o(\bar{\mathbf{d}}_{ij}^{\mathrm{T}}\mathbf{d}_o)\mathbf{d}_o$$

- Macroscopic deformation gradient

$$\mathbf{F}_{\mathrm{macro}} = \varepsilon_p\mathbf{d}_p\mathbf{d}_p^{\mathrm{T}} + \varepsilon_o\mathbf{d}_{\boldsymbol{o}}\mathbf{d}_o^{\mathrm{T}}$$

or $$\mathbf{F}_{\mathrm{macro}} = [\mathbf{x}_i - \mathbf{x}_j \quad \mathbf{x}_k - \mathbf{x}_l]\,[\mathbf{X}_i - \mathbf{X}_j \quad \mathbf{X}_k - \mathbf{X}_l]^{-1}$$



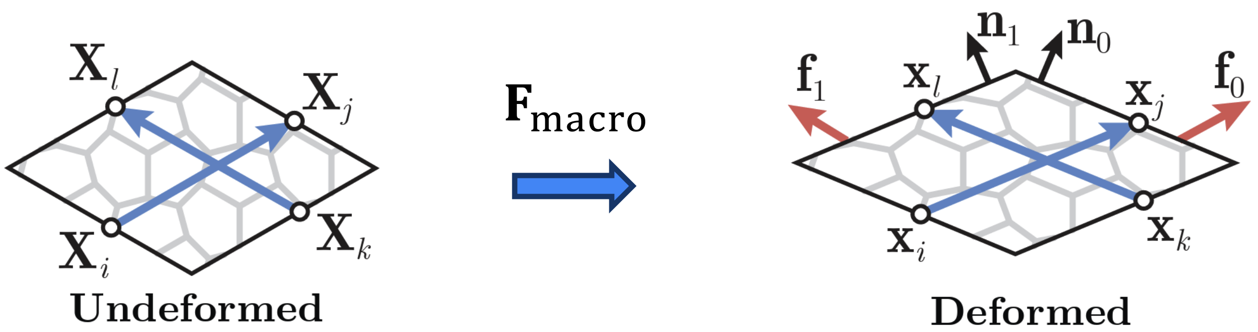
Macroscopic In-plane Deformation

- Anisotropic Kirchhoff plates membrane stress $\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\epsilon}$
- Macroscopic Cauchy strain tensor

$$\boldsymbol{\epsilon}_{\text{macro}} = \frac{1}{2}\left(\mathbf{F}_{\text{macro}} + \mathbf{F}_{\text{macro}}^{\text{T}}\right) - \mathbf{I}$$

- Macroscopic Cauchy stress tensor

$$\boldsymbol{\sigma}_{\text{macro}} = [\mathbf{f}_0 \quad \mathbf{f}_1][\mathbf{n}_0 \quad \mathbf{n}_1]^{-1}$$



Characterizing In-plane Mechanical Properties

- Fit the homogenized compliance tensor $\mathbb{S} = \mathbb{C}^{-1}$ by solving

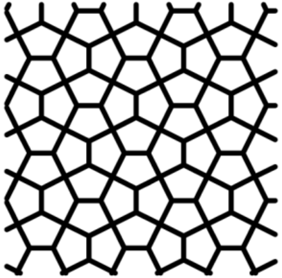
$$\mathbb{S}^{\mathrm{H}} = \underset{\mathbb{S}}{\operatorname{argmin}} \sum_{i=1}^{N} \frac{1}{||\boldsymbol{\epsilon}_{\mathbf{i}}||_F^2} ||\mathbb{S} : \boldsymbol{\sigma}_i - \boldsymbol{\epsilon}_i||_F^2$$

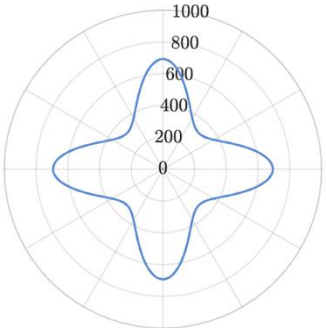
- Directional Young's modulus

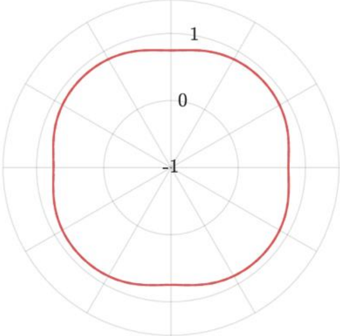
$$E(\mathbf{d}) = \frac{1}{(\mathbf{d}\mathbf{d}^{\mathrm{T}}) : \mathbb{S} : (\mathbf{d}\mathbf{d}^{\mathrm{T}})}$$

- Directional Poisson's ratio

$$\nu(\mathbf{d}) = -\frac{(\mathbf{d}\mathbf{d}^{\mathrm{T}}) : \mathbb{S} : (\mathbf{n}\mathbf{n}^{\mathrm{T}})}{(\mathbf{d}\mathbf{d}^{\mathrm{T}}) : \mathbb{S} : (\mathbf{d}\mathbf{d}^{\mathrm{T}})}$$



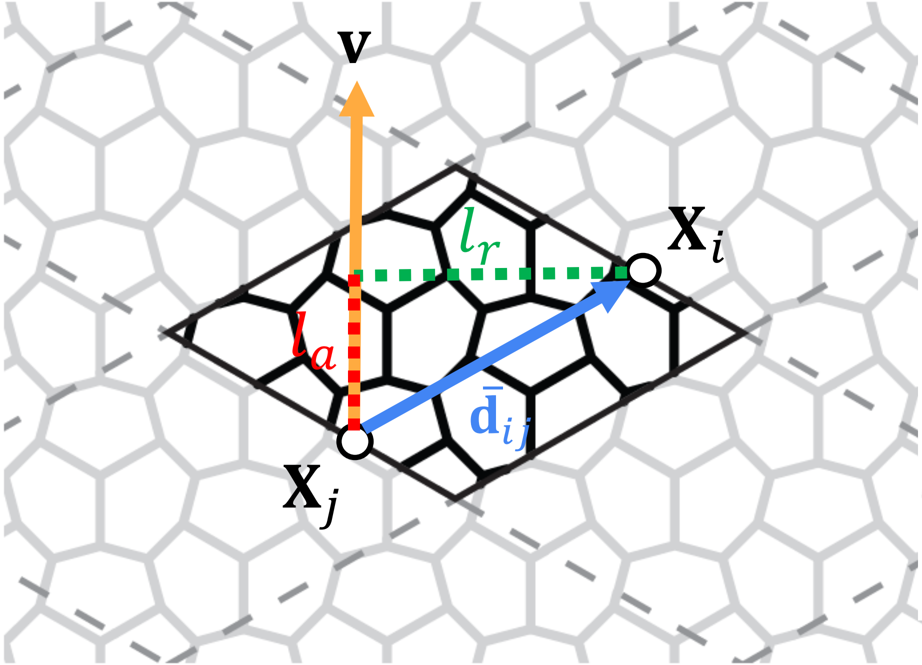


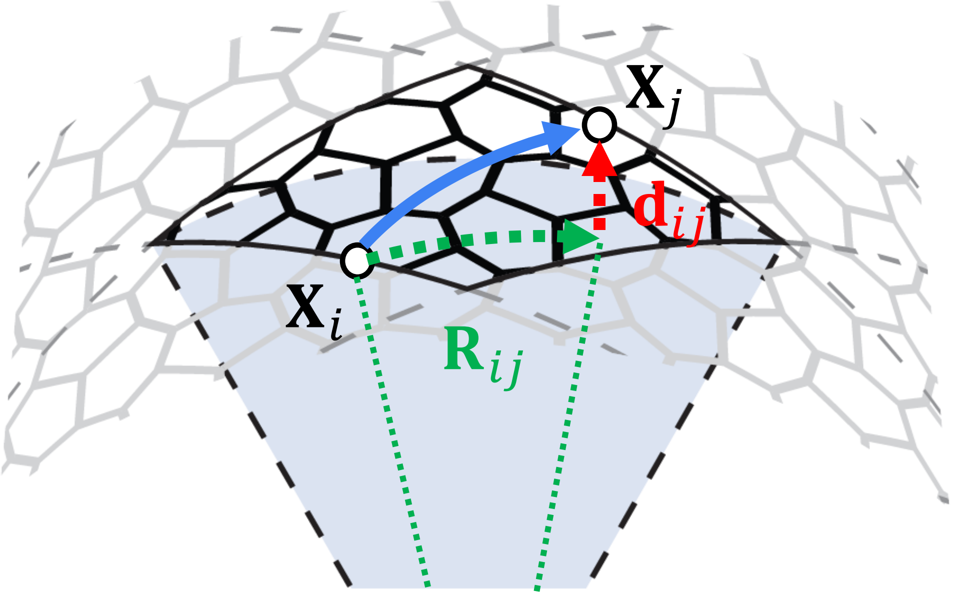


Bending Periodic Boundary Conditions

- Bending with single bending curvature κ_c with direction $\mathbf{v}$

$$\mathbf{x}_j = \mathbf{R}_{ij}\mathbf{x}_i + \mathbf{d}_{ij}$$





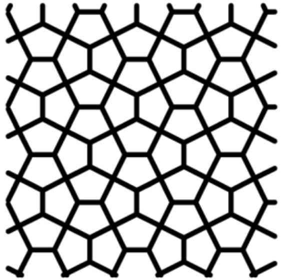
Characterizing Bending Mechanical Properties

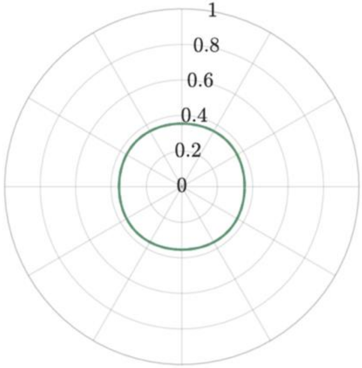
- Fit the homogenized bending stiffness by solving

$$\mathbb{B}^H = \arg\min_{\mathbb{B}} \sum_{i=0}^{M} \left(\frac{1}{2} \boldsymbol{\kappa}_i : \mathbb{B} : \boldsymbol{\kappa}_i - W_i \right)^2$$

- Directional bending stiffness

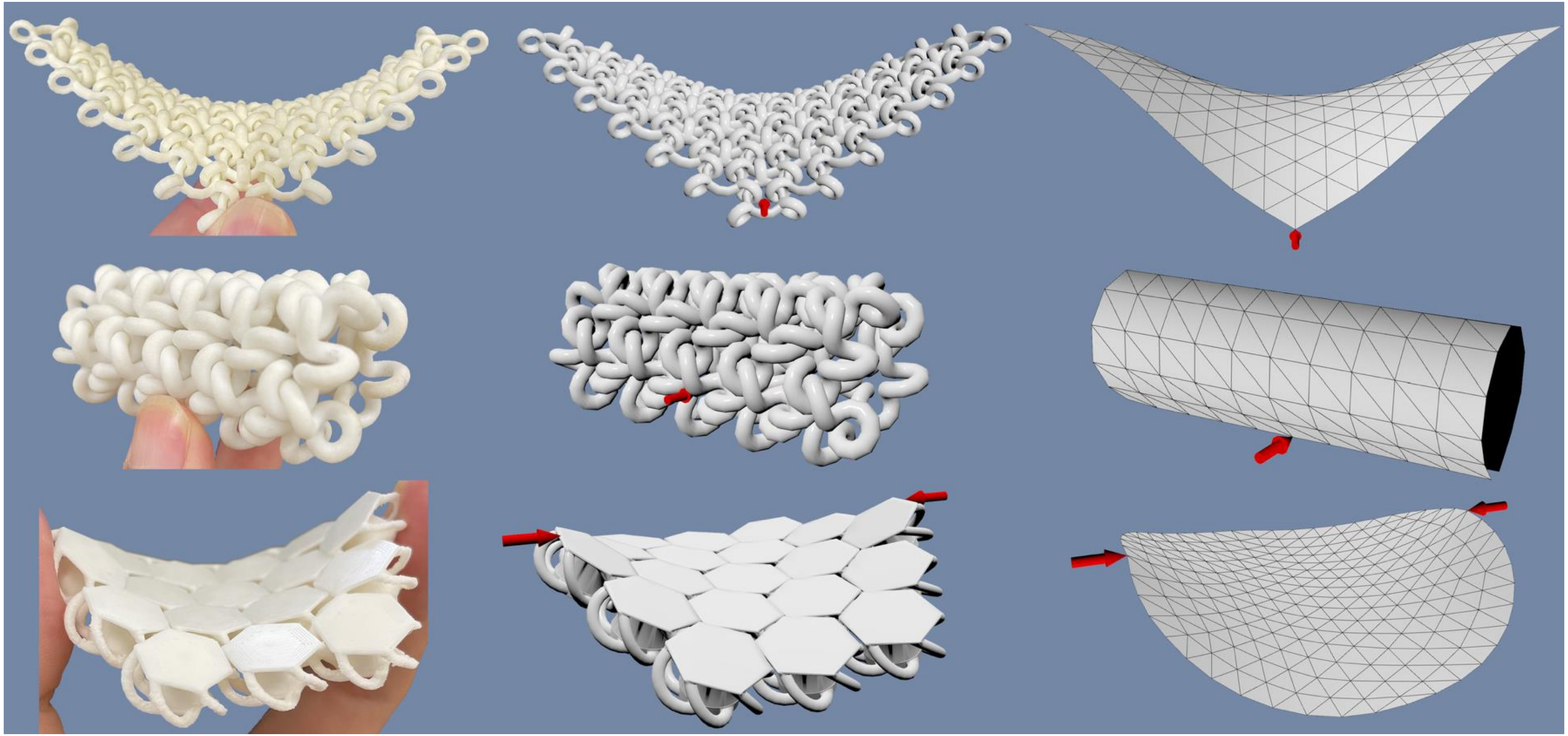
$$b(\mathbf{d}) = \left(\mathbf{d}\mathbf{d}^{\mathrm{T}}\right) : \mathbb{B} : \left(\mathbf{d}\mathbf{d}^{\mathrm{T}}\right)$$





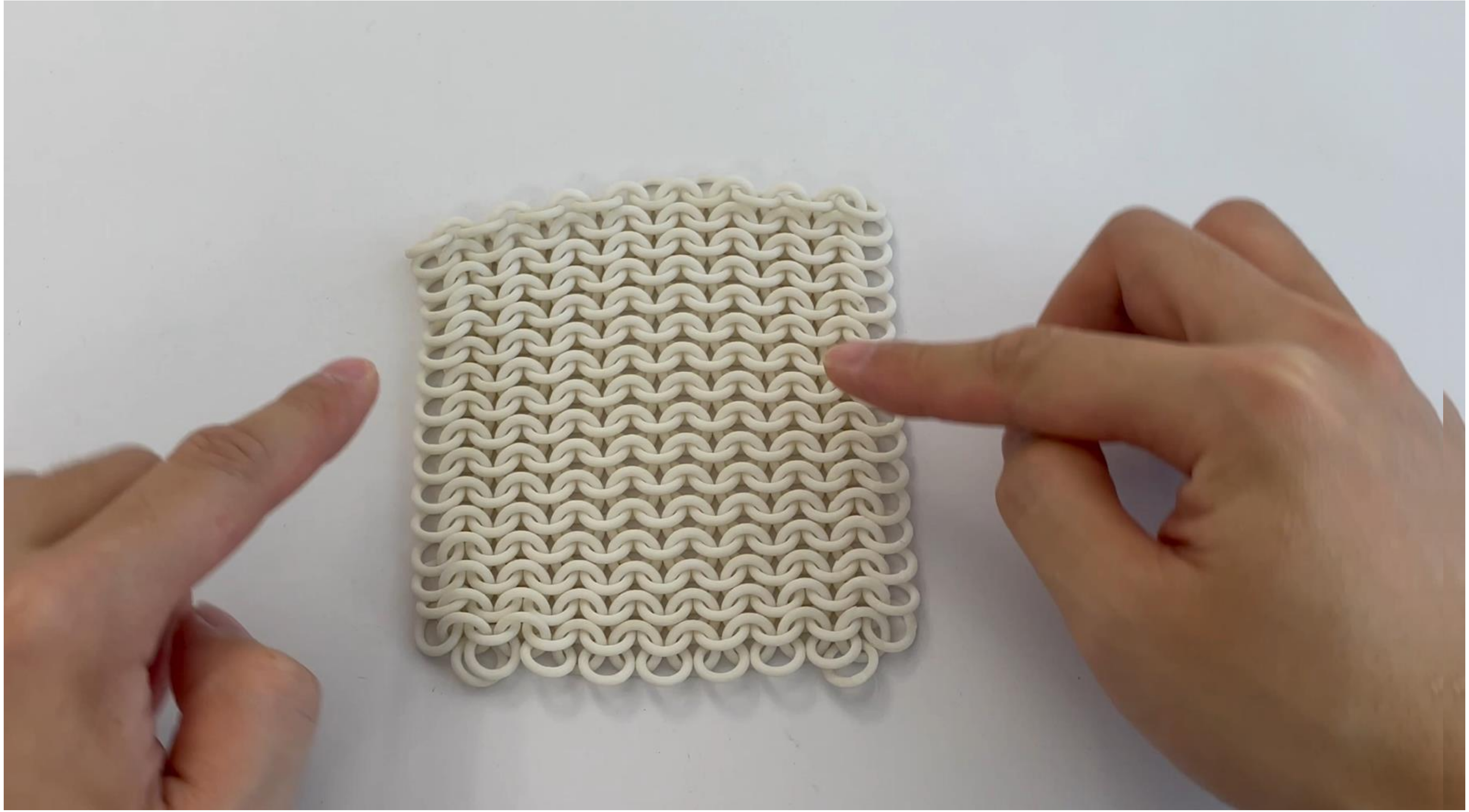
Outline Today

- Introduction to Computational Design of Metamaterials
- Computational Models
  - Rigid Body, Finite Element Method, Discrete Elastic Rods
- Numerical Homogenization
- Case Study1: Mechanical Characterization
  - Discrete Interlocking Materials
- Numerical Methods in Inverse Design
- Case Study2: Metamaterials Design with Desired Behaviors
  - Inverse Design of Structured Surfaces and Discrete Interlocking Materials



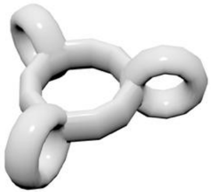
P. Tang, S. Coros, B. Thomaszewski. Beyond Chainmail: Computational Modeling of Discrete Interlocking Materials. ACM SIGGRAPH 2023

Discrete Interlocking Materials



Discrete Interlocking Materials

Element Shape + Connectivity



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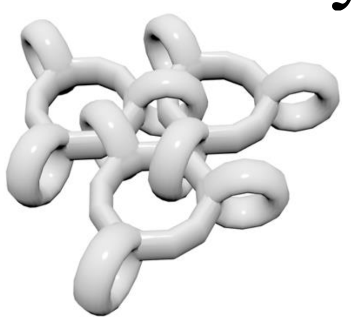
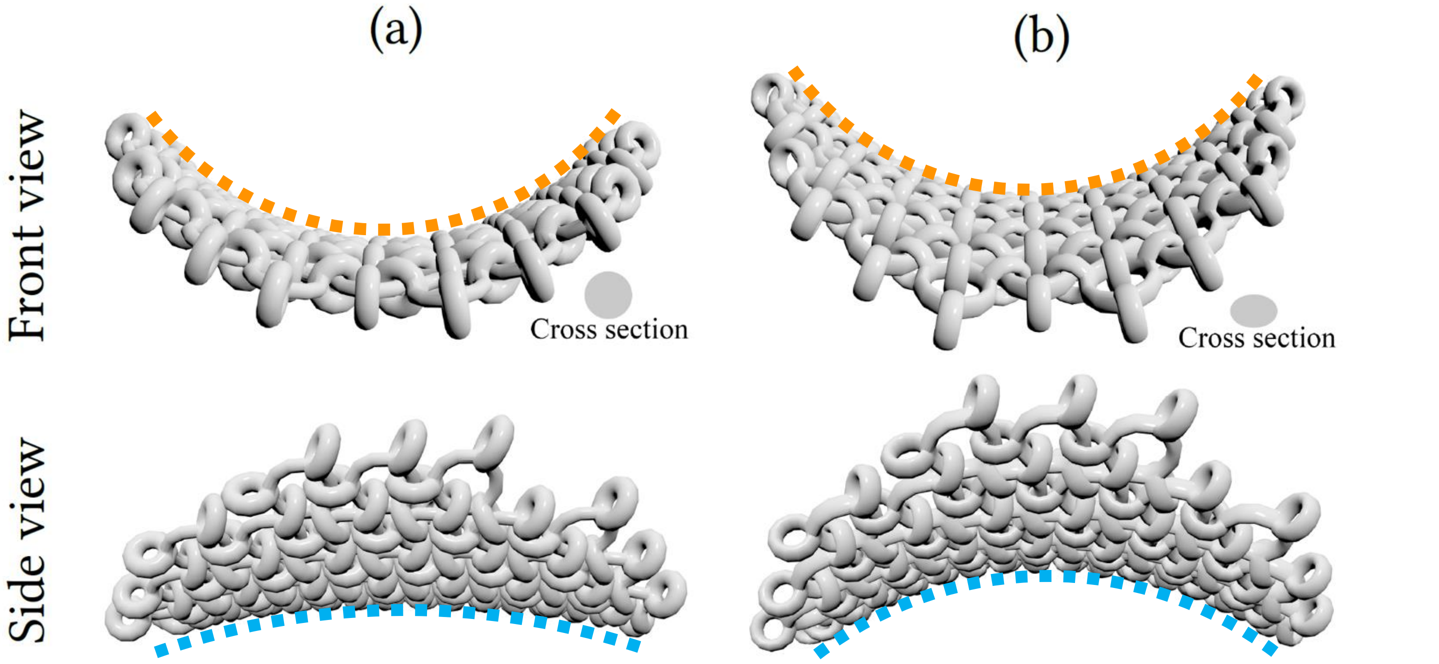


Macromechanical Properties

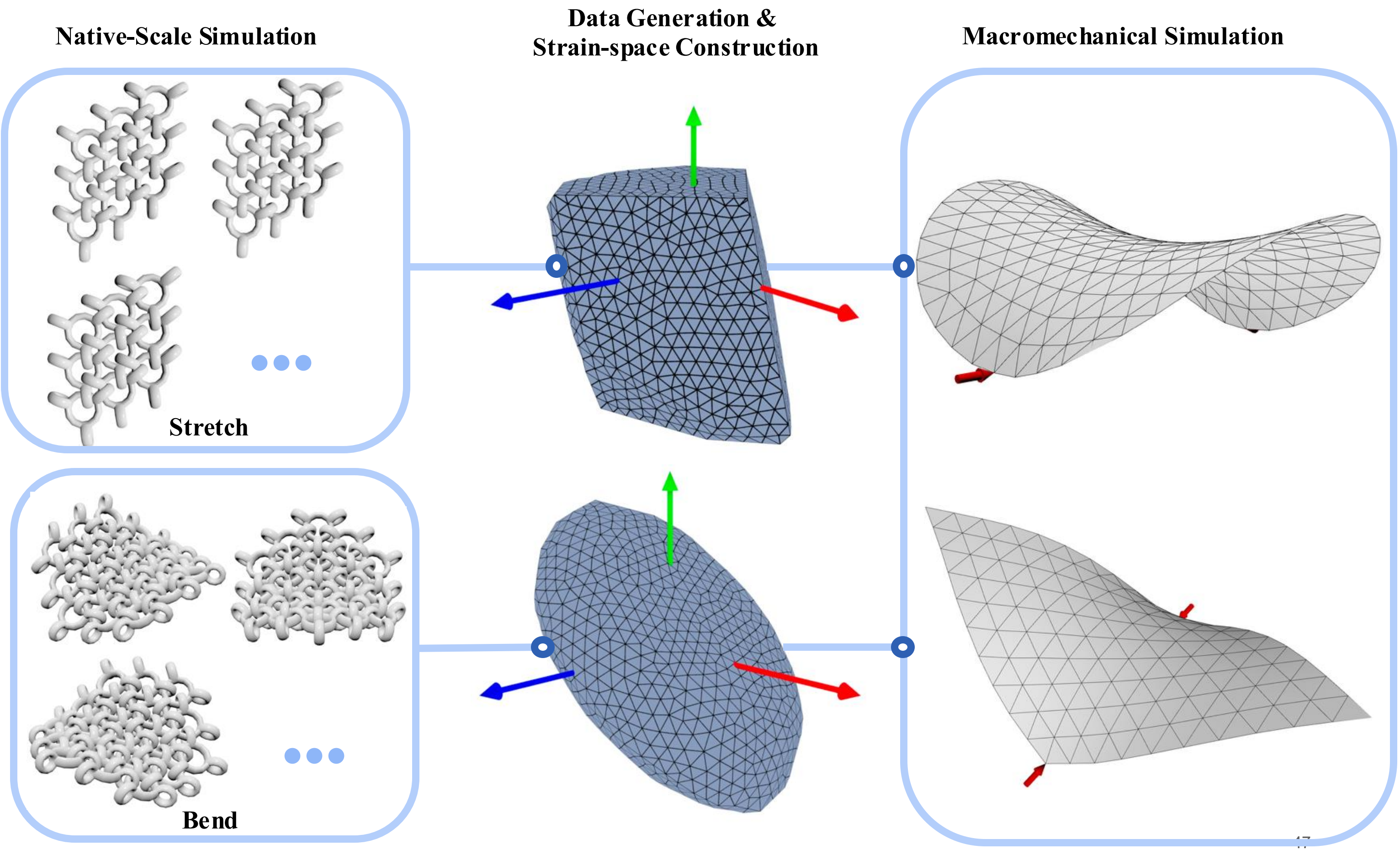
Discrete Interlocking Materials



Goal

A new computational framework for modeling and characterizing DIM composed of quasi-rigid elements.

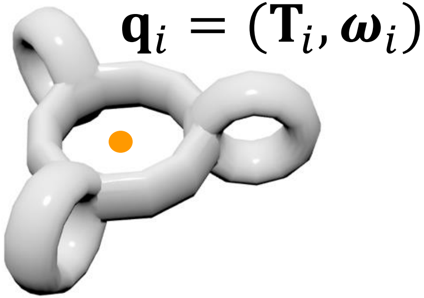
Overview

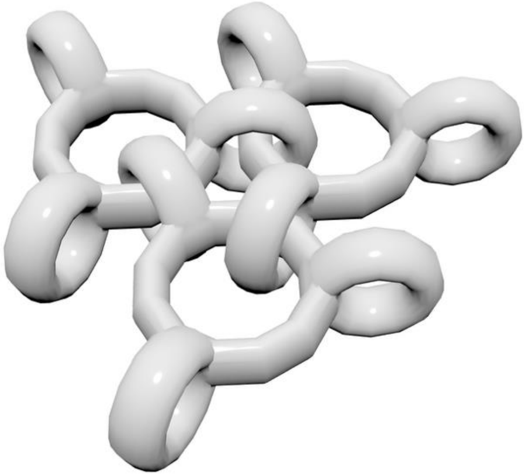

Native-Scale Simulation
Data Generation &
Strain-space Construction
Macromechanical Simulation
Stretch
Bend

Native-Scale Model

- We simulate static equilibrium states of DIM as rigid bodies with contact by an unconstrained minimization problem

$$\min_{\mathbf{q}} E_{\mathrm{Ext}}(\mathbf{q}) + E_{\mathrm{Coll}}(\mathbf{q})$$



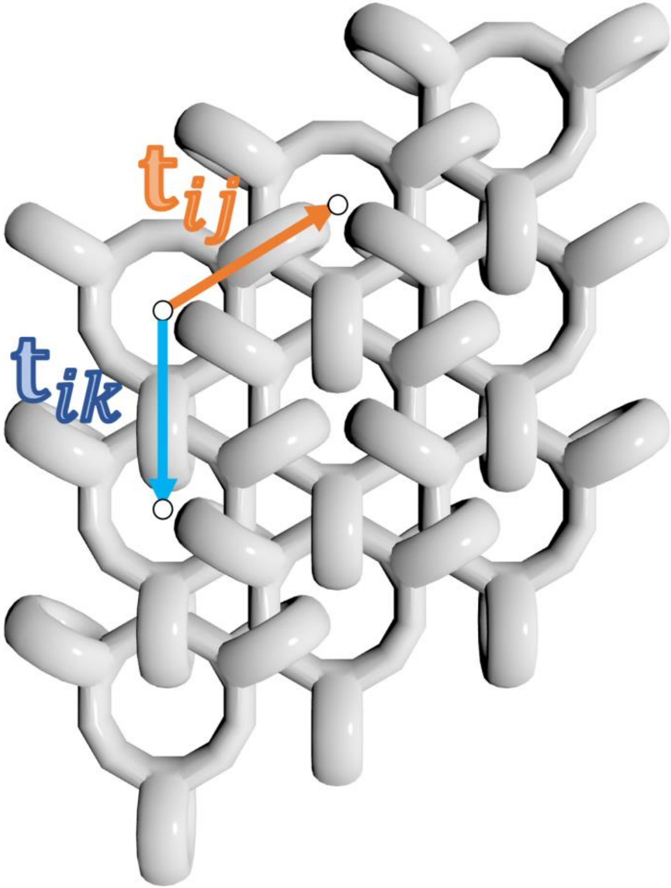


Macro-Scale Deformations – In-plane

Periodicity:

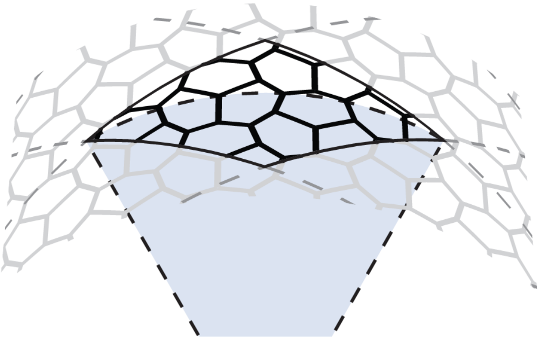
$\mathbf{T}_j = \mathbf{T}_i + \mathbf{t}_{ij}$

$\boldsymbol{\omega}_j = \boldsymbol{\omega}_i$



Macro-Scale Deformations – Out-of-plane

- Single curvature states with periodic boundary conditions can be conveniently modeled.

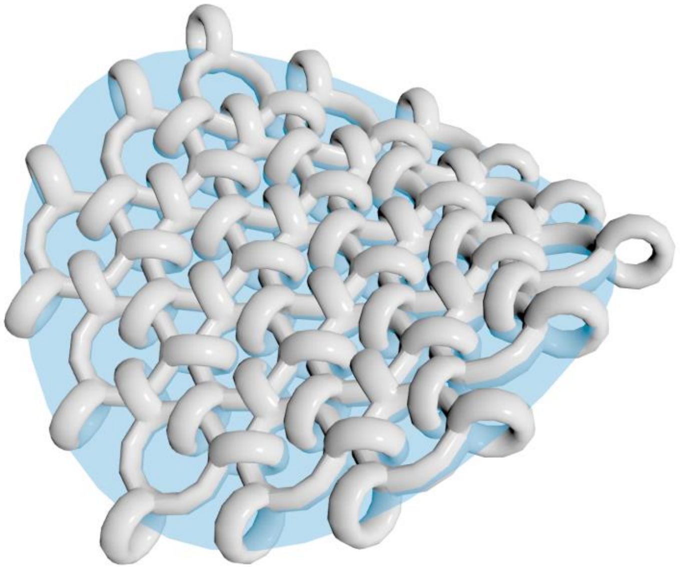


- However, one cannot, in Euclidean geometry, define a finite-sized, double-curvature patch that tiles with itself [Sausset and Tarjus 2007].

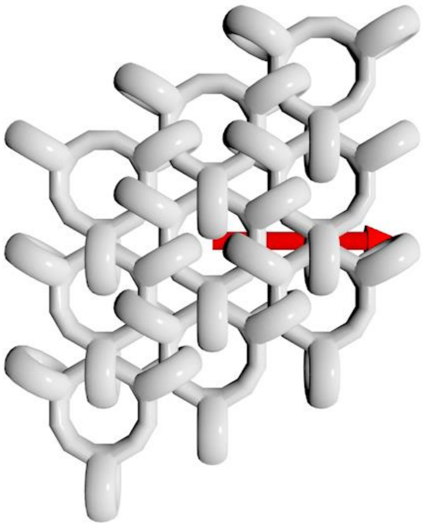
Macro-Scale Deformations – Out-of-plane

- Circular finite patches of paraboloid surfaces

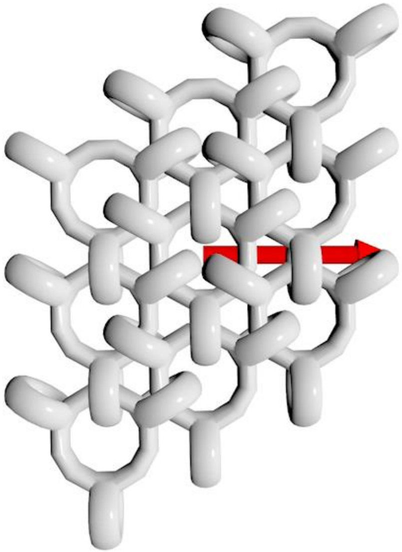
$$z = Ax^2 + By^2 + Cxy$$



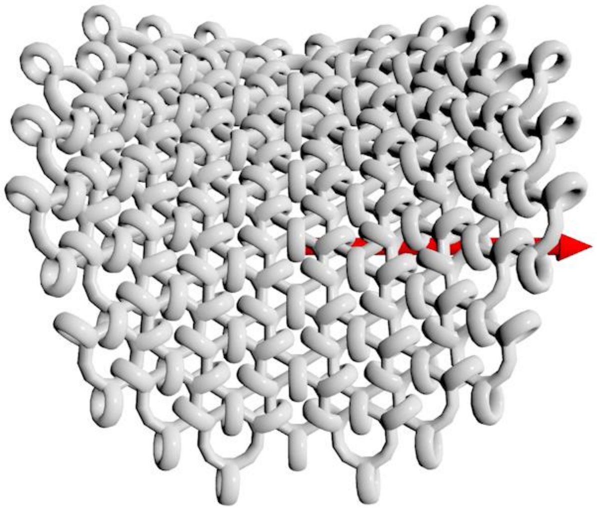
Native-Scale Simulations



Stretching

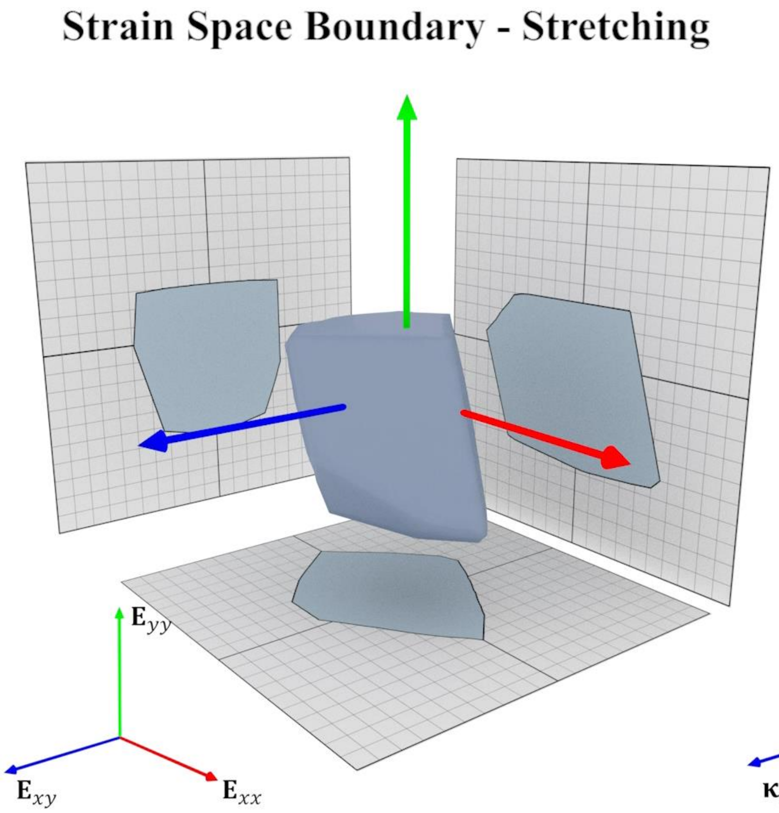


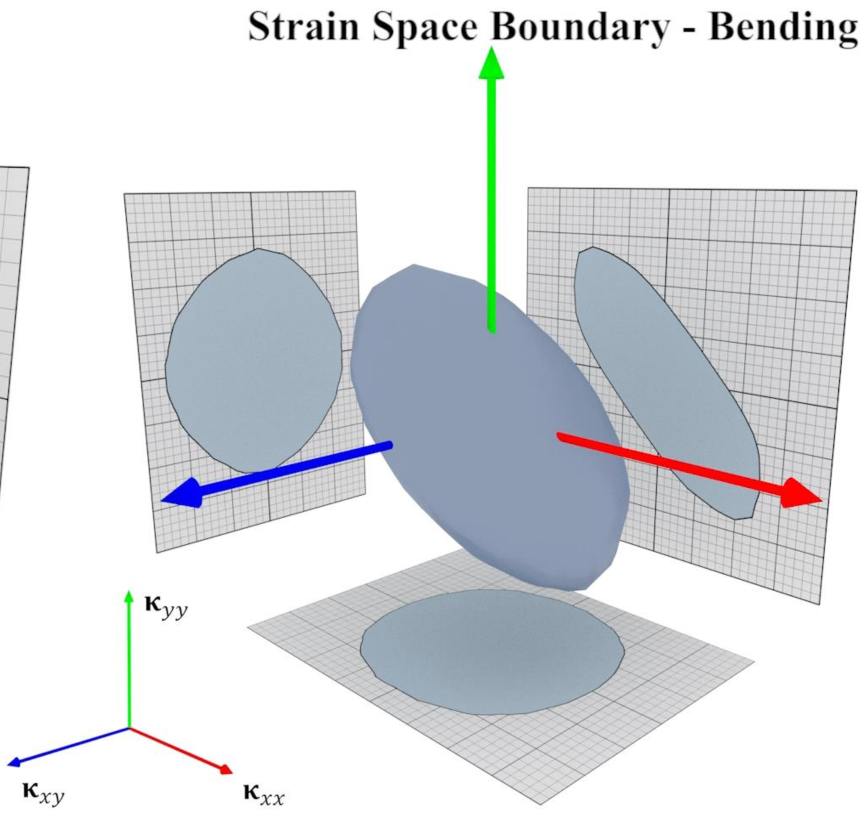
Compression



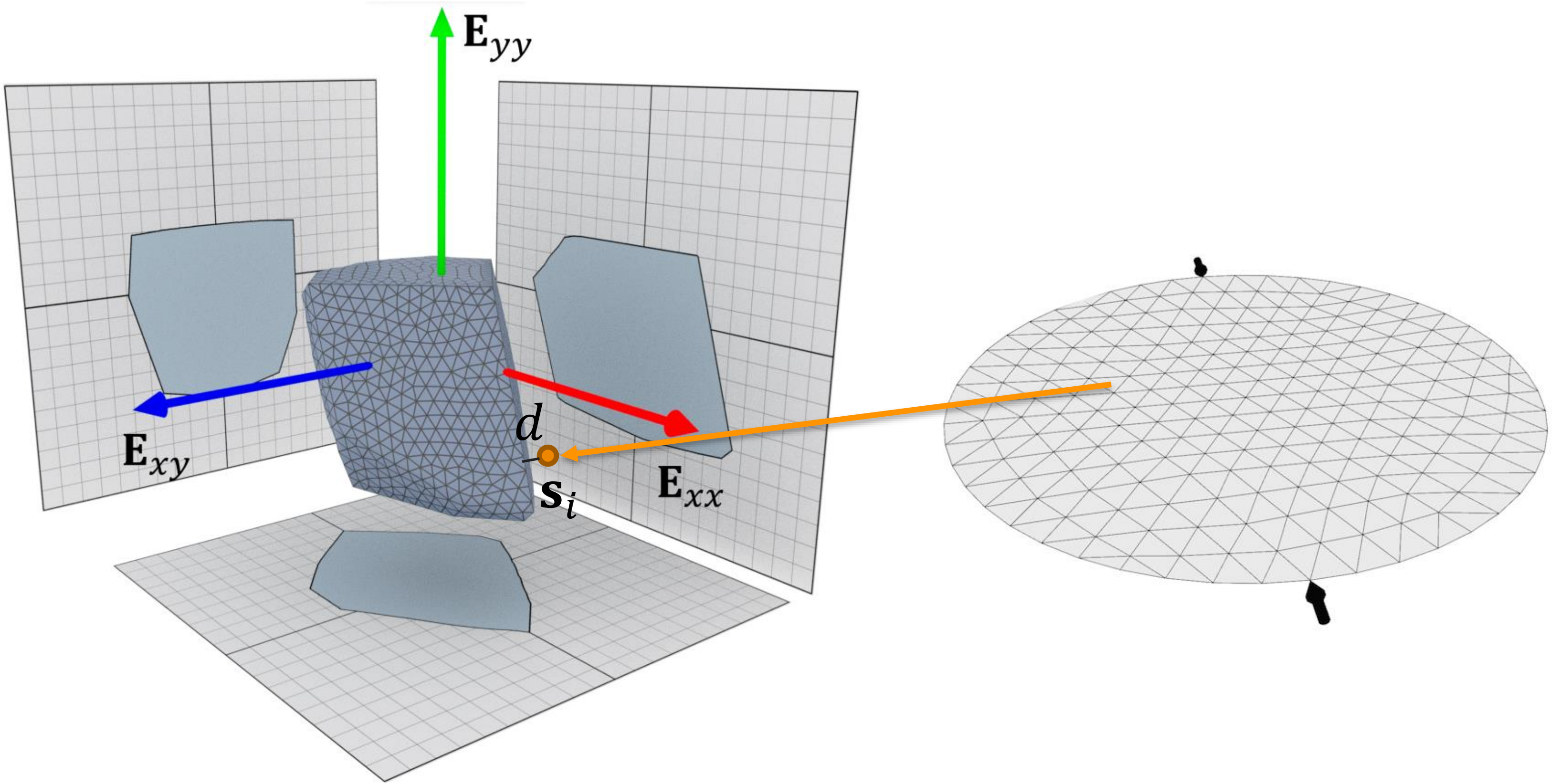
Bending

Strain-Space Representation

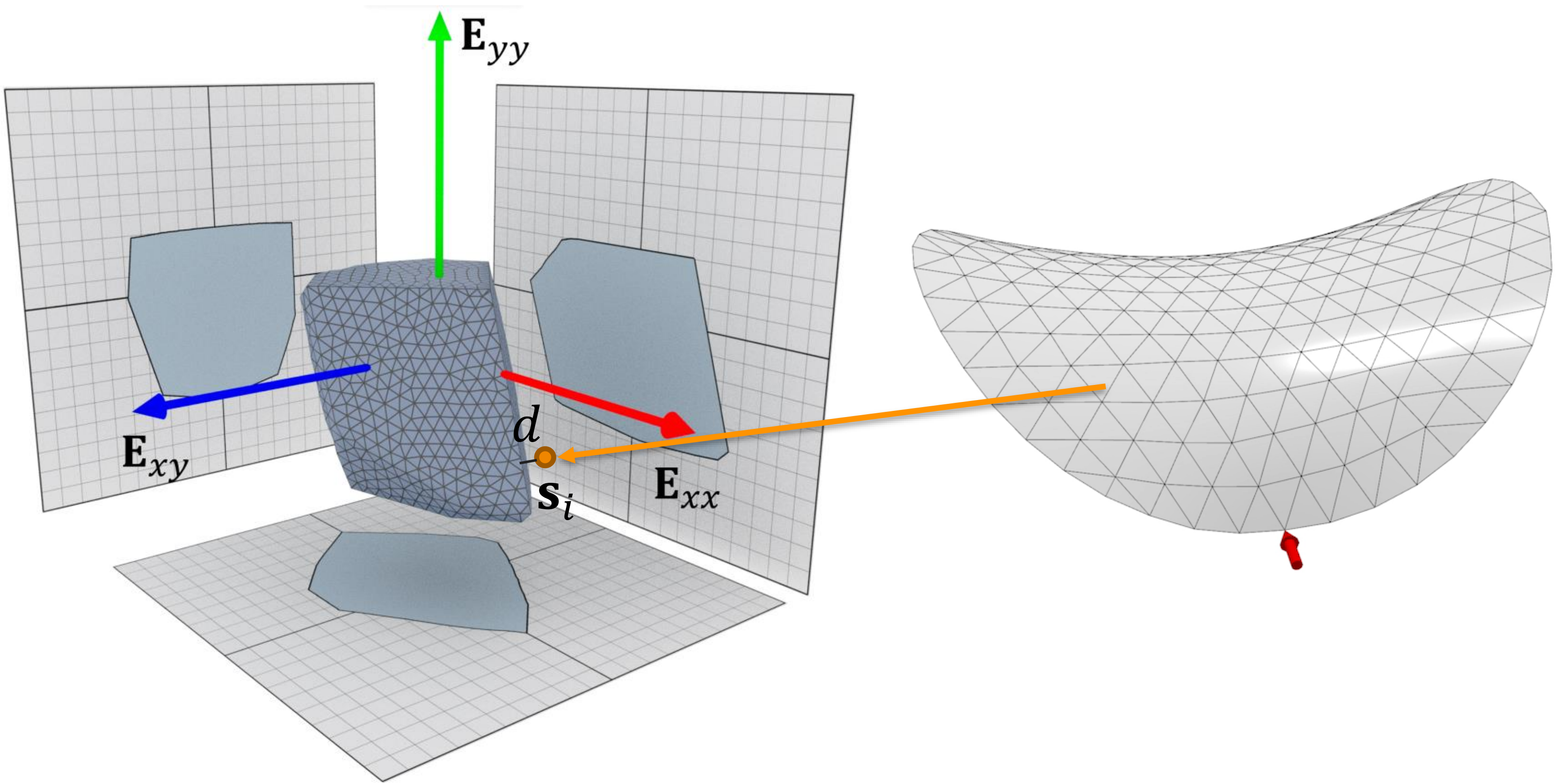




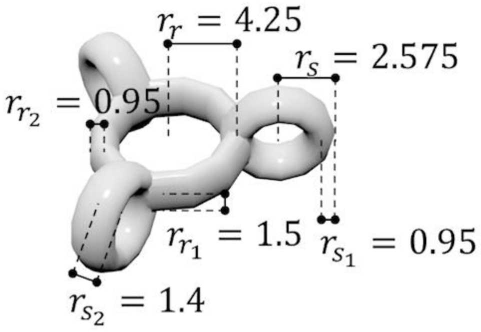
Macro-Scale Model

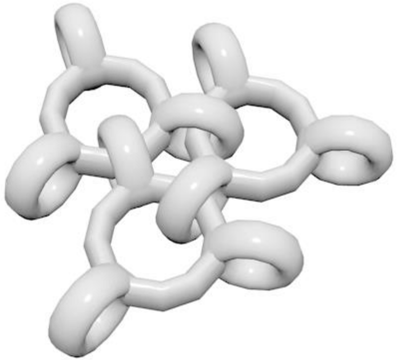


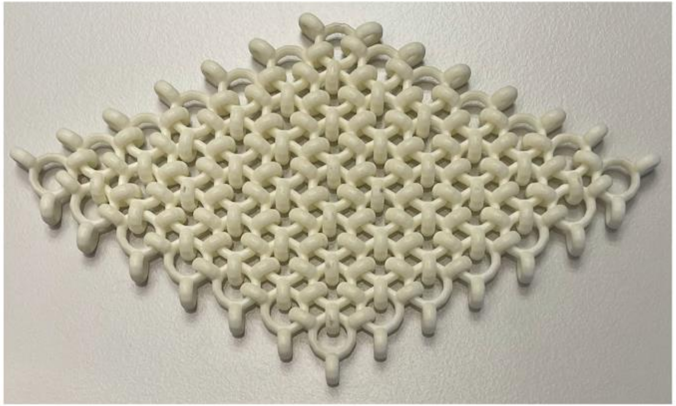
Macro-Scale Model



Threefold Symmetric Chainmail



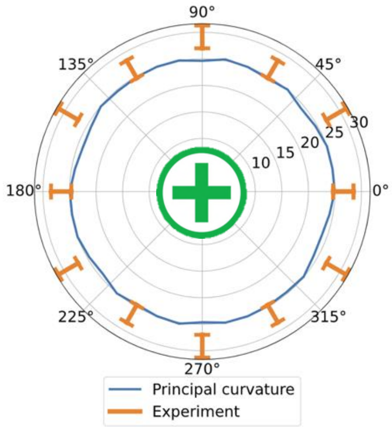




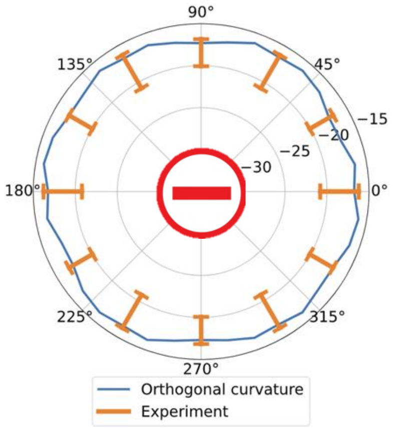
Threefold Symmetric Chainmail

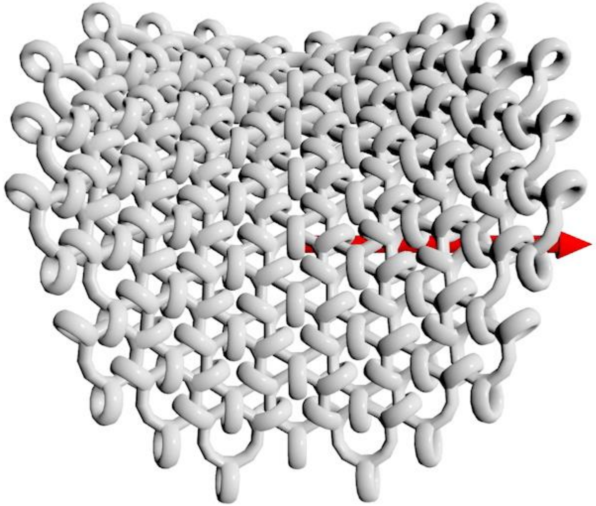
Planar State

Principal Curvature Limits



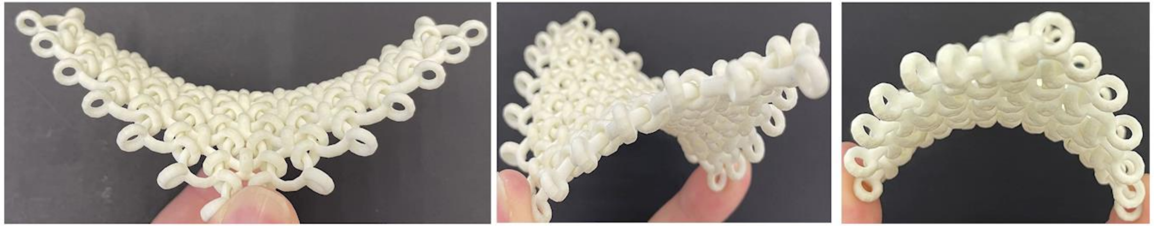
Orthogonal Curvature Limits

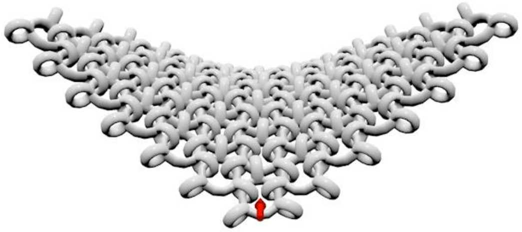


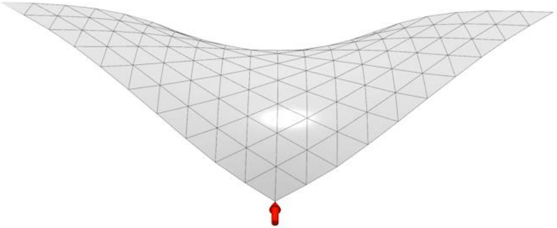


Bending

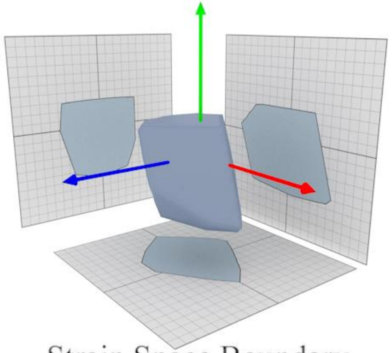
Threefold Symmetric Chainmail



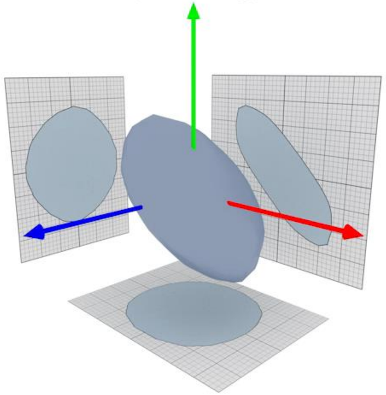




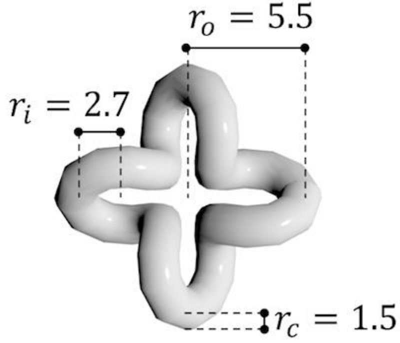
Strain Space Boundary
(Stretching)

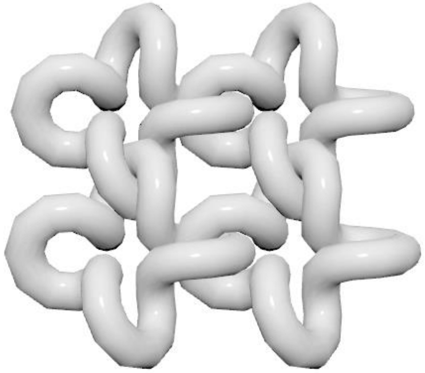


Strain Space Boundary
(Bending)

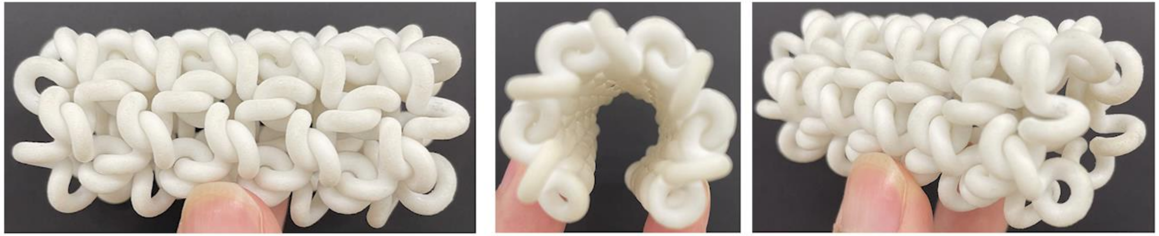


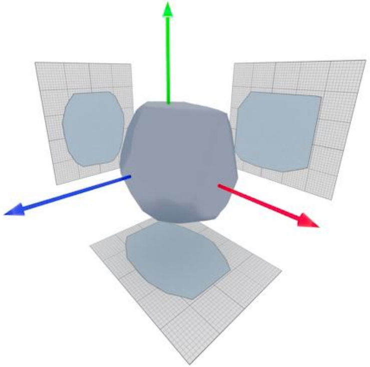
Torus Knot Material

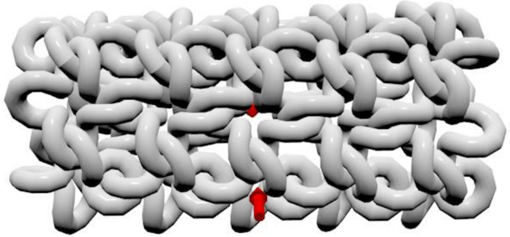


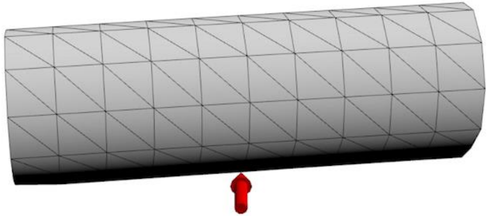


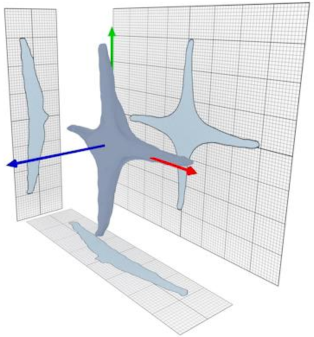
Torus Knot Material



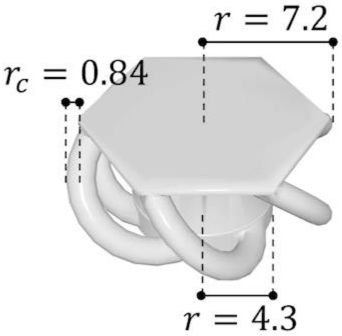


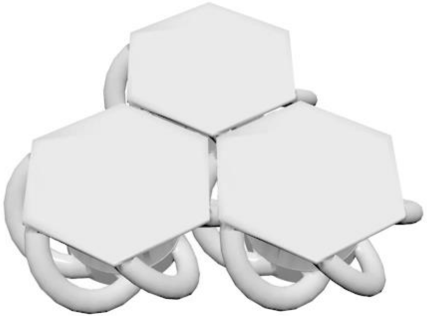






Scale Mail





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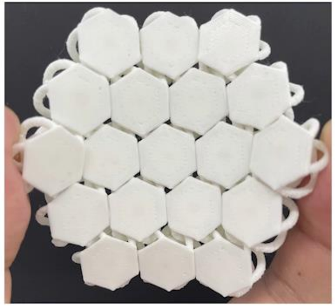

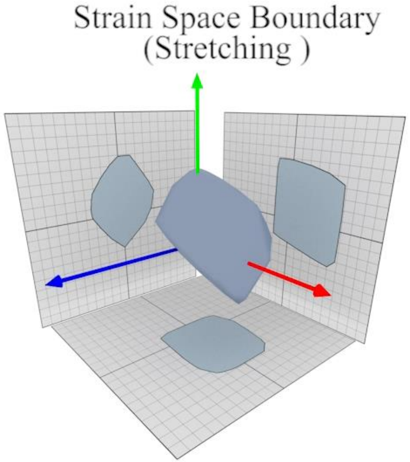
Strain Space Boundary
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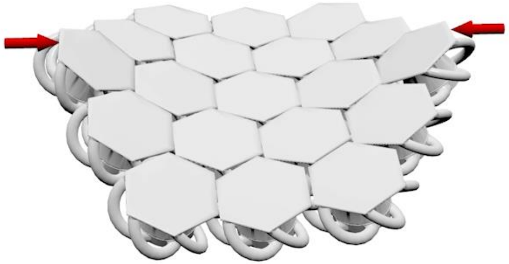
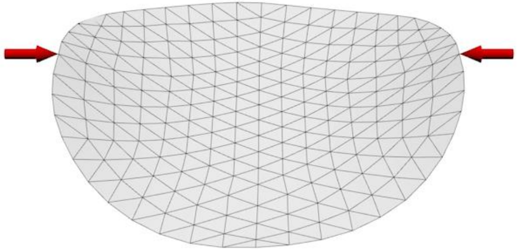
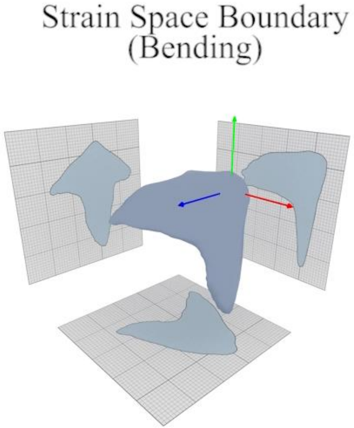
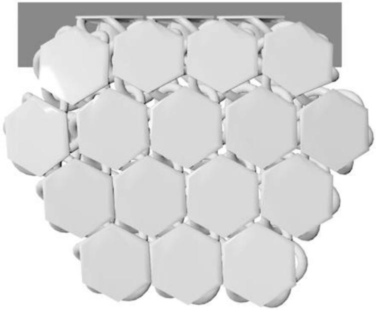


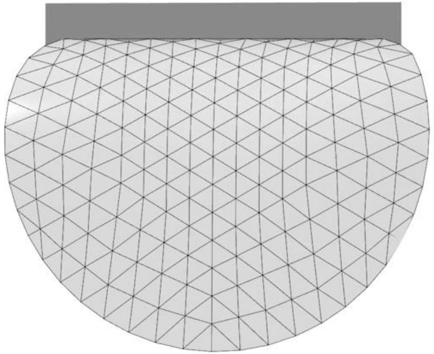



Strain Space Boundary
(Bending)

Scale Mail

Bending Under Gravity - Side 1





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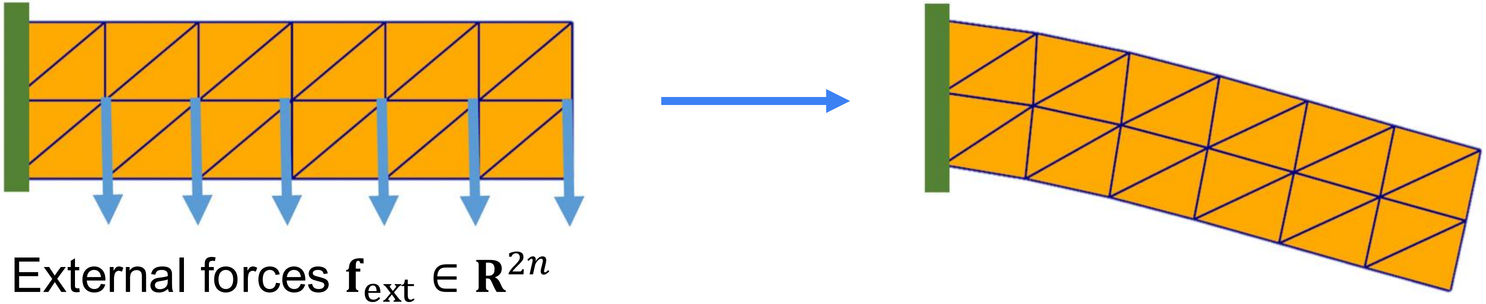
Forward Problem

- Consider a 2D elastic bar

Undeformed state $\mathbf{p} \in \mathbf{R}^{2n}$ Deformed state $\mathbf{x} \in \mathbf{R}^{2n}$



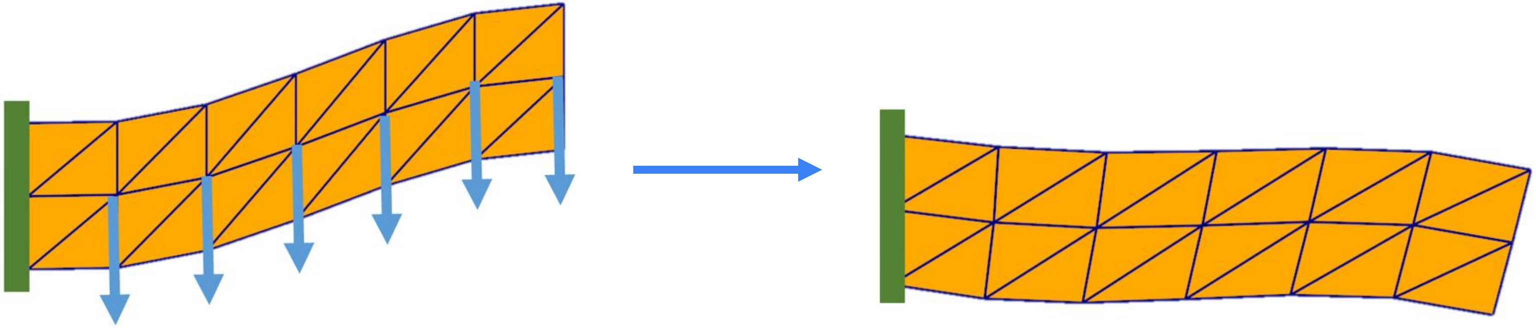
External forces $\mathbf{f}_{\text{ext}} \in \mathbf{R}^{2n}$

- Forward problem: given design parameter $\mathbf{p}$ and external force $\mathbf{f}_{\text{ext}}$, compute equilibrium configuration $\mathbf{x}$ by solving

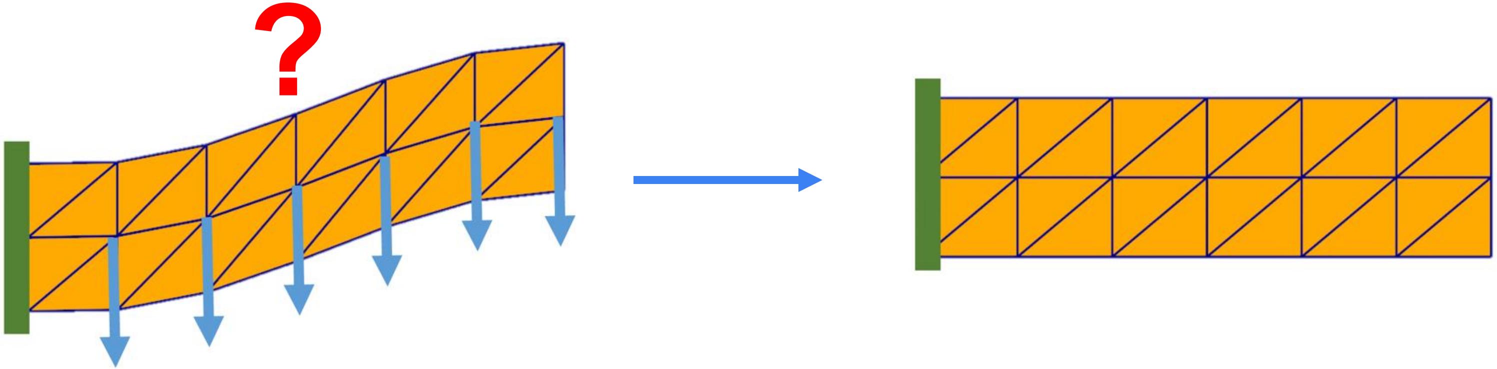
$$\mathbf{f}(\mathbf{x}, \mathbf{p}) = \mathbf{f}_{\text{ext}} + \mathbf{f}_{\text{int}}(\mathbf{x}, \mathbf{p}) = \mathbf{0}$$

Forward Problem

- Change the undeformed state $\mathbf{p}$ changes the equilibrium state $\mathbf{x}$



- How can we determine $\mathbf{p}$ that leads to a desired equilibrium state?



Inverse Design Objective

- Introduce objective that quantifies distance to target

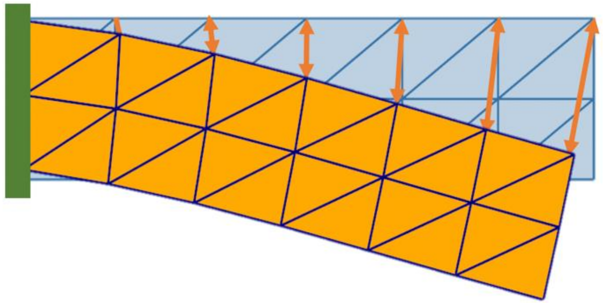
$$T(\mathbf{x}) = \frac{1}{2}\|\mathbf{x} - \mathbf{x}_{\text{tar}}\|^2$$

- Introduce objective that quantifies distance to target

$$T(\mathbf{x}) = \frac{1}{2}\|\mathbf{x} - \mathbf{x}_{\text{tar}}\|^2$$

- Objective: find $\mathbf{x}$ and $\mathbf{p}$ such that $\mathbf{x}$ minimizes T
- Constraint: $\mathbf{x}$ has to be an equilibrium state for $\mathbf{p}$, i.e., $\mathbf{f}(\mathbf{x}, \mathbf{p}) = \mathbf{0}$

Target shape $\mathbf{x}_{\text{tar}}$



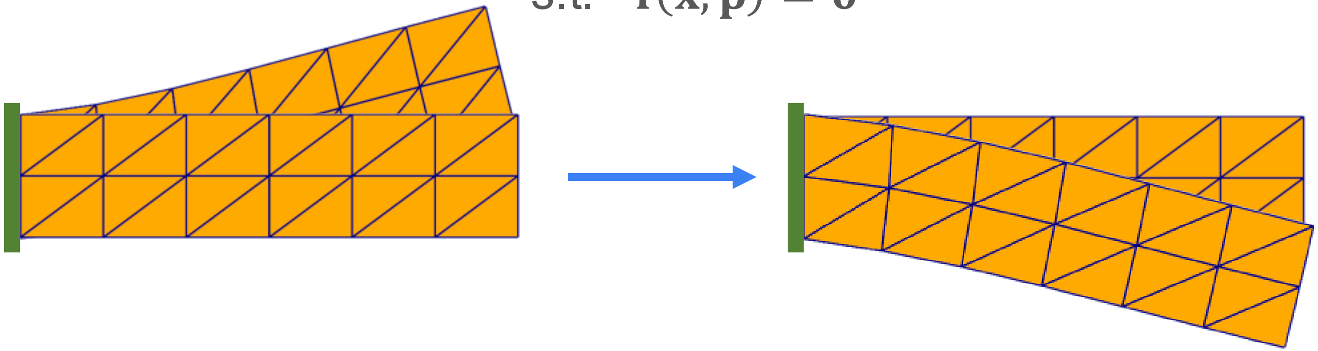
$\mathbf{x} - \mathbf{x}_{\text{tar}}$

- Objective: find $\mathbf{x}$ and $\mathbf{p}$ such that $\mathbf{x}$ minimizes T
- Constraint: $\mathbf{x}$ has to be an equilibrium state for $\mathbf{p}$, i.e., $\mathbf{f}(\mathbf{x}, \mathbf{p}) = \mathbf{0}$

Inverse Problem

- Formulation

$$\min_{\mathbf{x}} T(\mathbf{x}, \mathbf{p})$$
$$\text{s.t.} \quad \mathbf{f}(\mathbf{x}, \mathbf{p}) = \mathbf{0}$$



- Interpretation:

From all possible equilibrium states $\mathbf{x}$,
i.e., those $\mathbf{x}$ for which there exists $\mathbf{p}$ such that $\mathbf{f}(\mathbf{x}, \mathbf{p}) = \mathbf{0}$,
find the one that minimizes $T(\mathbf{x})$.

Constrained Optimization

- Generic optimization problem

$$\min_{\mathbf{x}} f(\mathbf{x}) \quad \text{s.t.} \quad \mathbf{C}(\mathbf{x}) = \mathbf{0}$$

- Unknowns $\mathbf{x} \in \mathbf{R}^n$
- Objective function $f(\mathbf{x}): \mathbf{R}^n \to \mathbf{R}$
- Constraints $\mathbf{C}(\mathbf{x}): \mathbf{R}^n \to \mathbf{R}^{\mathbf{m}}$

How can we solve this optimization problem?

Numerical Methods in Inverse Design

- Sequential Quadratic Programming (SQP)
- Sensitivity Analysis
- Interior Point Methods
- Augmented Lagrangian Method
- …

SQP for Inverse Problems

- Lagrangian $L(\mathbf{x}, \mathbf{p}, \boldsymbol{\lambda}) = T(\mathbf{x}) + \mathbf{f}(\mathbf{x}, \mathbf{p})^{\mathrm{T}} \boldsymbol{\lambda}$

$$\left.\begin{array}{lll} - & \mathbf{x} & \text{deformed positions} \\ - & \mathbf{p} & \text{undeformed positions} \\ - & \boldsymbol{\lambda} & \text{Lagrangian multipliers} \end{array}\right\} \quad \mathbf{s} = (\mathbf{x}, \mathbf{p}, \boldsymbol{\lambda})^{\mathrm{T}} \in \mathbf{R}^{3 \cdot D \cdot n}$$

- First order optimality conditions: $\nabla_s L = \mathbf{0}$

$$\boxed{\begin{aligned} \nabla_{\mathbf{x}} L &= \nabla_{\mathbf{x}} T(\mathbf{x}) + \nabla_{\mathbf{x}} \mathbf{f}(\mathbf{x}, \mathbf{p})^{\mathrm{T}} \boldsymbol{\lambda} = 0 \\ \nabla_{\mathbf{p}} L &= \nabla_{\mathbf{p}} T(\mathbf{x}) + \nabla_{\mathbf{p}} \mathbf{f}(\mathbf{x}, \mathbf{p})^{\mathrm{T}} \boldsymbol{\lambda} = 0 \\ \nabla_{\lambda} L &= \qquad\qquad\qquad\quad \mathbf{f}(\mathbf{x}, \mathbf{p}) = 0 \end{aligned}}$$

SQP for Inverse Problems

- Given $\boldsymbol{s}$, find $\Delta\boldsymbol{s}$ such that

$$\nabla_{\boldsymbol{s}} L(\mathbf{s} + \Delta\mathbf{s}) = \mathbf{0} \quad \rightarrow \quad \nabla_{\boldsymbol{ss}} L \cdot \Delta\mathbf{s} = -\nabla_{\boldsymbol{s}} L$$

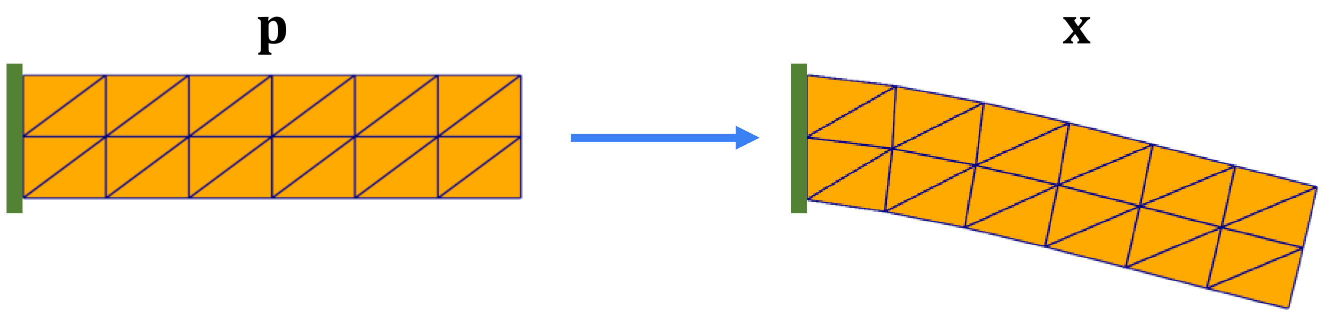
$$\begin{bmatrix} \nabla_{\mathbf{xx}} T + \nabla_{\mathbf{xx}} \mathbf{f}^{\mathrm{T}} \boldsymbol{\lambda} & \nabla_{\mathbf{xp}} \mathbf{f}^{\mathrm{T}} \boldsymbol{\lambda} & \nabla_{\mathbf{x}} \mathbf{f}^{\mathrm{T}} \\ \boldsymbol{\lambda}^{\mathrm{T}} \nabla_{\mathbf{xp}} \mathbf{f} & \nabla_{\mathbf{pp}} \mathbf{f}^{\mathrm{T}} \boldsymbol{\lambda} & \nabla_{\mathbf{p}} \mathbf{f}^{\mathrm{T}} \\ \nabla_{\mathbf{x}} \mathbf{f} & \nabla_{\mathbf{p}} \mathbf{f} & \mathbf{0} \end{bmatrix} \cdot \begin{bmatrix} \Delta\mathbf{x} \\ \Delta\mathbf{p} \\ \Delta\boldsymbol{\lambda} \end{bmatrix} = - \begin{bmatrix} \nabla_{\mathbf{x}} L \\ \nabla_{\mathbf{p}} L \\ \nabla_{\boldsymbol{\lambda}} L \end{bmatrix}$$

- Indefinite matrix
  - Quadratic programming solver (MOSEK, GUROBI…)
- Apply Newton’s method to solve the problem.
  - Merit function, e.g., l_1 merit function $\phi(\mathbf{s}) = T(\mathbf{s}) + \mu \sum_i |c_i(\mathbf{s})|$

SQP Discussion

- SQP is a powerful optimization method, and it can be very fast
- Hessian of Lagrangian involves higher-order derivatives
  - Difficult and expensive to compute
  - can introduce indefiniteness
  - Alternative: use Quasi-newton methods to approximate Hessian
- SQP leads to large number of variables
  - One variable per DoF
  - One variable per parameter
  - One Lagrange multiplier per constraint

Sensitivity Analysis



- In this this problem, the design parameters $\mathbf{p}$ are effective DoFs.
- $\mathbf{x} = \text{simulation}(\mathbf{p})$
- For design, we need derivatives

$$\frac{dT}{d\mathbf{p}} = \frac{\partial T}{\partial \mathbf{x}} \frac{d\mathbf{x}}{d\mathbf{p}} + \frac{\partial T}{\partial \mathbf{p}}$$

- How to compute?

$$\frac{d\mathbf{x}}{d\mathbf{p}} = \frac{d\ \text{simulation}}{d\mathbf{p}}$$

Sensitivity Analysis

- Simulation map: $\mathbf{x} = \mathrm{simulation}(\mathbf{p})$

$$\mathbf{f}(\mathbf{x}, \mathbf{p}) = \mathbf{0} \qquad \text{has to hold always}$$

- Any change in design parameters $\mathbf{p}$ should lead to corresponding change in state $\mathbf{x}$ such that $\mathbf{f}(\mathbf{x}, \mathbf{p}) = \mathbf{0}$ is still satisfied.

$$\frac{d\mathbf{f}}{d\mathbf{p}} = 0 \quad \rightarrow \quad \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \frac{d\mathbf{x}}{d\mathbf{p}} + \frac{\partial \mathbf{f}}{\partial \mathbf{p}} = 0$$

Sensitivity Matrix $\qquad \dfrac{d\mathbf{x}}{d\mathbf{p}} = -\left(\dfrac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^{-1} \dfrac{\partial \mathbf{f}}{\partial \mathbf{p}}$

Sensitivity Analysis

- Design objective gradient

$$\nabla_{\mathbf{p}} T = \frac{\partial T}{\partial \mathbf{x}} \frac{d\mathbf{x}}{d\mathbf{p}} + \frac{\partial T}{\partial \mathbf{p}}$$

- Solve the problem by using Gradient Descent or LBSGS

Gradient Descent
Until Convergence:
    Compute search direction $\Delta\mathbf{p} = -\nabla_{\mathbf{p}} T$
    $\alpha = 1$
    Line search Loop:
        $\mathbf{p}_{\mathrm{L+1}} = \mathbf{p} + \alpha\Delta\mathbf{p}$
        $\mathbf{x}_{\mathrm{L+1}} = \mathrm{Simulation}(\mathbf{p}_{\mathrm{L+1}})$
        $\alpha = \alpha/2$
        Until $T_{L+1} < T_L$
End

Adjoint Method

- Design objective gradient

$$\nabla_{\mathbf{p}} T = \frac{\partial T}{\partial \mathbf{x}} \frac{d\mathbf{x}}{d\mathbf{p}} + \frac{\partial T}{\partial \mathbf{p}} = -\boxed{\frac{\partial T}{\partial \mathbf{x}} \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^{-1}} \frac{\partial \mathbf{f}}{\partial \mathbf{p}} + \frac{\partial T}{\partial \mathbf{p}}$$

- The expensive part here is computing $\frac{d\mathbf{x}}{d\mathbf{p}} = -\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^{-1} \frac{\partial \mathbf{f}}{\partial \mathbf{p}}$
  - if number of state variables $\mathbf{x}$ is large
  - If number of design parameters $\mathbf{p}$ is large
- Avoid computing $\frac{d\mathbf{x}}{d\mathbf{p}}$ explicitly, defining adjoint vector $\boldsymbol{\lambda} \in \mathbf{R}^{\mathrm{n}}$ as

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}}^{\mathrm{T}} \boldsymbol{\lambda} = \frac{\partial T}{\partial \mathbf{x}}^{\mathrm{T}}$$

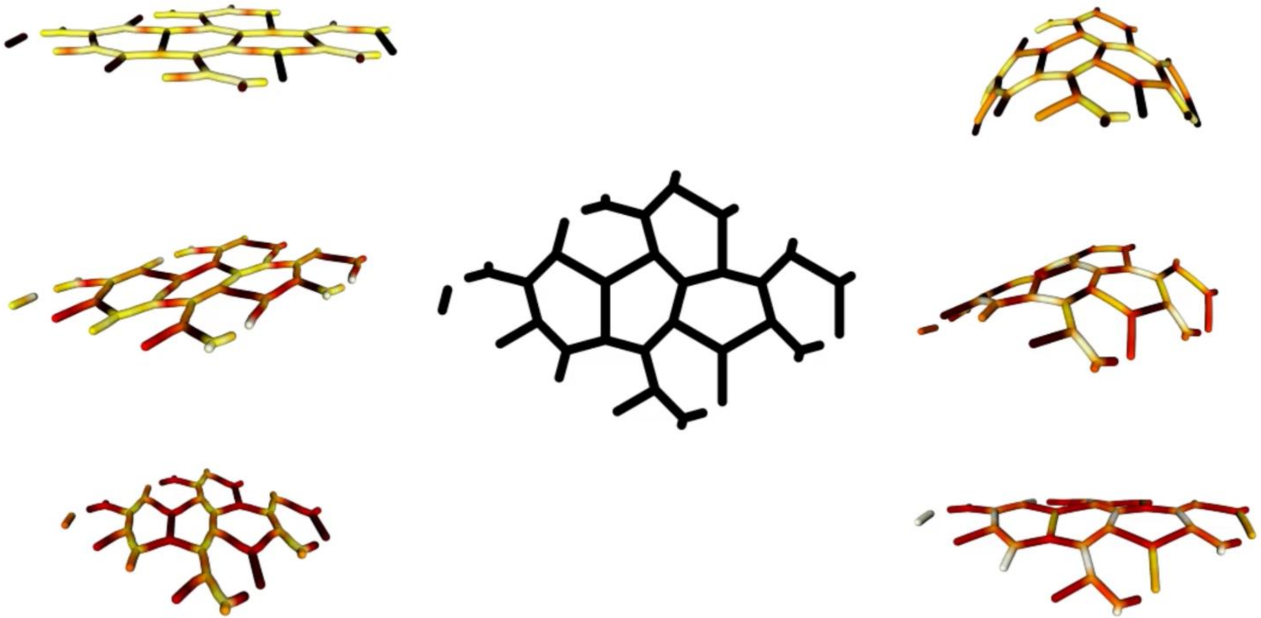
- Design objective gradient

$$\nabla_{\mathbf{p}} T = -\boldsymbol{\lambda}^{\mathrm{T}} \frac{\partial \mathbf{f}}{\partial \mathbf{p}} + \frac{\partial T}{\partial \mathbf{p}}$$

Inverse Design of Metamaterials

- Forward problem, given design parameter $\mathbf{p}$, compute equilibrium configuration $\mathbf{x}$ by solving

$$\mathbf{f}(\mathbf{x}, \mathbf{p}) = \mathbf{f}_{\text{ext}} + \mathbf{f}_{\text{int}}(\mathbf{x}, \mathbf{p}) = \mathbf{0}$$



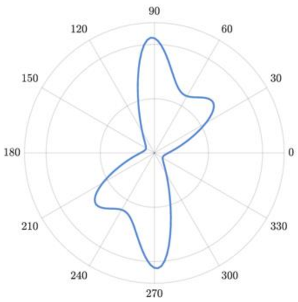
Inverse Design of Metamaterials

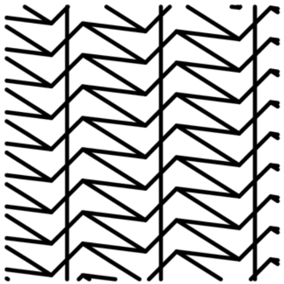
- Target: **Microscopic** geometry from **macroscopic** material properties

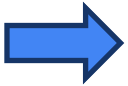
Directional stiffness / Poisson's ratio

Microscopic structure

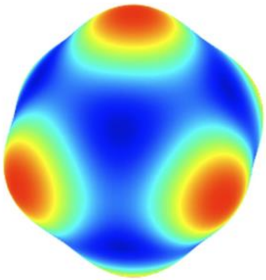
2D

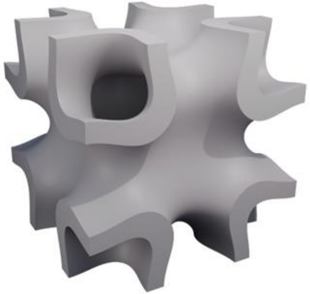






3D

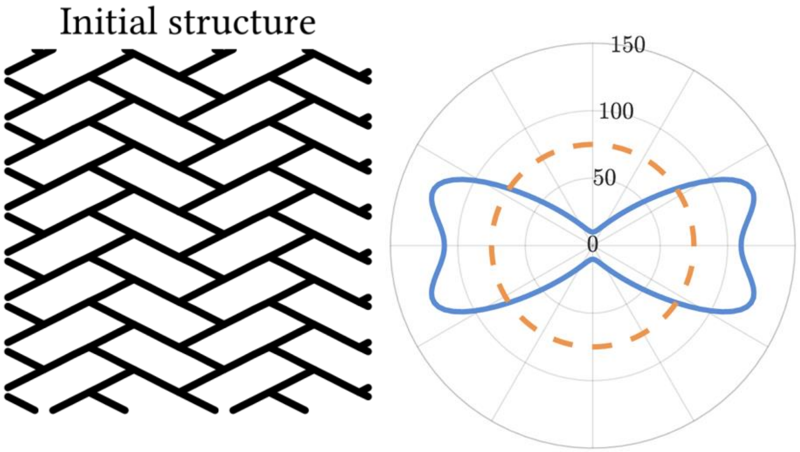


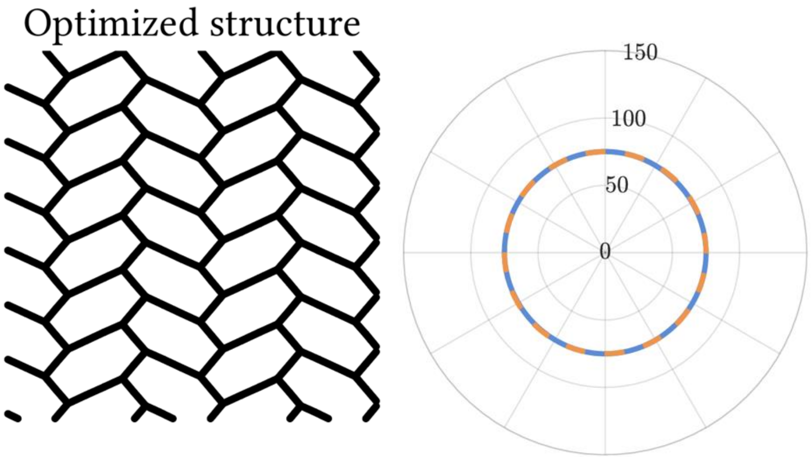


Inverse Design Objective

- Introduce design objective that quantifies the distance to target

$$T(\mathbf{x}) = \frac{1}{2n}\sum_{i}^{n}\left(\frac{E_H(\mathbf{d}_i)}{E_{tar}} - 1\right)^2$$



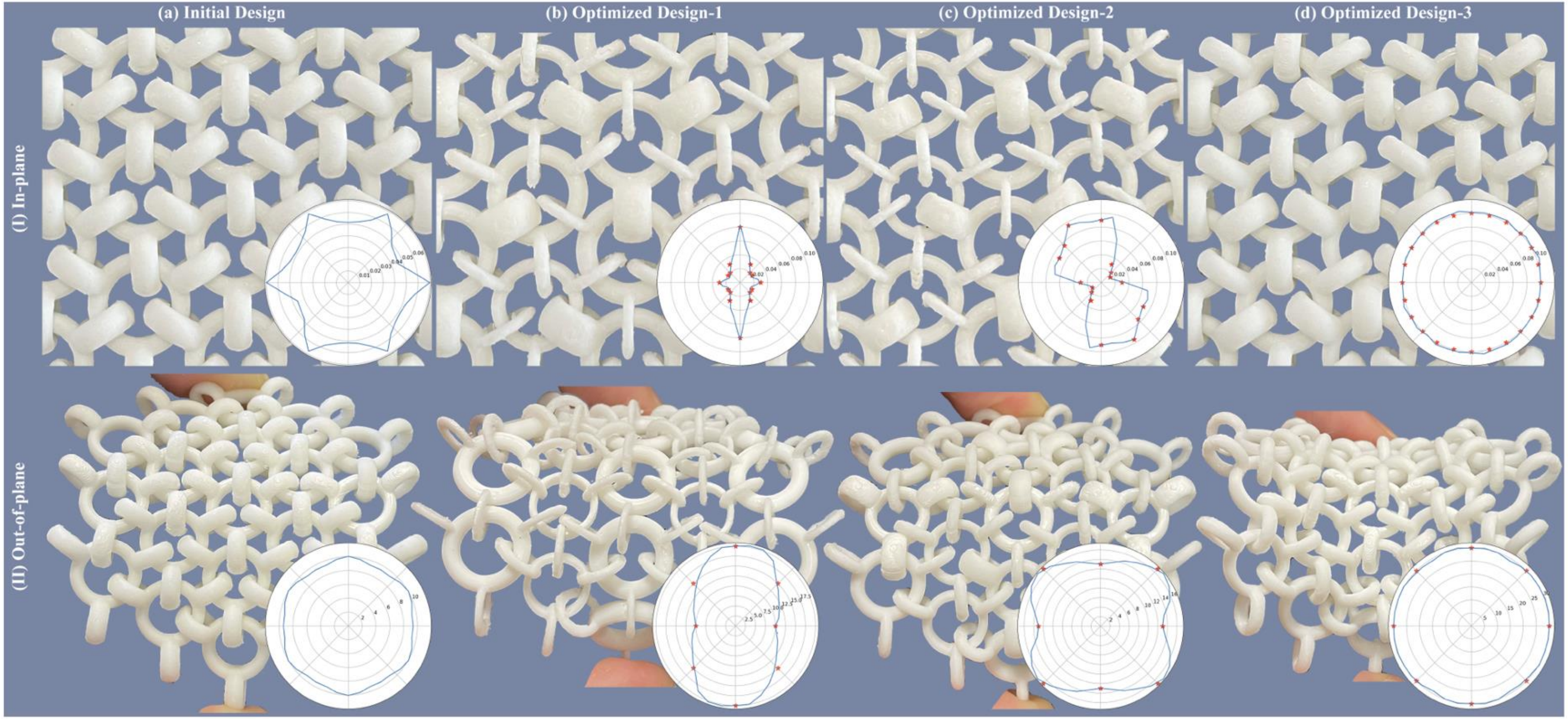


Homogenized Young's modulus

Target Young's modulus

Outline Today

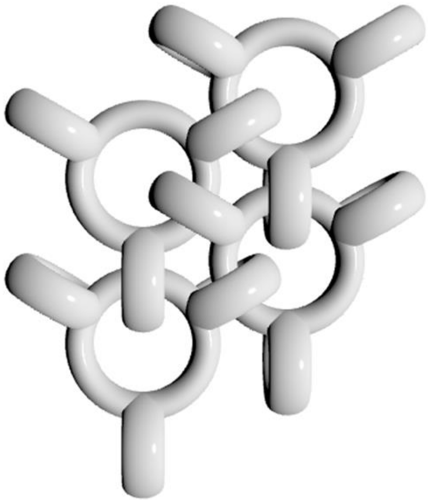
- Introduction to Computational Design of Metamaterials
- Computational Models
  - Rigid Body, Finite Element Method, Discrete Elastic Rods
- Numerical Homogenization
- Case Study1: Mechanical Characterization
  - Discrete Interlocking Materials
- Numerical Methods in Inverse Design
- Case Study2: Metamaterials Design with Desired Behaviors
  - Inverse Design of Discrete Interlocking Materials and Structured Surfaces

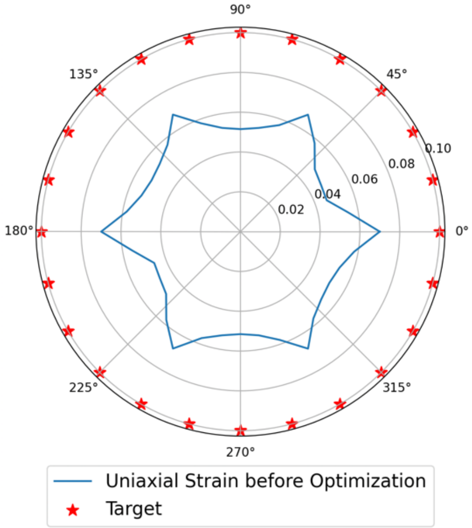


P. Tang, B. Thomaszewski, S. Coros, B. Bickel. Inverse Design of Discrete Interlocking Materials with Desired Mechanical Behavior. ACM SIGGRAPH 2025

Challenge

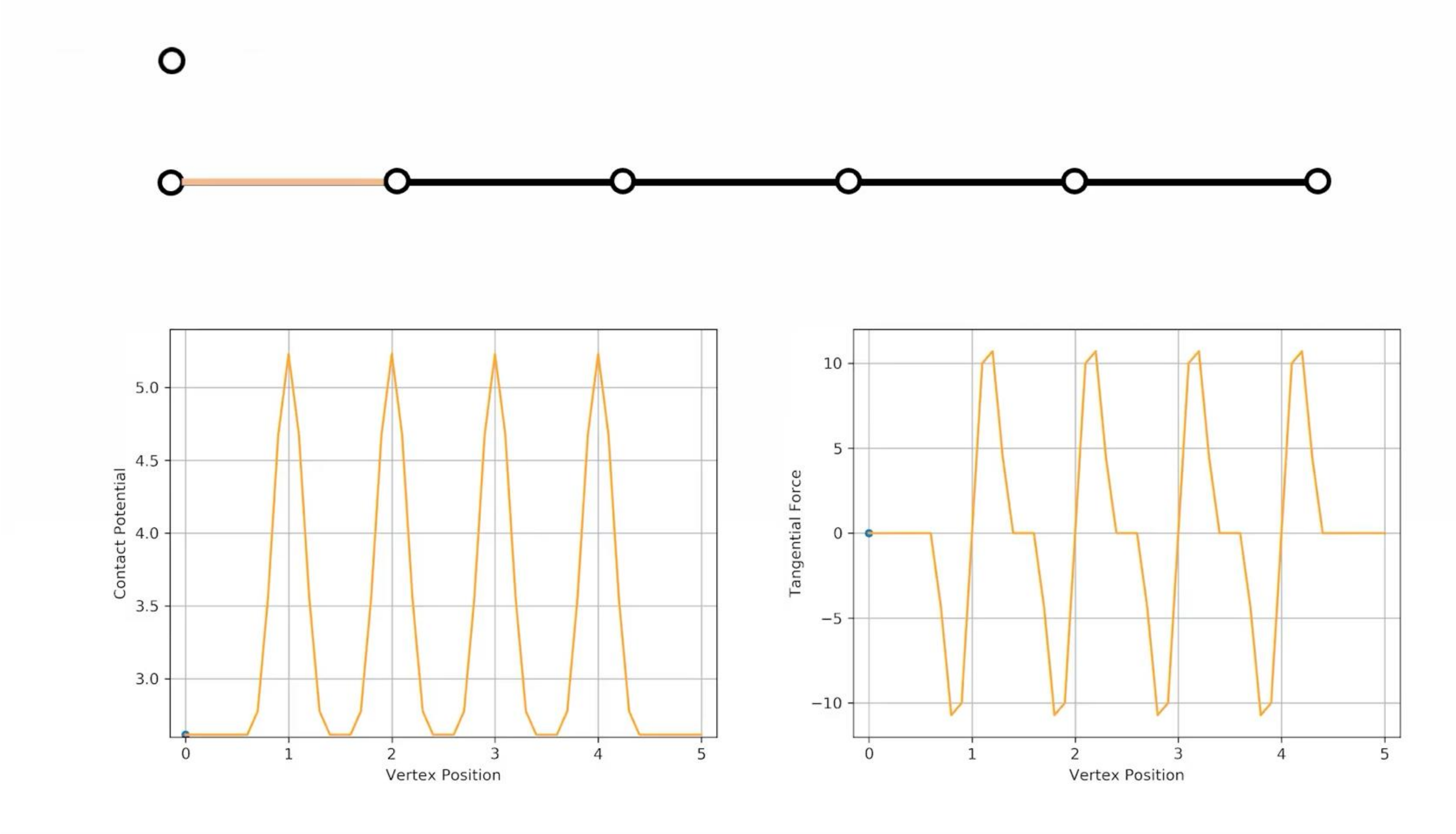
- How to inverse design Discrete Interlocking Materials with desired kinematic deformation limits?





- Designing with explicit triangle meshes is computational expensive.

Challenge

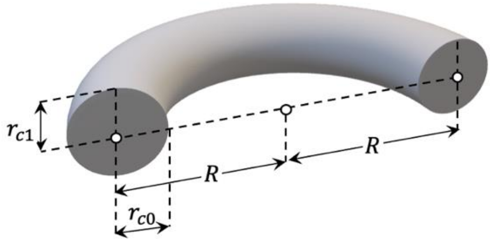


[Du et al. 2024]

Implicit Contact Model

- Represent by parametric torus

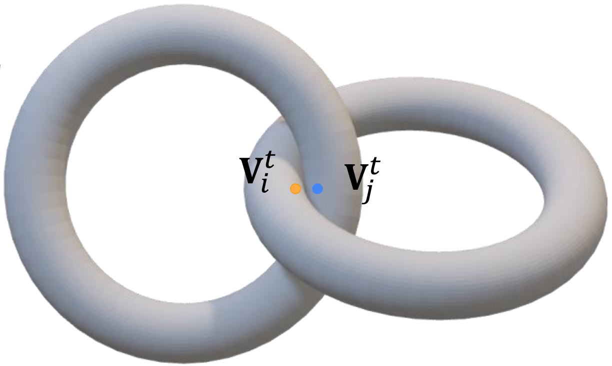
$$V_x(u,v) = (R + r_{c0}\cos(v))\cos(u)$$
$$V_y(u,v) = (R + r_{c0}\cos(v))\sin(u)$$
$$V_z(u,v) = r_{c1}\sin(v)$$



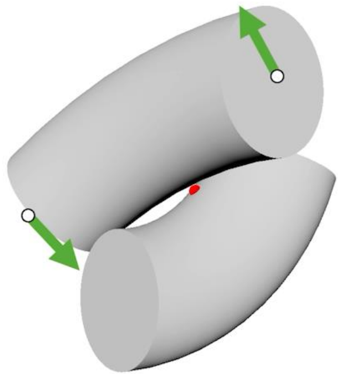
- Contact potential between tori $b(d,\hat{d}) = \begin{cases} -(d-\hat{d})^2 \ln(d/\hat{d}) & 0 < d \\ 0 & d \geq \hat{d} \end{cases}$

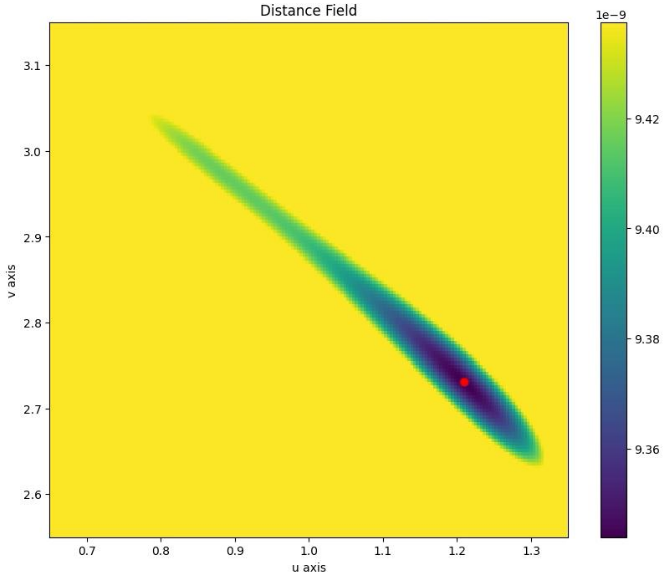
- Minimum squared distance

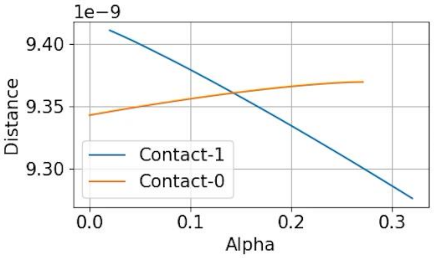
$$\min_{\mathbf{c}_{ij}} d(\mathbf{c}_{ij}, \mathbf{q}_{ij}) = \left\| \mathbf{V}_i^t - \mathbf{V}_j^t \right\|^2$$

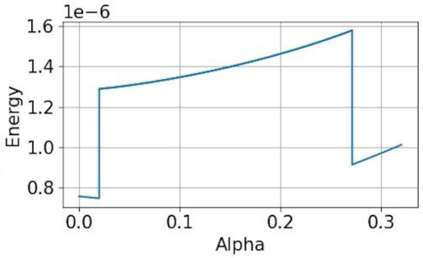


Singularity









Implicit Contact Model

- Revised contact potential $E_{Coll} = \kappa \sum_{k \in C} s(\mathbf{c}, \mathbf{q}) \cdot b(\mathbf{c}, \mathbf{q}, \hat{d})$
- Compute static equilibrium states by solving

$$\min_{\mathbf{q}} E_{\text{Ext}}(\mathbf{q}) + E_{\text{Coll}}(\mathbf{q})$$

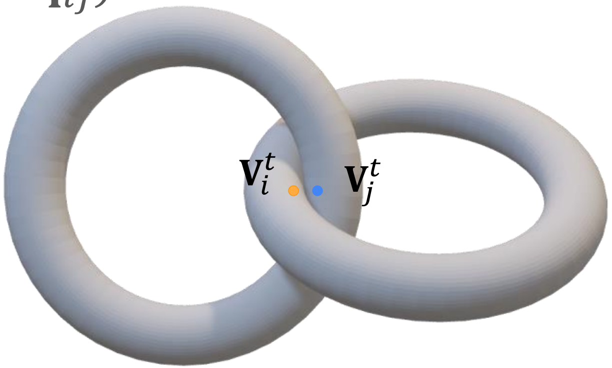
- CCD to find maximum intersection-free step size α_t

$$\min_{\alpha_t} d$$

$$\text{s.t. } d(\alpha_t) = \min_{\mathbf{c}_{ij}} d(\mathbf{c}_{ij}, \mathbf{q}_{ij} + \alpha_t \Delta \mathbf{q}_{ij})$$

$$0 \leq \alpha_t \leq \alpha_{hi}$$

  - If $d < d_{th}$, we shrink α_{hi} by 0.9 until $d > d_{th}$.



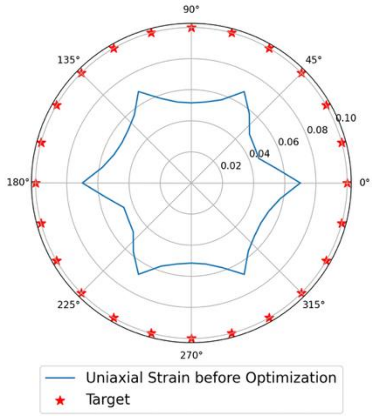
Inverse Design of Deformation Limits

- In-plane objective function

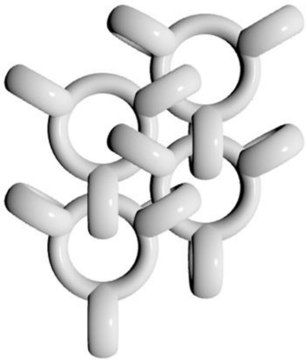
$$\min_{\mathbf{p}} T = \sum_i \frac{1}{2}\left(\boldsymbol{\varepsilon}(\mathbf{p},\theta_i) - \boldsymbol{\varepsilon}_t(\theta_i)\right)^2$$
$$\text{s.t.} \quad \mathbf{f}_{\text{planar}}(\mathbf{y}(\mathbf{p}),\mathbf{p},\theta_i) = 0, \forall i$$
$$\mathbf{C}_{ij}(\mathbf{p}) > \epsilon_c, \forall (i,j) \in \mathbf{N}$$
$$\epsilon_l < \mathbf{p} < \epsilon_h$$

- Out-of-plane objective function

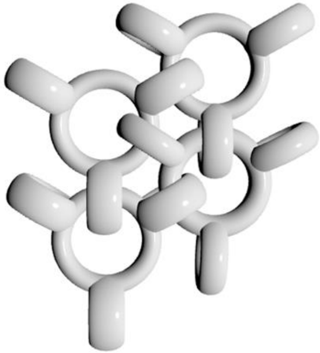
$$\min_{\mathbf{p}} T = \sum_i \frac{1}{2}\left(\boldsymbol{\kappa}(\mathbf{p},\theta_i) - \boldsymbol{\kappa}_t(\theta_i)\right)^2$$
$$\text{s.t.} \quad \mathbf{f}_{\text{bending}}(\mathbf{y}(\mathbf{p}),\mathbf{p},\theta_i) = 0, \forall i$$
$$\mathbf{C}_{ij}(\mathbf{p}) > \epsilon_c, \forall (i,j) \in \mathbf{N}$$
$$\epsilon_l < \mathbf{p} < \epsilon_h$$



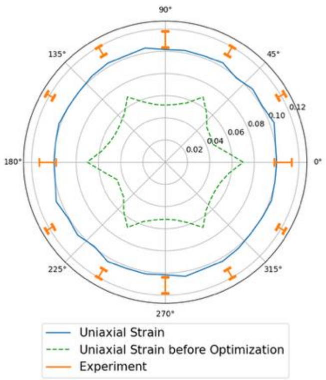
In-plane Deformation Limits



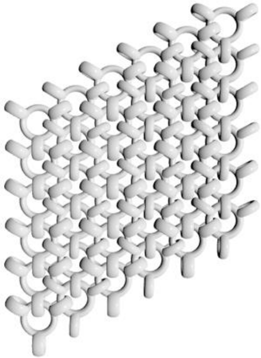
Before optimization

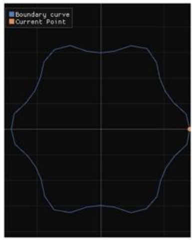


After optimization

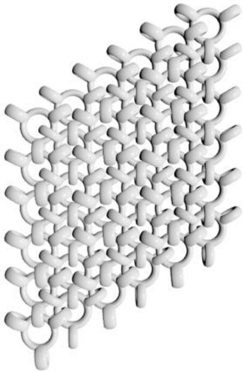


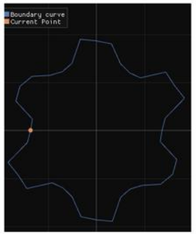
Stretching



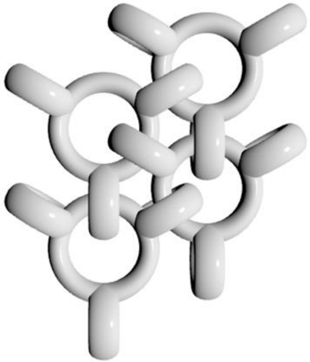


Compression

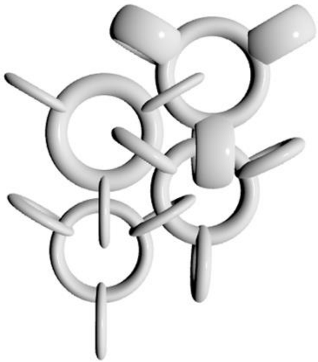




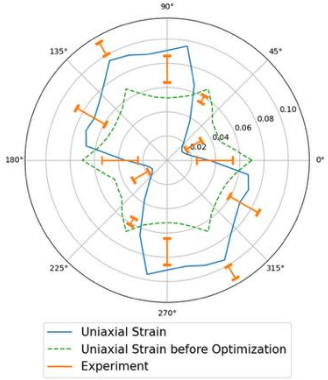
In-plane Deformation Limits



Before optimization



After optimization



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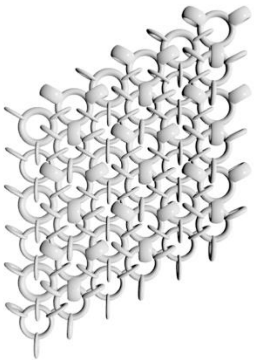

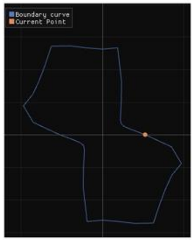

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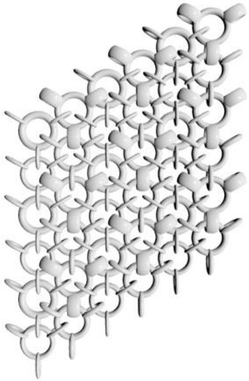
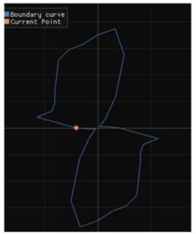
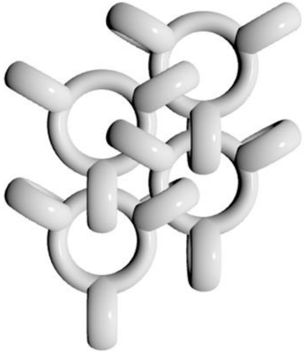


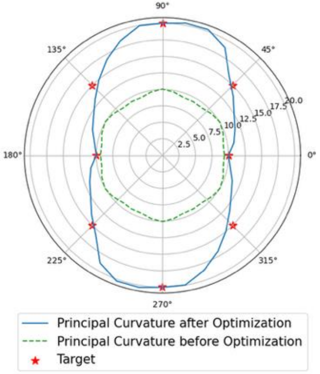


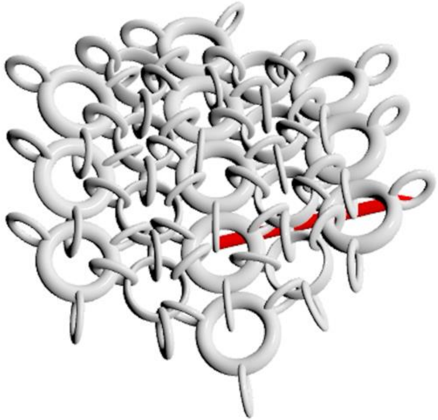
Out-of-plane Deformation Limits

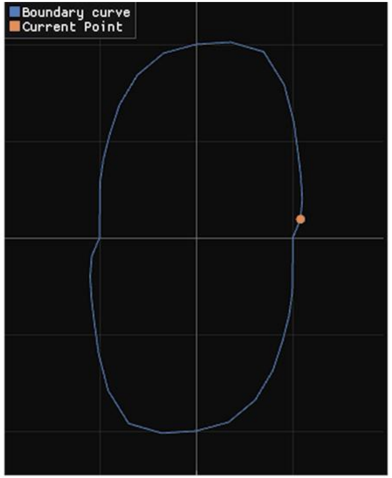


Before optimization

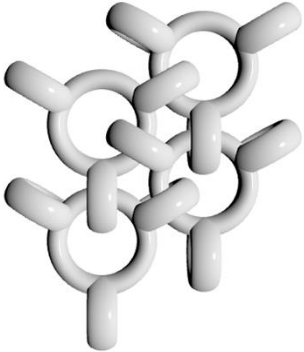
After optimization





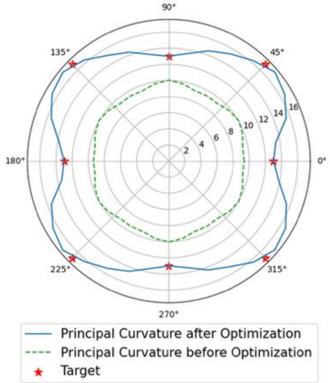


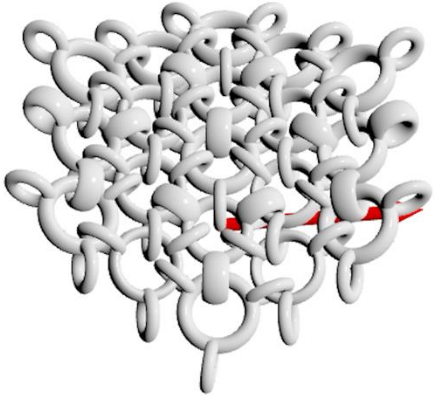
Out-of-plane Deformation Limits

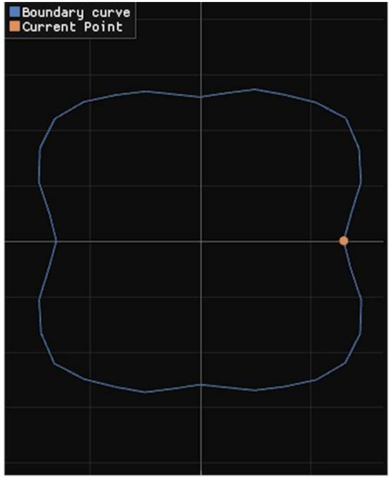


Before optimization

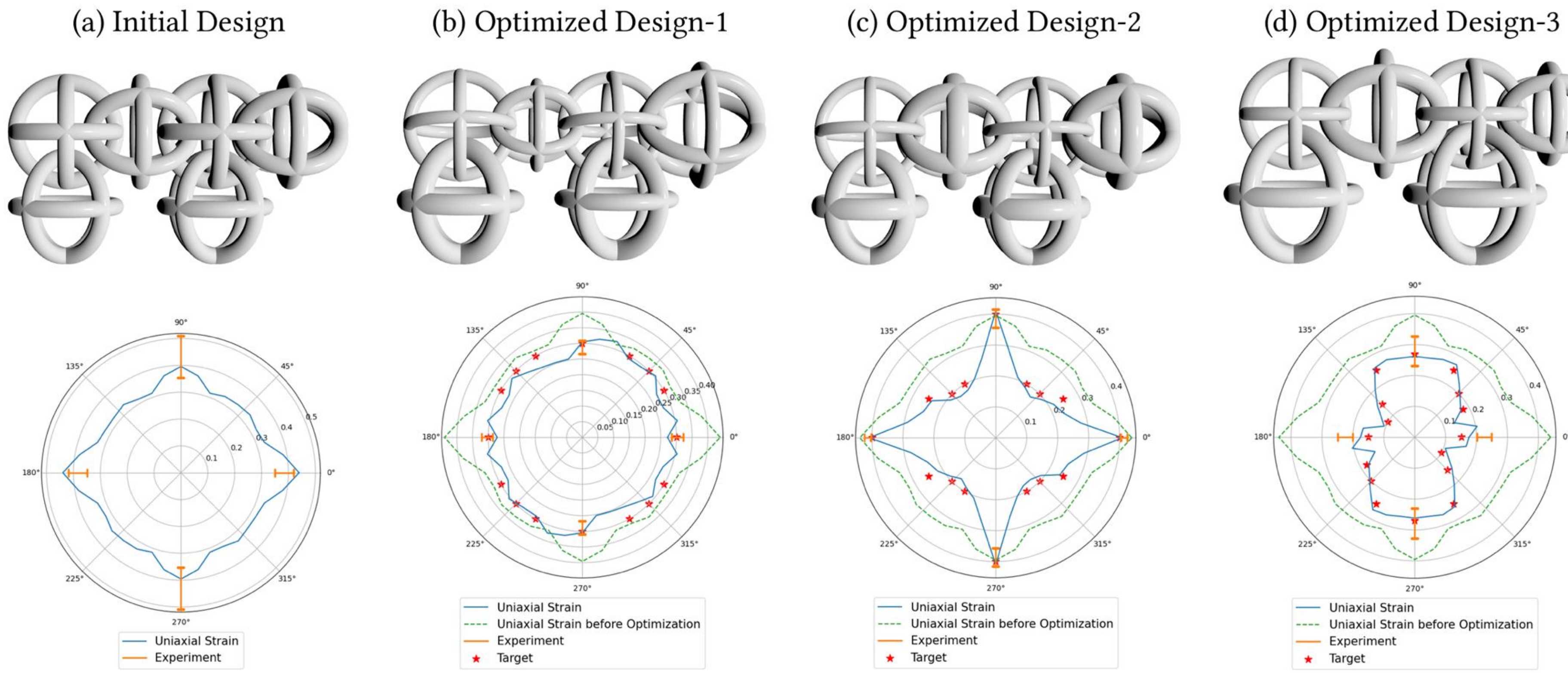
After optimization



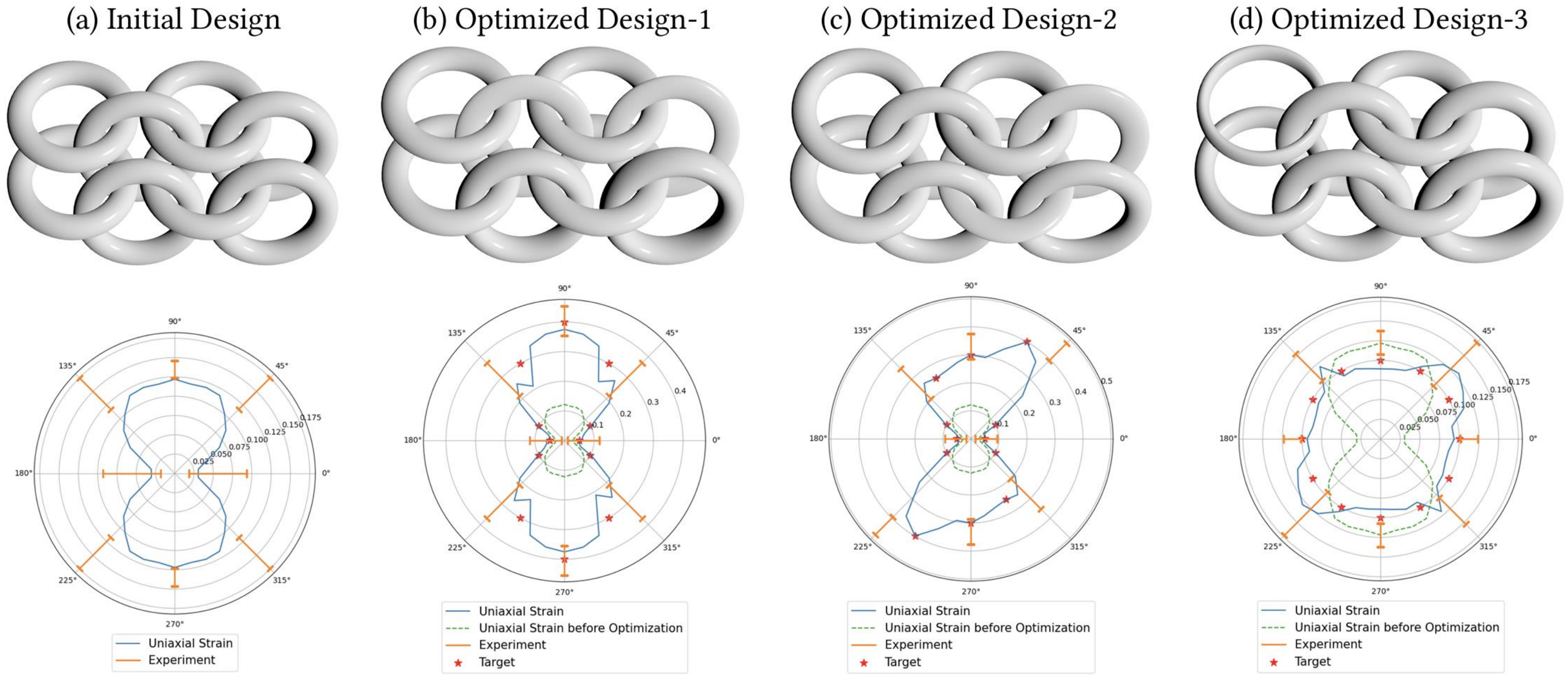


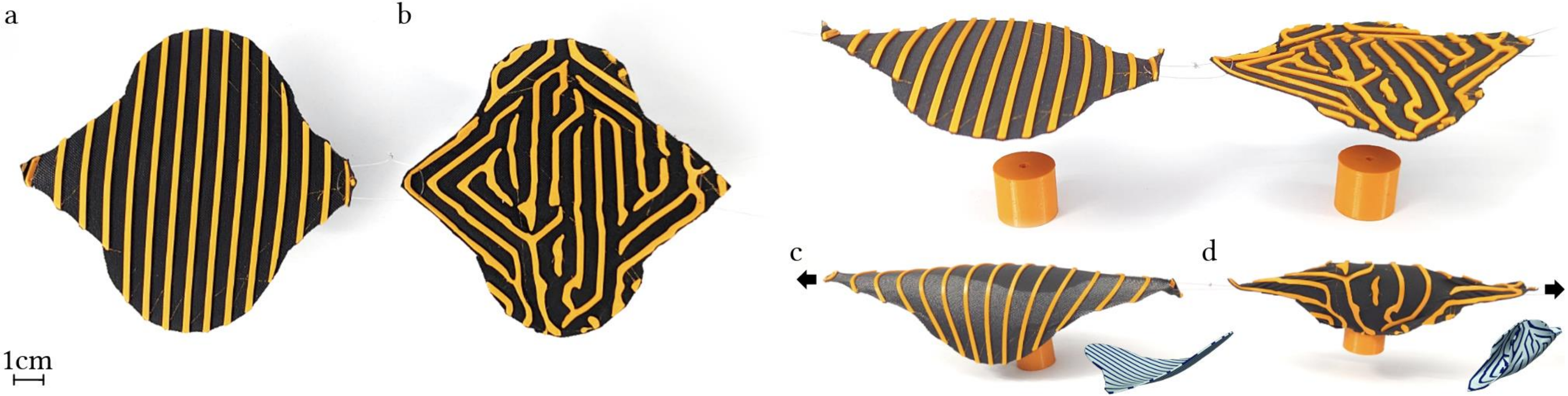


Fourfold Symmetric Material



4-in-1 Chainmail



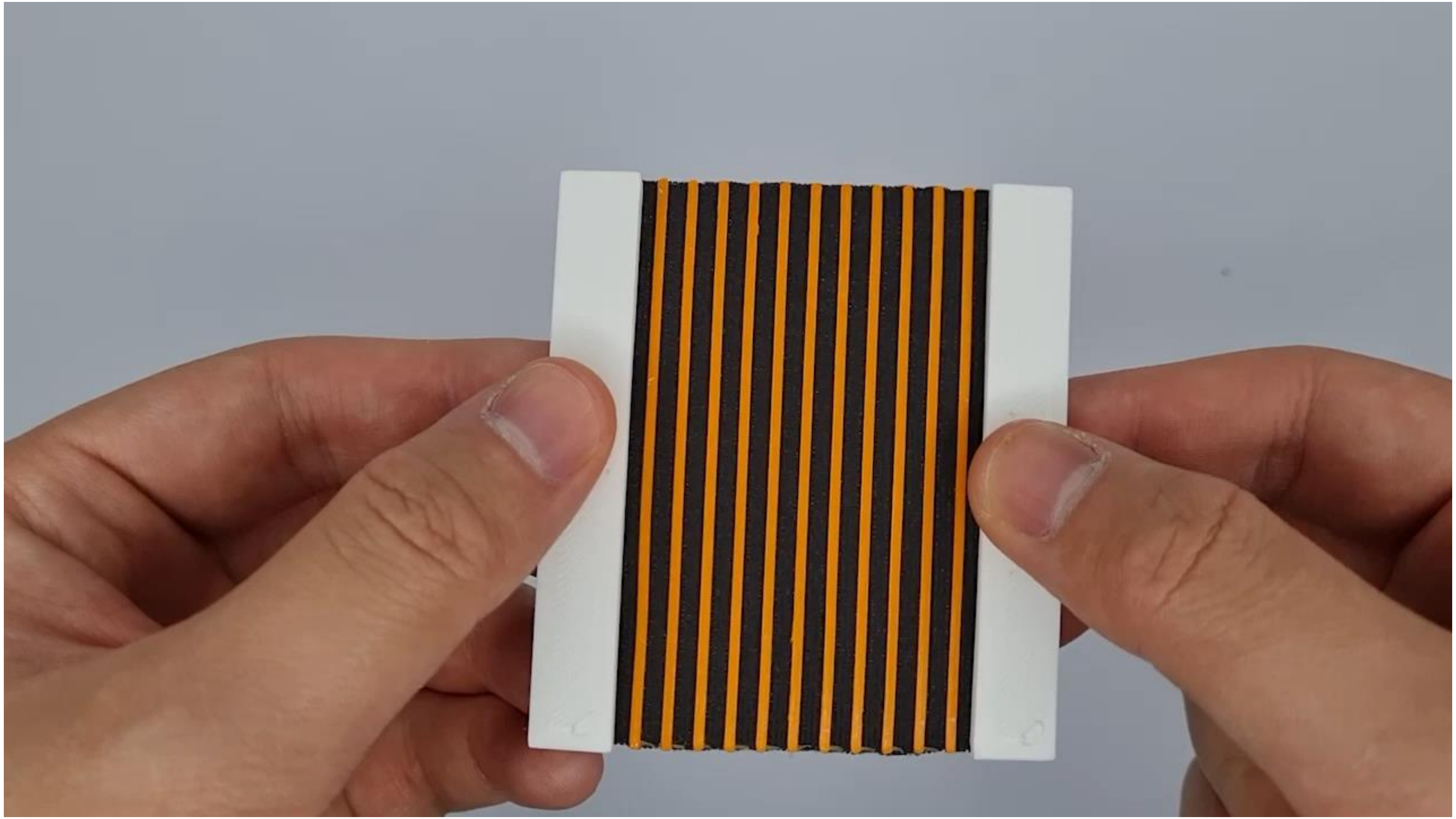


J. Montes, Y. Du, R. Hinchet, S. Coros, B. Thomaszewski. Differentiable Stripe Patterns for Inverse Design of Structured Surfaces. ACM SIGGRAPH 2023

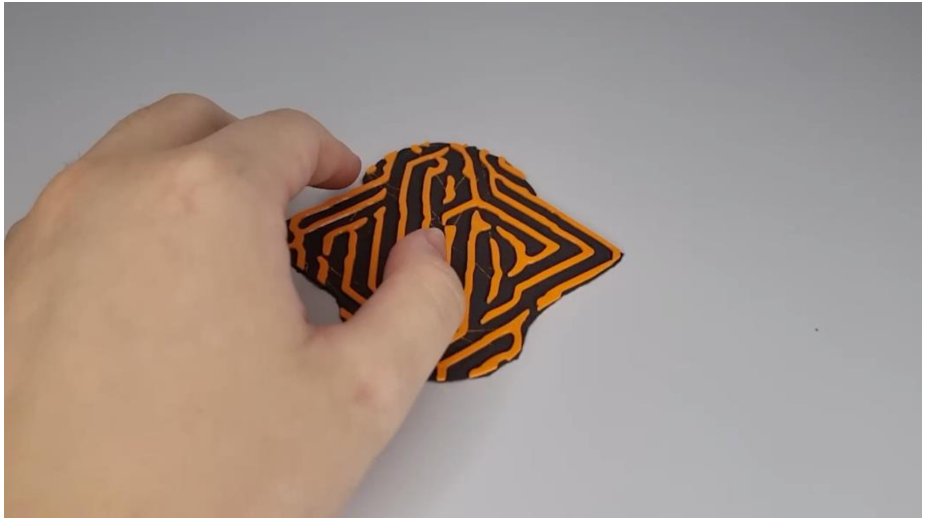
Motivation

[Knöppel et al. 2015]

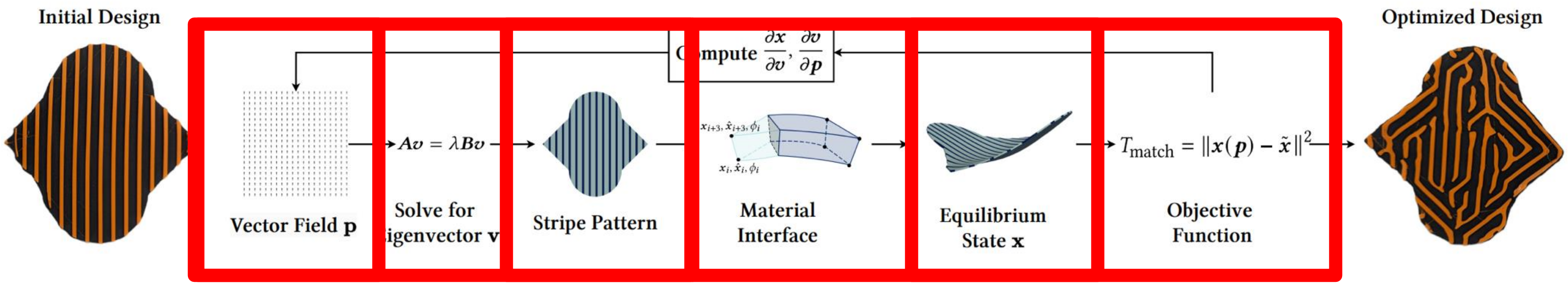
Motivation



Motivation



Goal



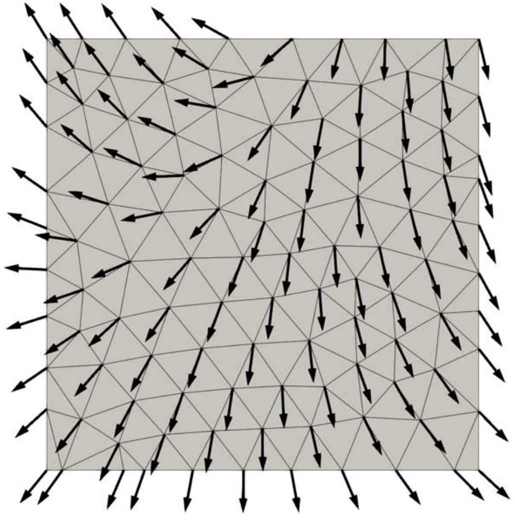
$$\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{p}}$$

Stripes eigenvector sensitivities

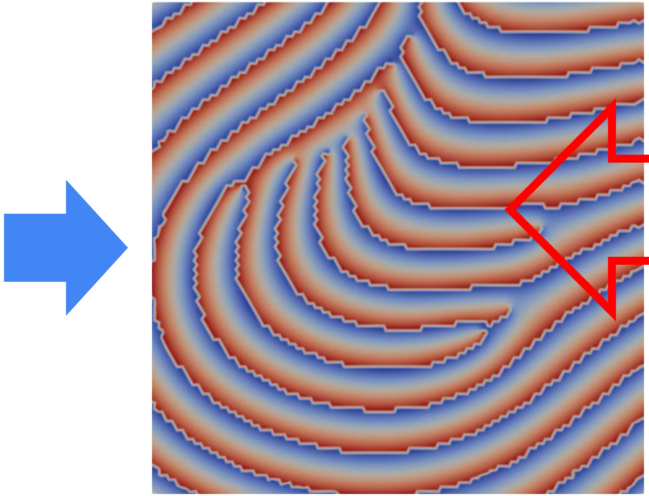
$$\frac{\partial (\boldsymbol{x}, \hat{\boldsymbol{x}}_{\boldsymbol{i}})}{\partial \boldsymbol{v}}$$

Simulation sensitivities

Generation of Stripe Patterns

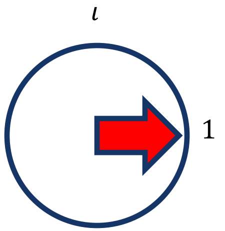


Vector field $\boldsymbol{p}$



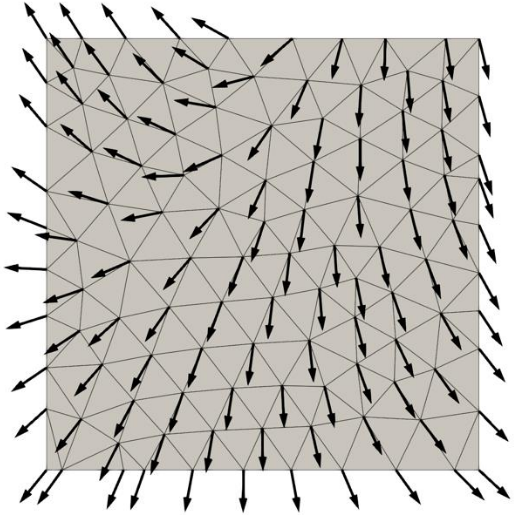
Phases $\boldsymbol{v}$

$$\boldsymbol{v}_i = a_i + \iota b_i \rightarrow (a_i, b_i)$$

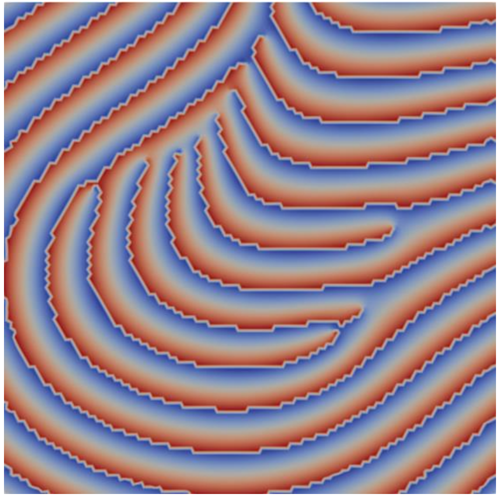


$$\min_{\boldsymbol{v}} E_\psi = \frac{1}{2}\boldsymbol{v}^T\boldsymbol{A}(\boldsymbol{p})\boldsymbol{v} \quad \text{s.t.} \quad \boxed{\boldsymbol{v}^T\boldsymbol{B}\boldsymbol{v} = 1}$$

Generation of Stripe Patterns



Vector field $\boldsymbol{p}$



Phases $\boldsymbol{v}$

Levelset $\boldsymbol{\phi}$

Generalized eigenvalue problem

$$[\boldsymbol{A}(\boldsymbol{p}) - \lambda \boldsymbol{B}]\boldsymbol{v} = 0$$

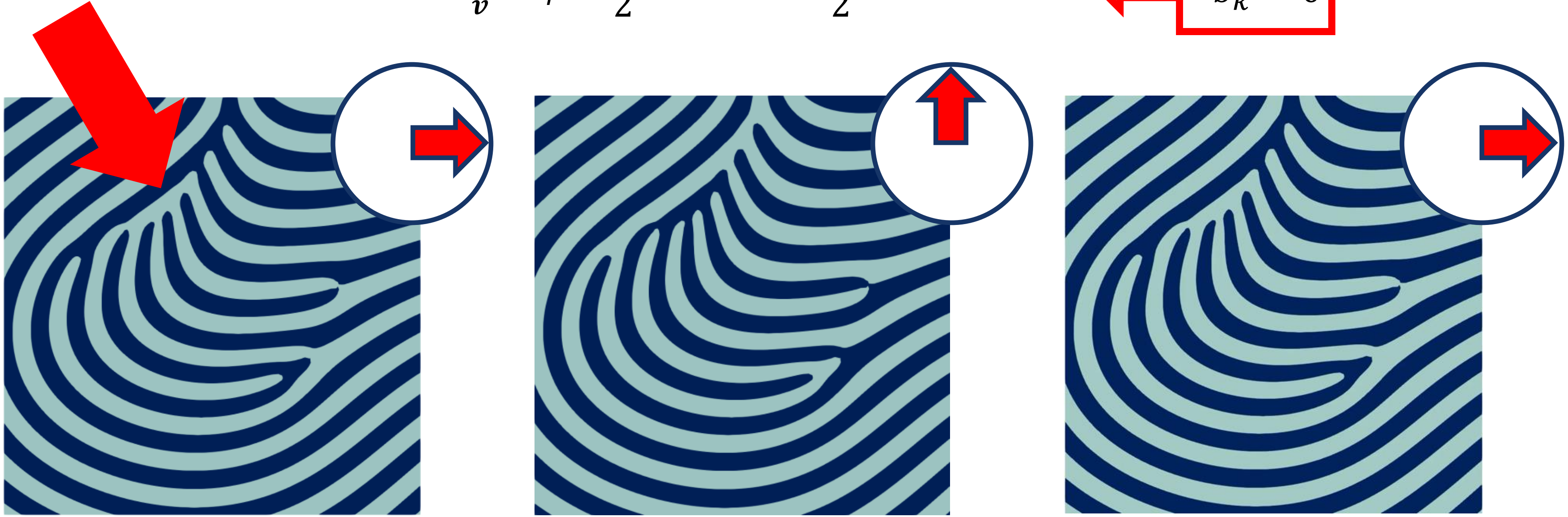
$$\boldsymbol{\phi}(\boldsymbol{v})$$

Multiplicity Two Eigenspace

Constraining the eigenspace

$$\min_{\boldsymbol{v}} E_\psi = \frac{1}{2}\boldsymbol{v}^T\boldsymbol{A}(\boldsymbol{p})\boldsymbol{v} - \frac{1}{2}\lambda\boldsymbol{v}^T\boldsymbol{B}\boldsymbol{v} - \boldsymbol{\mu}\boldsymbol{b}_k \Leftarrow \boxed{b_k = 0}$$

$v_k = (a_k, b_k)$



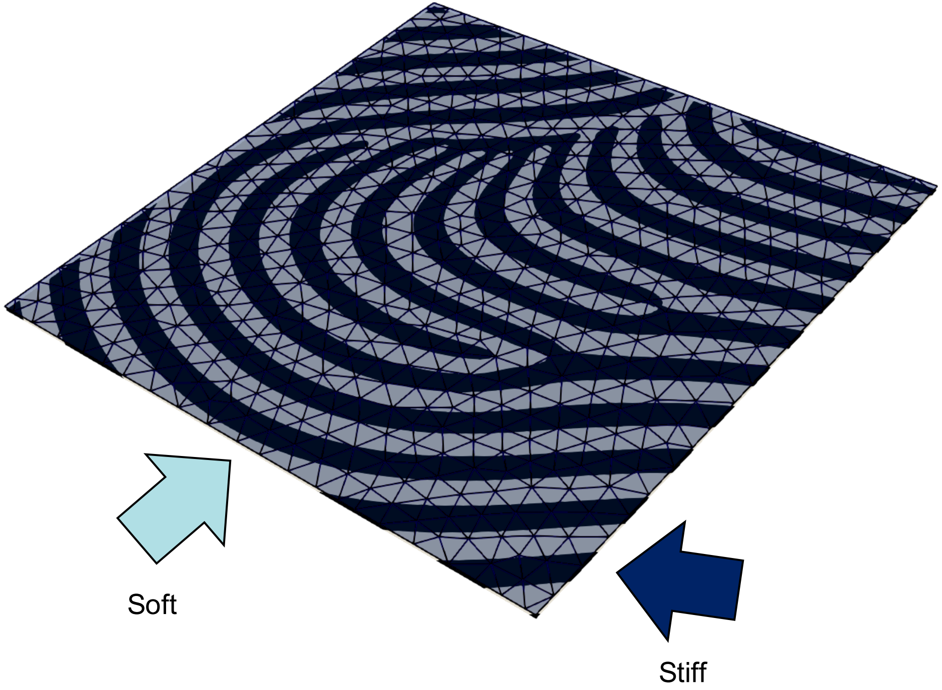
$v_i = (a_i, b_i)$ $\quad v_i^\perp = (-b_i, a_i)$ $\quad v^\theta = \cos(\theta)\, v + \sin(\theta)\, v^\perp$

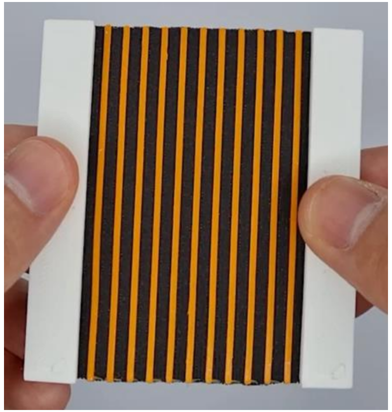
Constraining the eigenspace

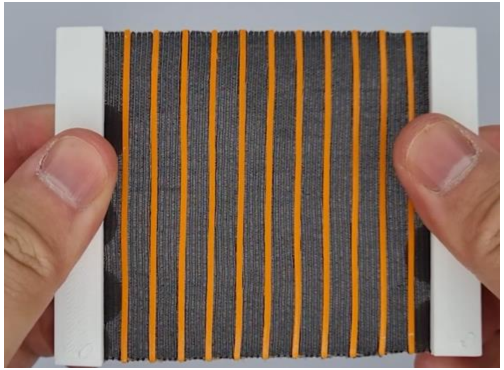
$$\min_{\boldsymbol{v}} E_\psi = \frac{1}{2}\boldsymbol{v}^T\boldsymbol{A}(\boldsymbol{p})\boldsymbol{v} - \frac{1}{2}\lambda\boldsymbol{v}^T\boldsymbol{B}\boldsymbol{v} - \boldsymbol{\mu}\boldsymbol{b}_k$$

$$\begin{pmatrix} \boldsymbol{A}(p) - \lambda\boldsymbol{v} & -\boldsymbol{B}\boldsymbol{v} & \boldsymbol{e}_{b_k} \\ (-\boldsymbol{B}\boldsymbol{v})^T & 0 & 0 \\ \boldsymbol{e}_{b_k}^t & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial v}{\partial p} \\ \frac{\partial v}{\partial \lambda} \\ 0 \end{pmatrix} = \begin{pmatrix} -\frac{\partial^2 E}{\partial \boldsymbol{v} \partial \boldsymbol{p}} \\ 0 \\ 0 \end{pmatrix}$$

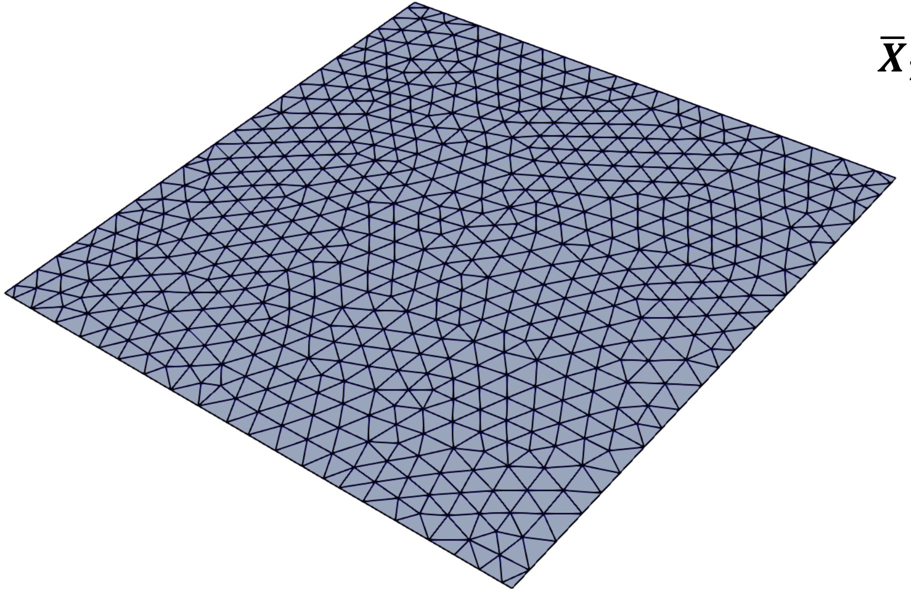
Simulation and X-Fem





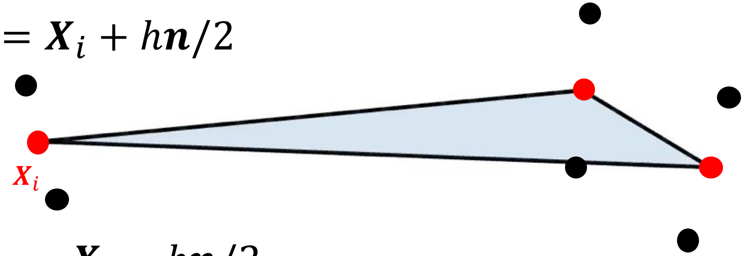


Simulation (Solid SHells)



Midsurface $\boldsymbol{X}_i$

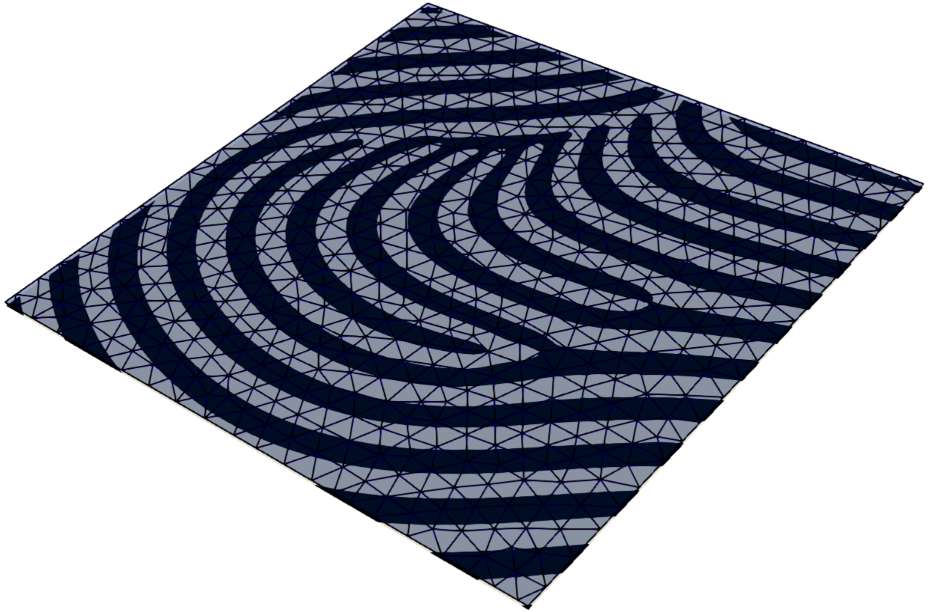
$\bar{\boldsymbol{X}}_{2i+1} = \boldsymbol{X}_i + h\boldsymbol{n}/2$

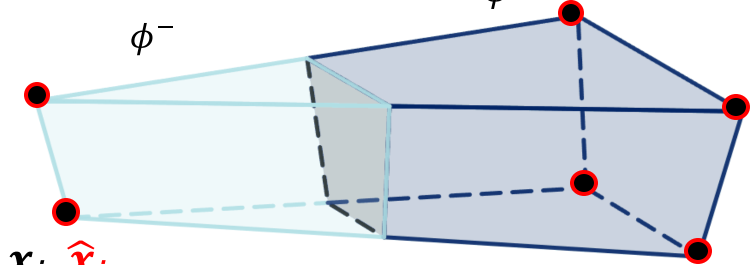


$\bar{\boldsymbol{X}}_{2i} = \boldsymbol{X}_i - h\boldsymbol{n}/2$

$$\boldsymbol{X} = \sum_i N_i \bar{\boldsymbol{X}}_i$$

Solid shells and X-Fem

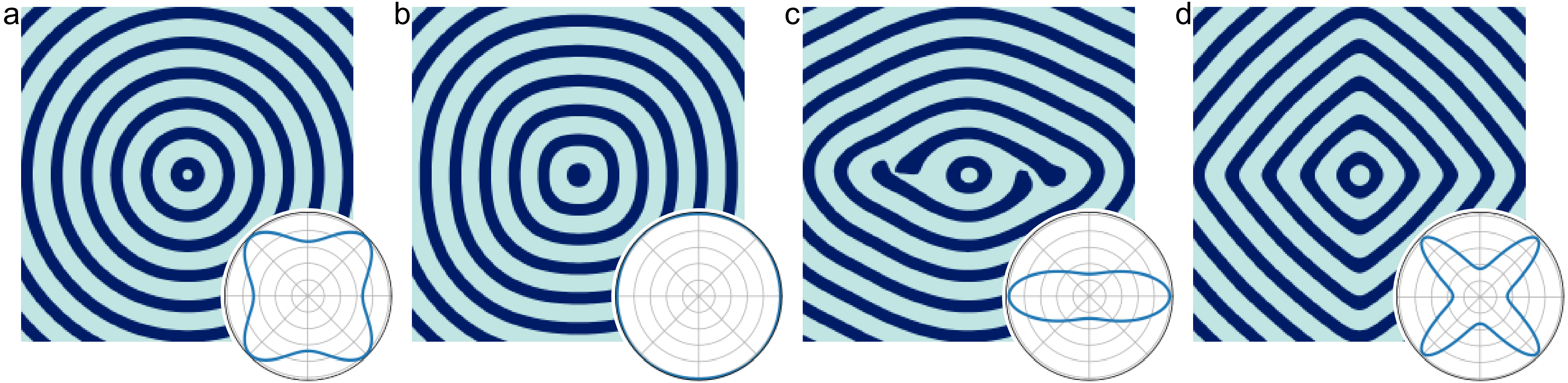




$$\phi = \sum_i N_i \phi_i$$

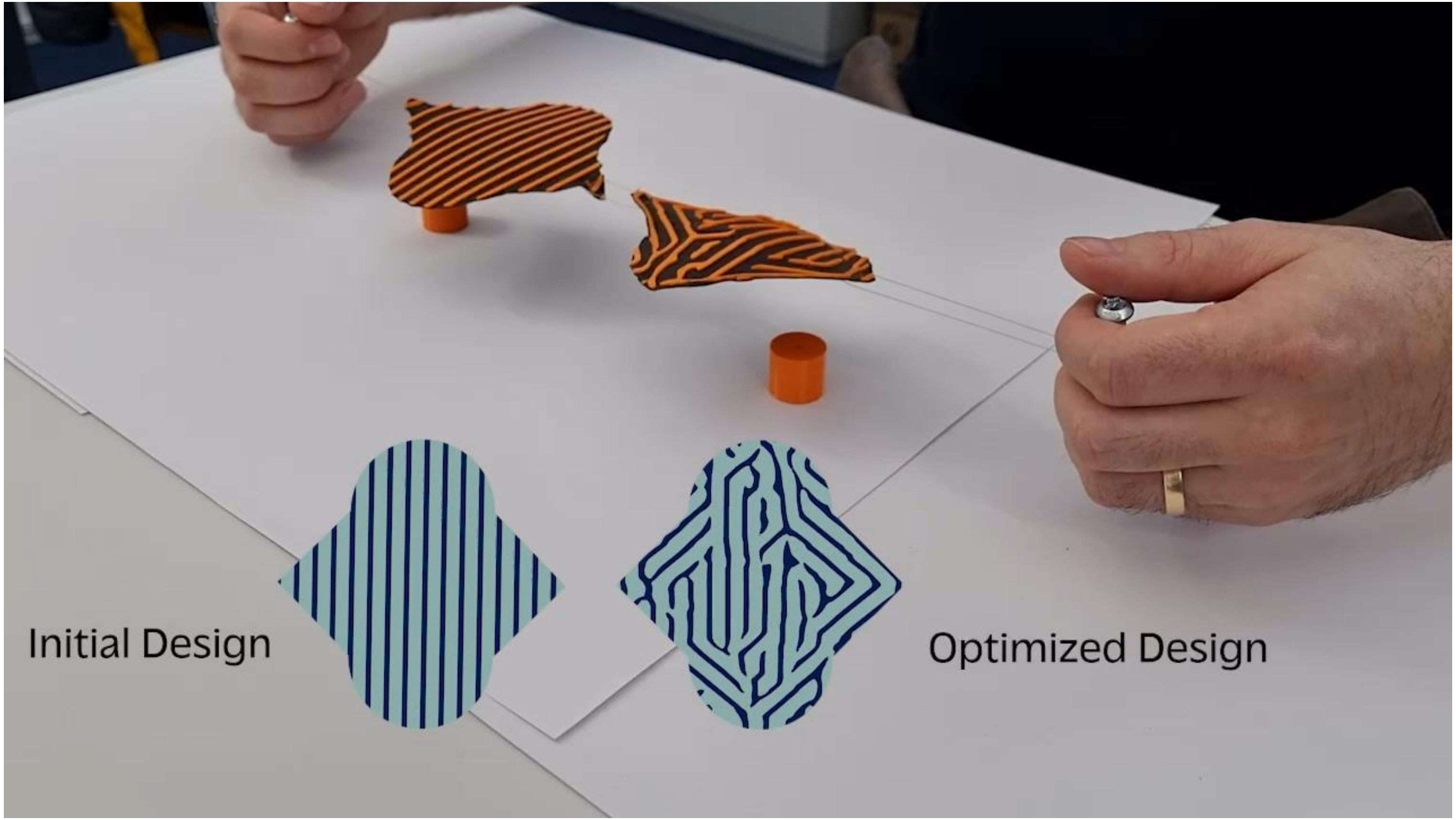
$$\mathbf{x} = \sum_i N_i \boldsymbol{x}_i + \sum_i \psi(\phi) N_i \hat{\boldsymbol{x}}_i$$

Macro-Mechanical Modulation



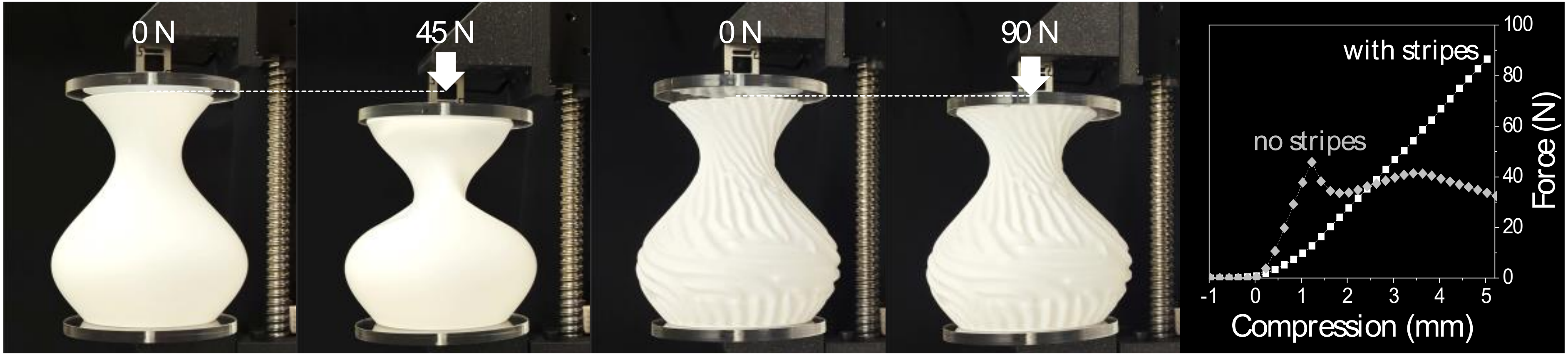
Variable Stiffness Materials

Compliant Gripper



Soft Pneumatic Actuator

Structural Optimization of Thin Shells



Unoptimized

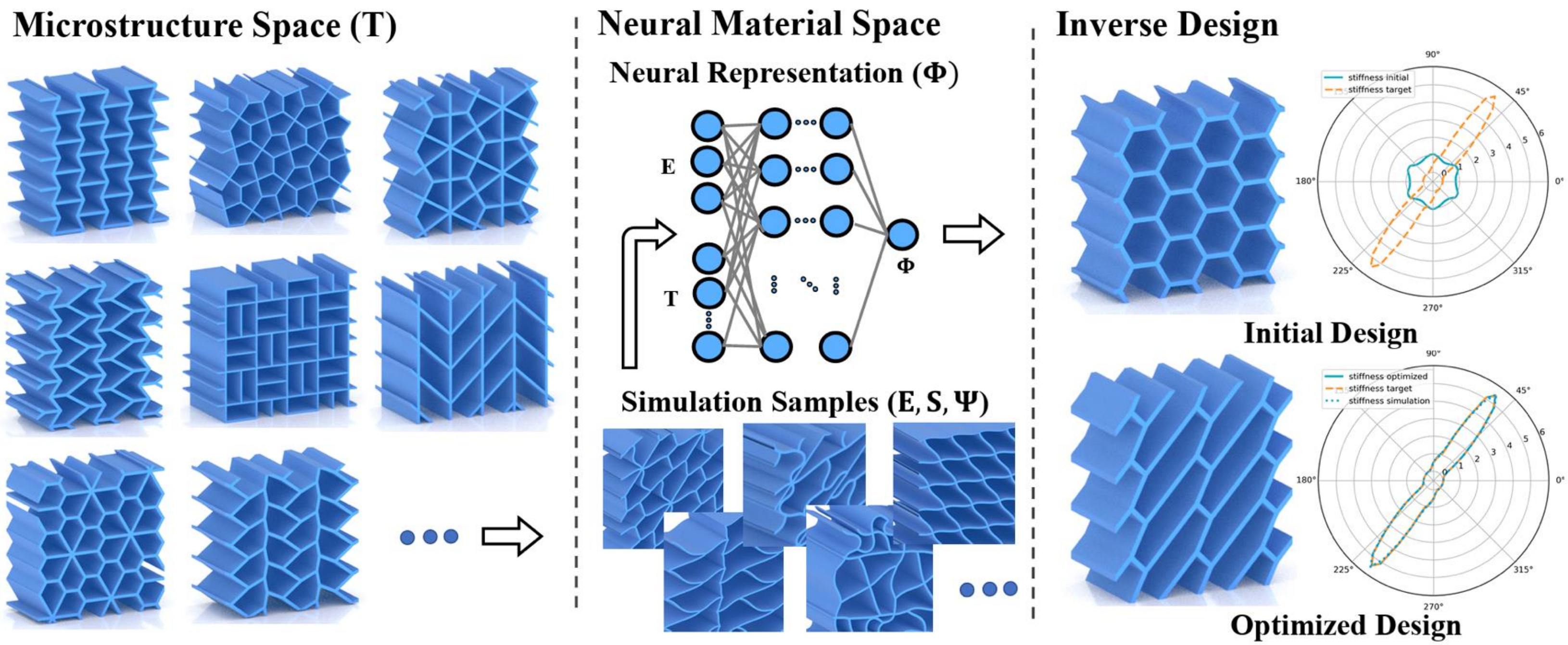
Optimized

Outline Today

- Introduction to Computational Design of Metamaterials
- Computational Models
  - Rigid Body, Finite Element Method, Discrete Elastic Rods
- Numerical Homogenization
- Case Study1: Mechanical Characterization
  - Discrete Interlocking Materials
- Numerical Methods in Inverse Design
- Case Study2: Metamaterials Design with Desired Behaviors
  - Inverse Design of Structured Surfaces and Discrete Interlocking Materials

Outlook

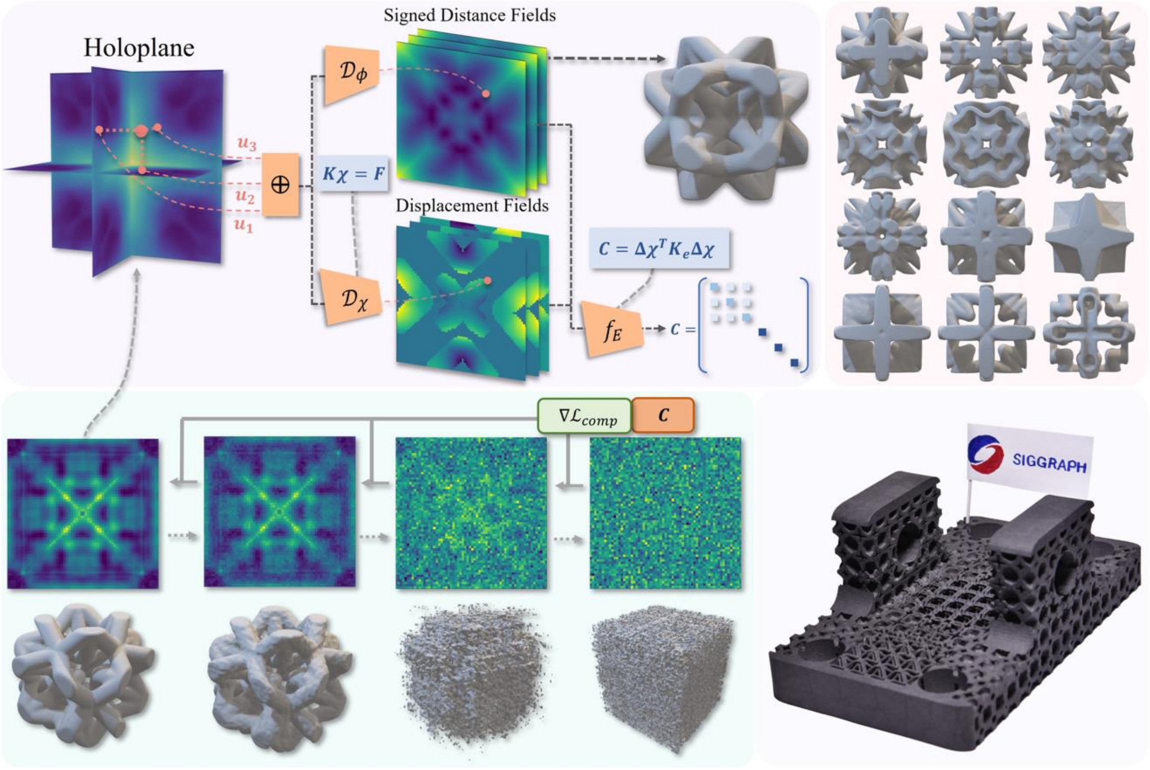
- Neural metamaterial design.



[Li et al. 2023]

Outlook

- Generative AI for metamaterial design.



[Xue et al. 2025]

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Thank you!