# Inverse-designed spinodoid metamaterials

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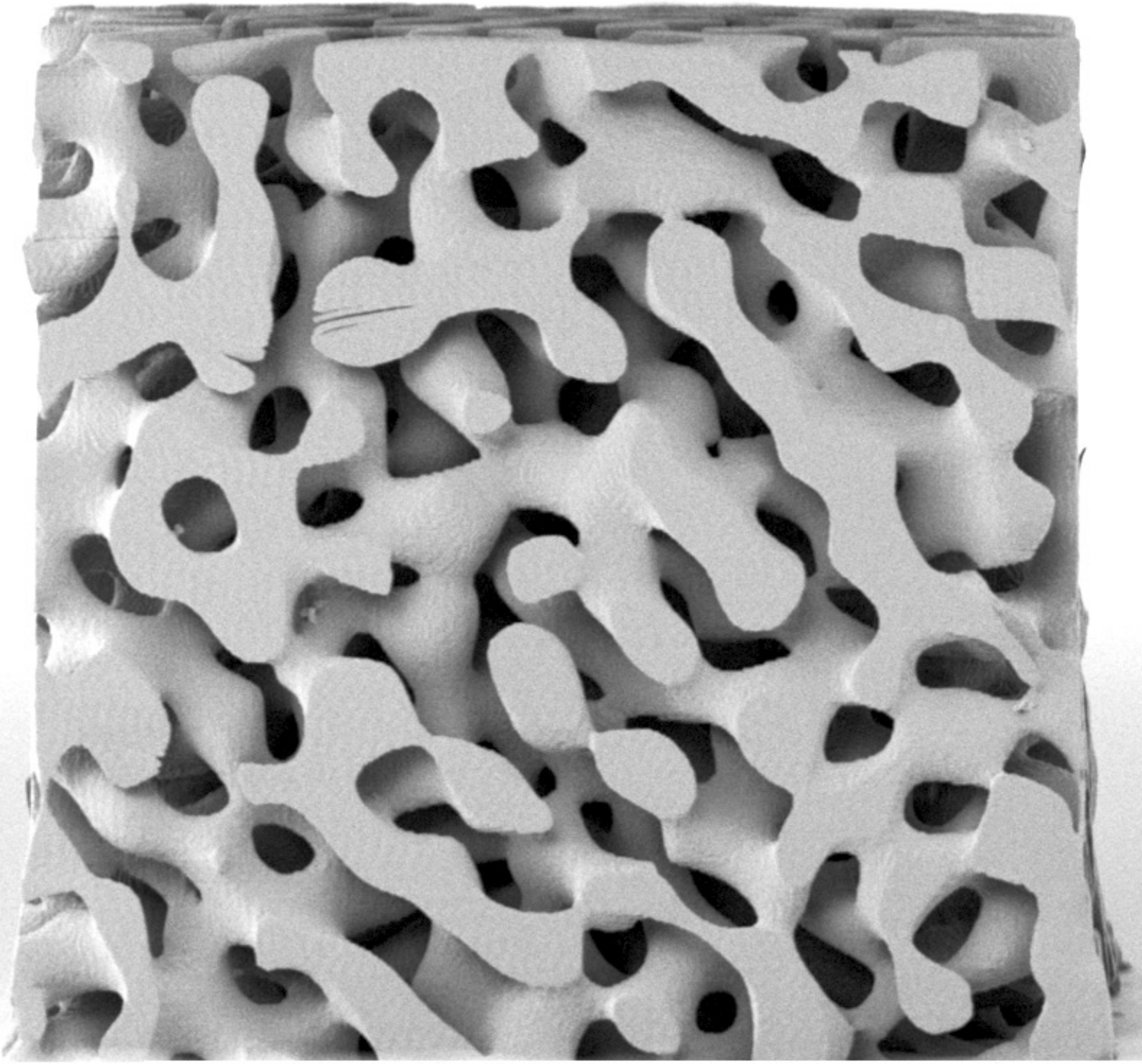
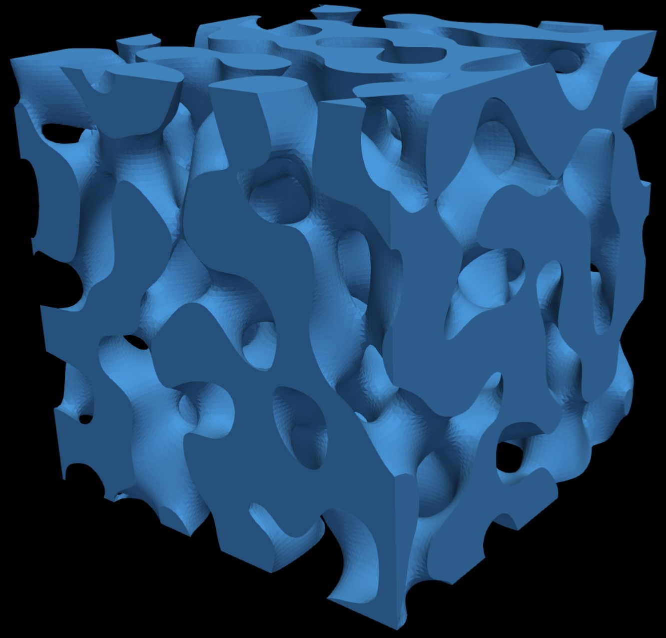
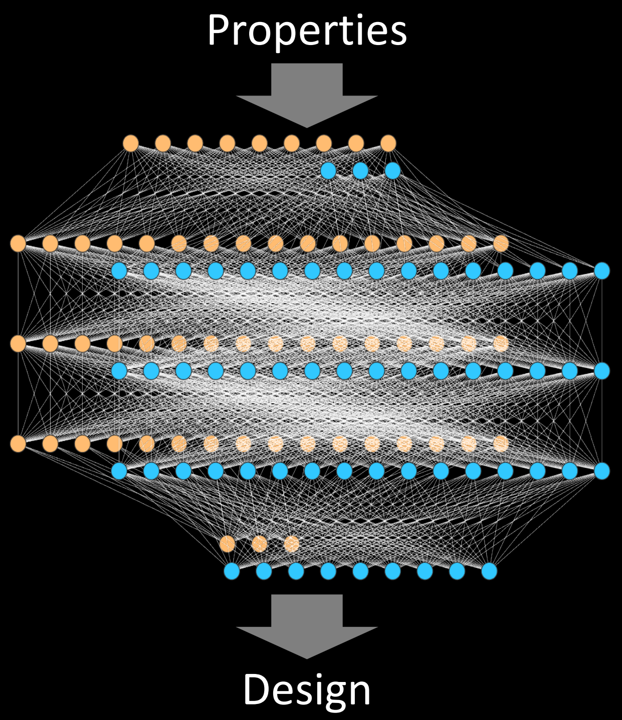


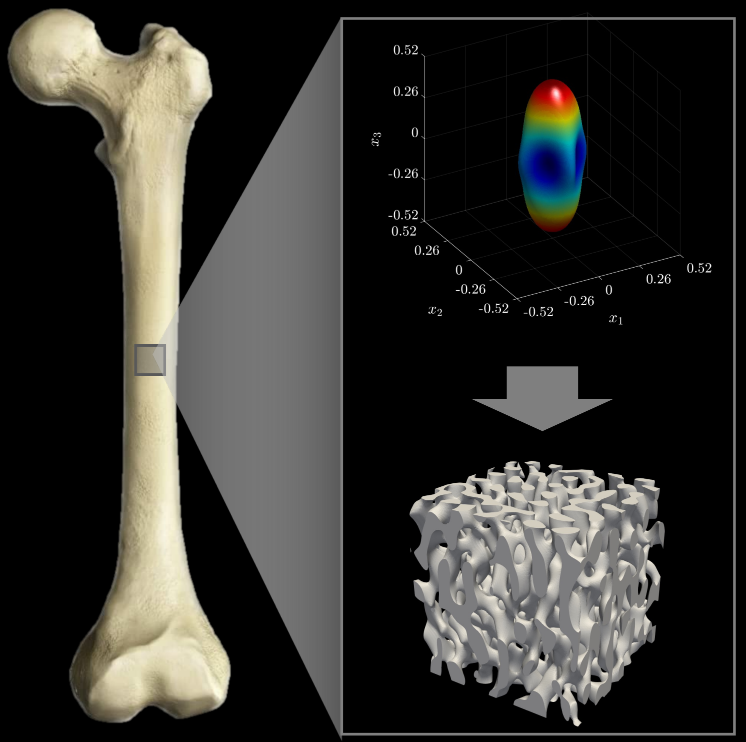
# What we will talk about



A new class of metamaterials for anisotropic tunability: **Spinodoids**

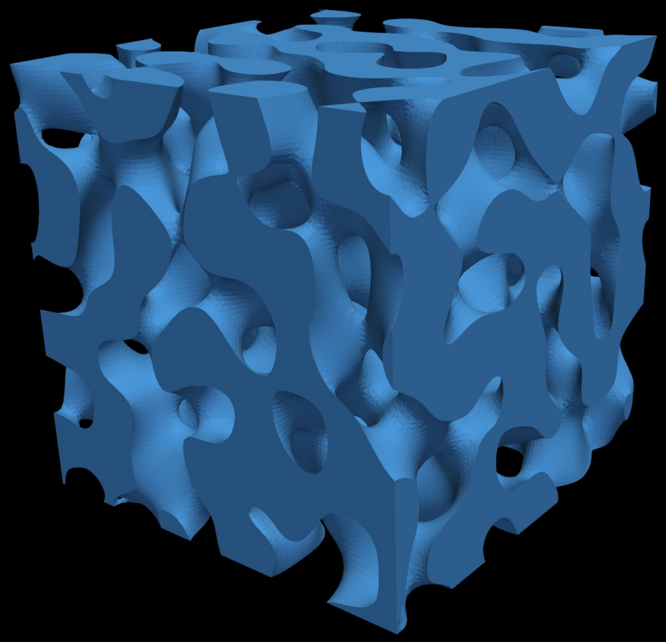



**Inverse design** using machine learning

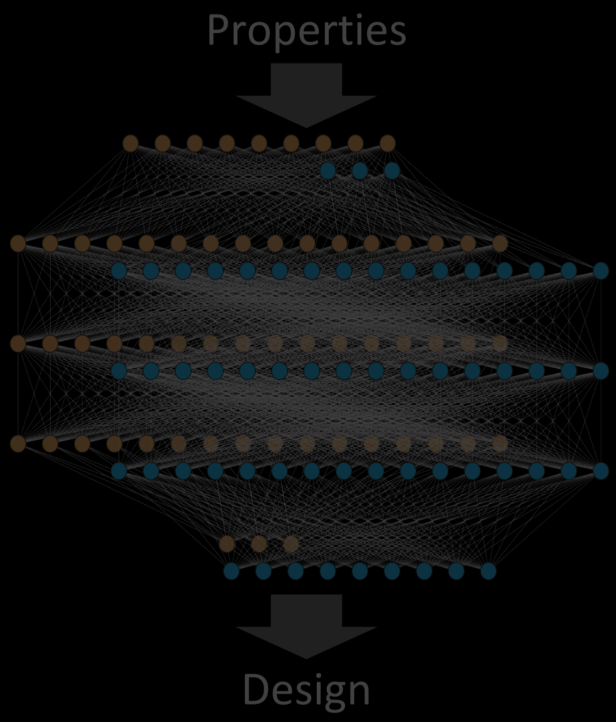


Applications to **synthetic bones** & **lightweight structures**

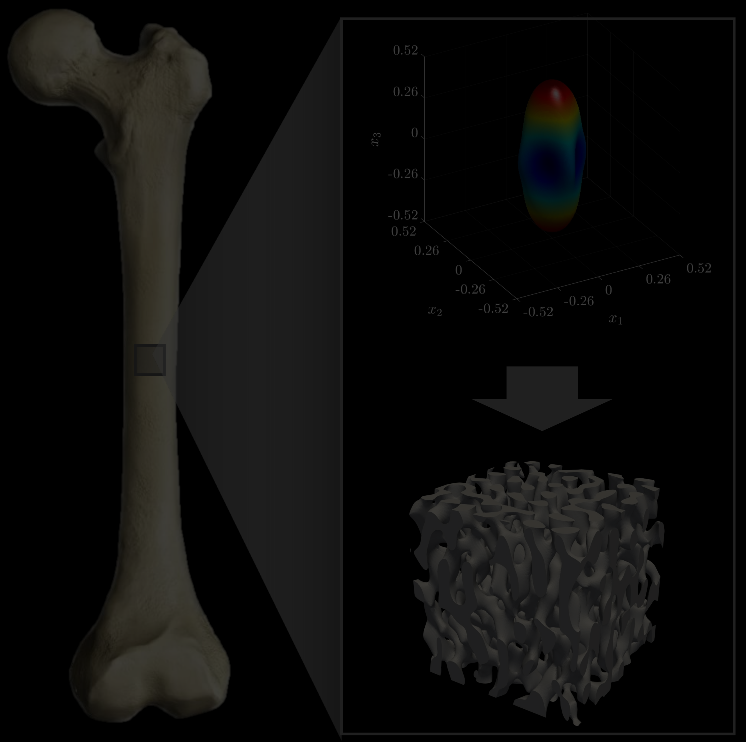
# What we will talk about



A new class of metamaterials for anisotropic tunability: **Spinodoids**

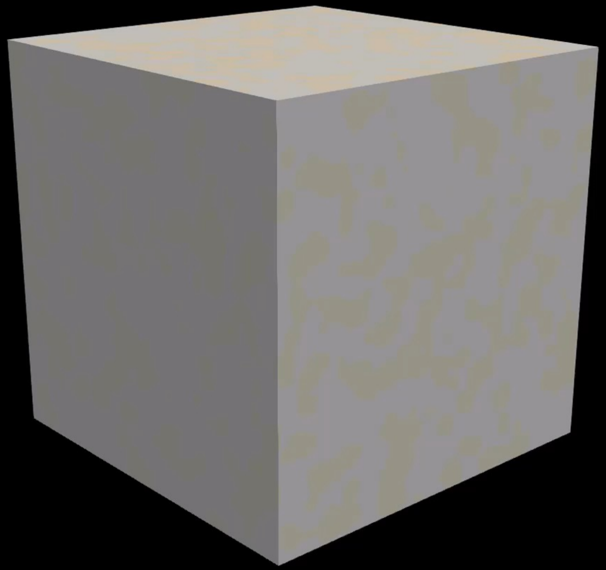



**Inverse design** using machine learning

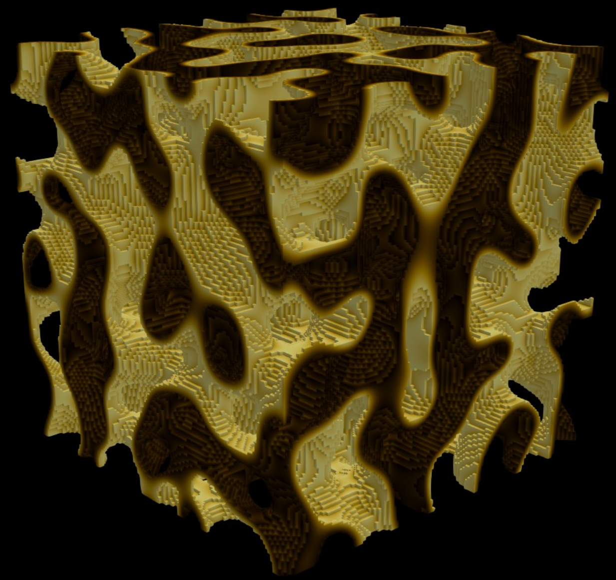


Applications to **synthetic bones** & **lightweight structures**

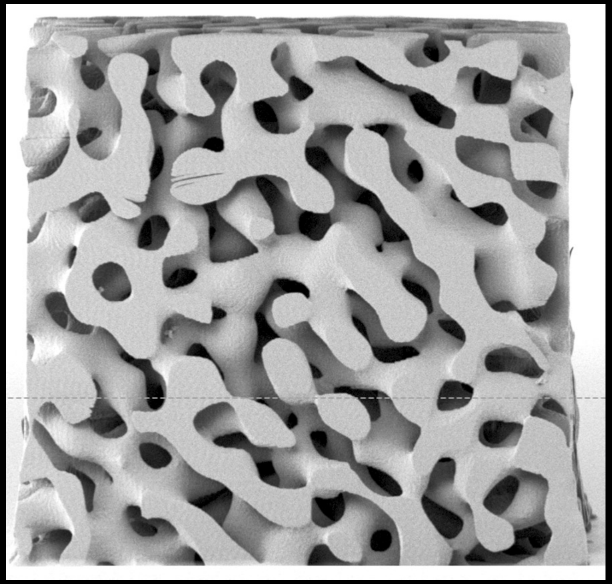
# Spinodal metamaterials



Spinodal simulation
*(Vidyasagar et al., PRSA 2018)*

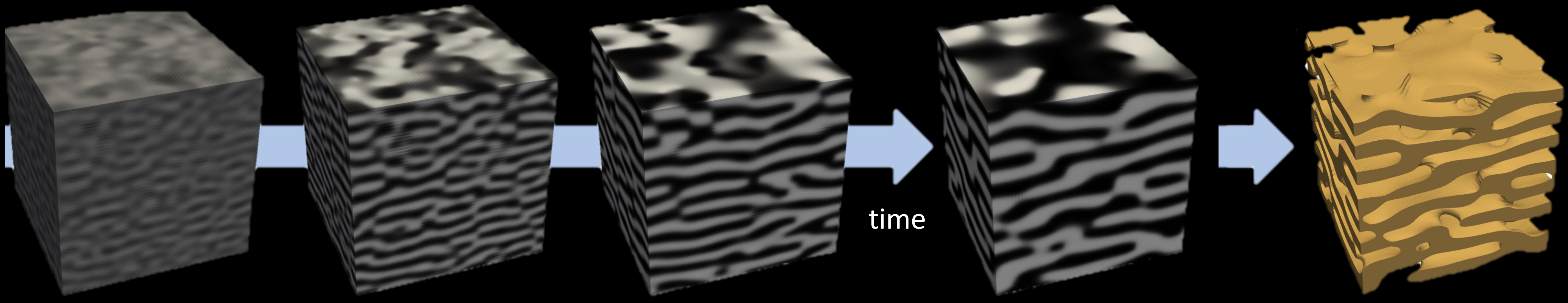


Extract topology



Additive manufacturing

# Diffusion-driven phase separation: a shortcut




$$\varphi(\boldsymbol{x}) = \sqrt{\frac{2}{N}} \sum_{i=1}^{N \gg 1} \cos\left(\beta\, \boldsymbol{n}_i \cdot \boldsymbol{x} - \gamma_i\right)$$

random phases: $\gamma_i \sim \mathcal{U}([0, 2\pi))$

random wave vectors: $\boldsymbol{n}_i \sim \mathcal{U}(S^2)$

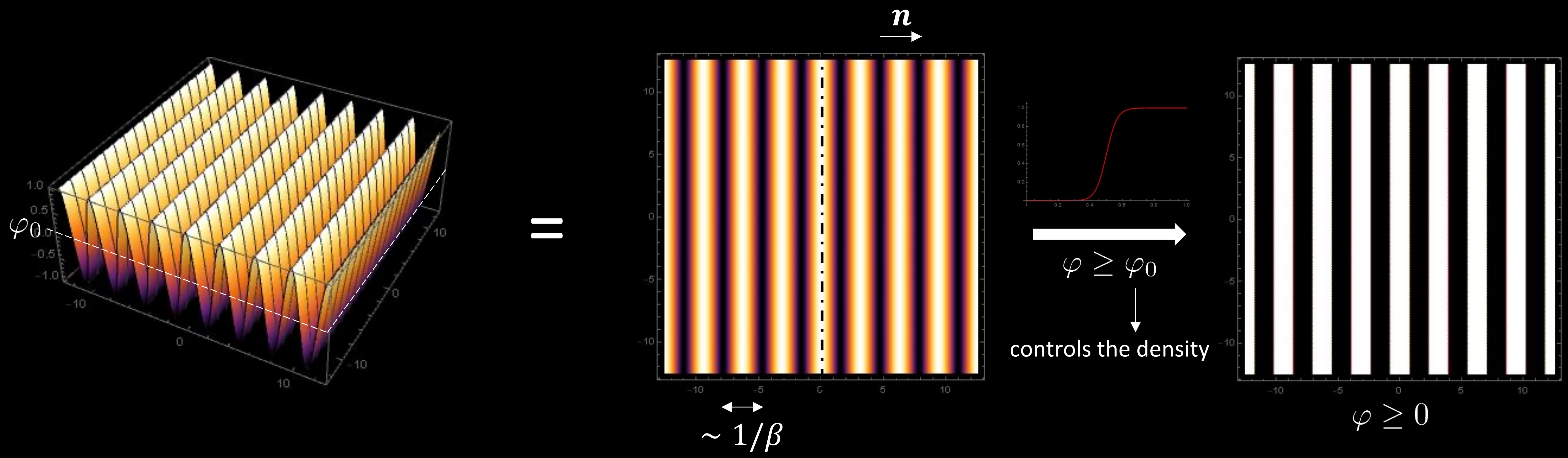
Physics modeling (based on Cahn-Hilliard partial differential equation)

Threshold

**Gaussian Random Field**

*(Cahn, J. Chem. Phys. 1965; Soyarslan et al., Acta Mater 2018)*

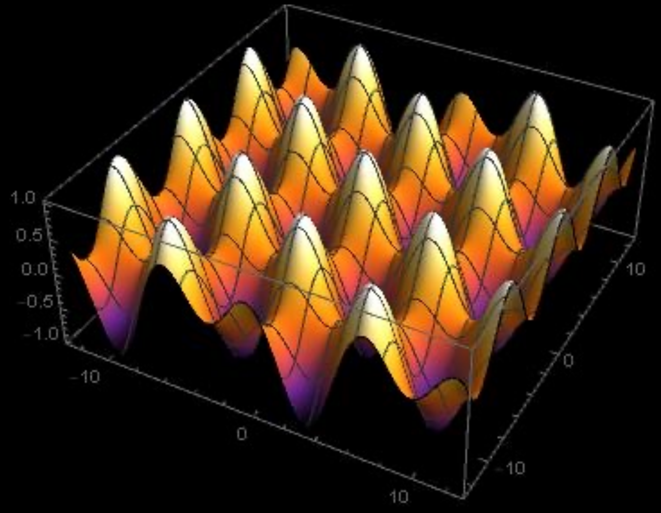
# Gaussian random fields (GRFs)




a simple example:

$$\varphi(\boldsymbol{x}) = \cos\left(\beta\, \boldsymbol{n} \cdot \boldsymbol{x} - \gamma\right)$$

# Gaussian random fields (GRFs)

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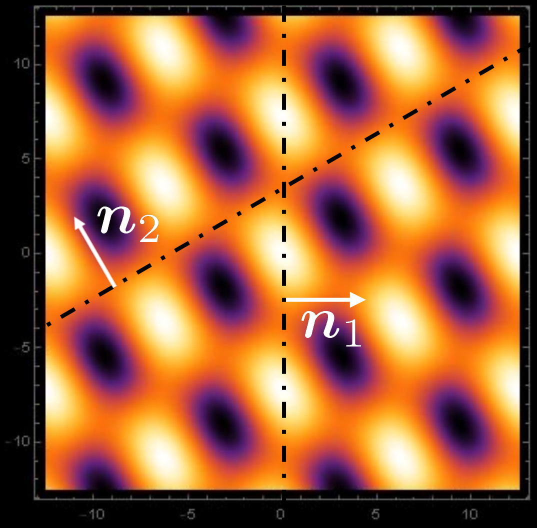
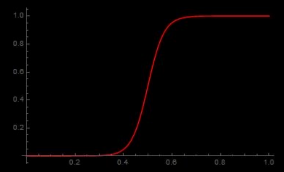
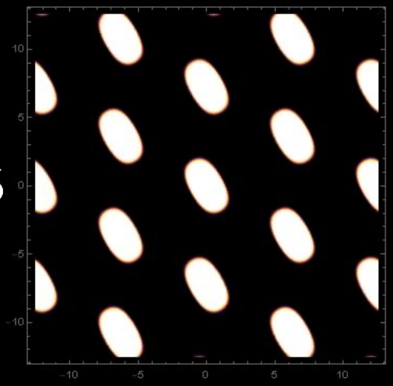


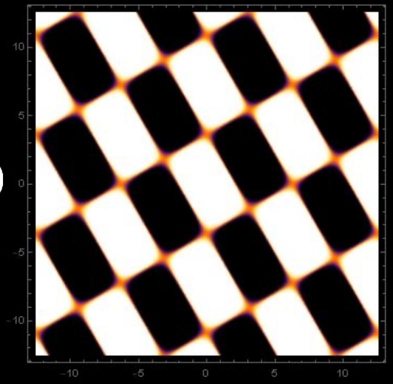
$\varphi \geq \varphi_0$

controls the density

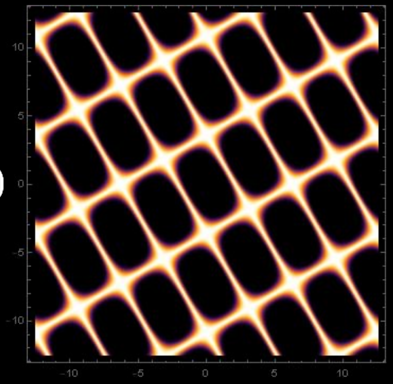
$\varphi \geq 0.5$



$\varphi \geq 0$



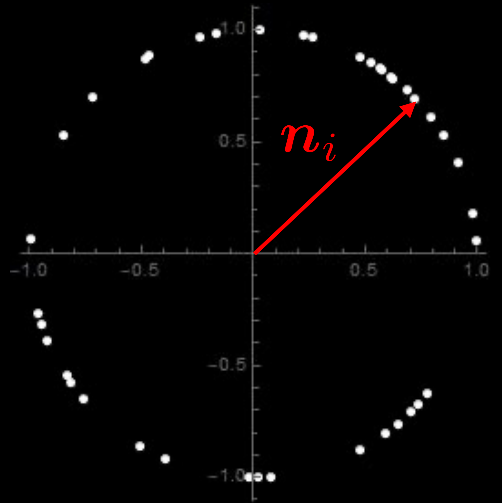
$\varphi \approx 0$



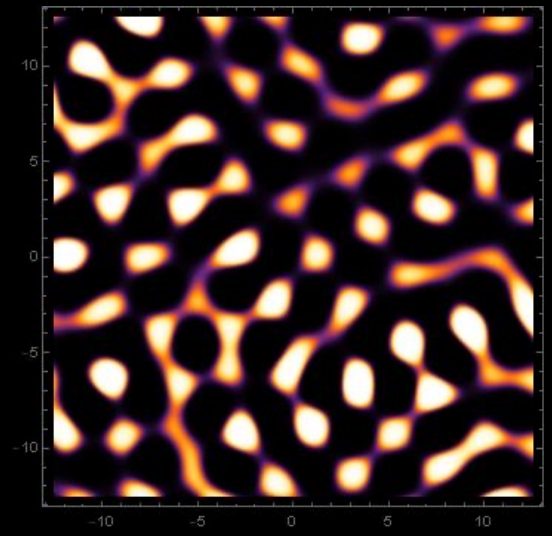
a simple example:

$$\varphi(\boldsymbol{x}) = \frac{1}{2}\left[\cos\left(\beta\, \boldsymbol{n}_1 \cdot \boldsymbol{x} - \gamma_1\right) + \cos\left(\beta\, \boldsymbol{n}_2 \cdot \boldsymbol{x} - \gamma_2\right)\right]$$

# Isotropic Gaussian random field




$N = 40$



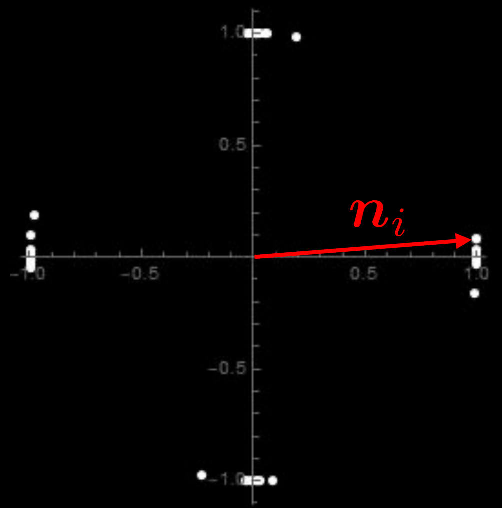

$$\varphi(\boldsymbol{x}) = \sqrt{\frac{2}{N}} \sum_{i=1}^{N=40} \cos\left(\beta\, \boldsymbol{n}_i \cdot \boldsymbol{x} - \gamma_i\right)$$

random phases: $\gamma_i \sim \mathcal{U}([0, 2\pi))$

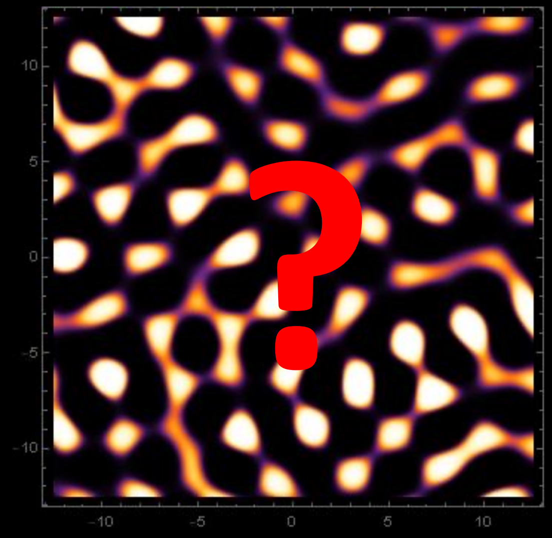
random wave vectors: $\boldsymbol{n}_i \sim \mathcal{U}(S^1)$

**Smooth bi-continuous structures which are also solutions to spinodal decomposition PDE**

# Anisotropic Gaussian random field




$N = 40$




$$\varphi(\boldsymbol{x}) = \sqrt{\frac{2}{N}} \sum_{i=1}^{N=40} \cos\left(\beta\, \boldsymbol{n}_i \cdot \boldsymbol{x} - \gamma_i\right)$$

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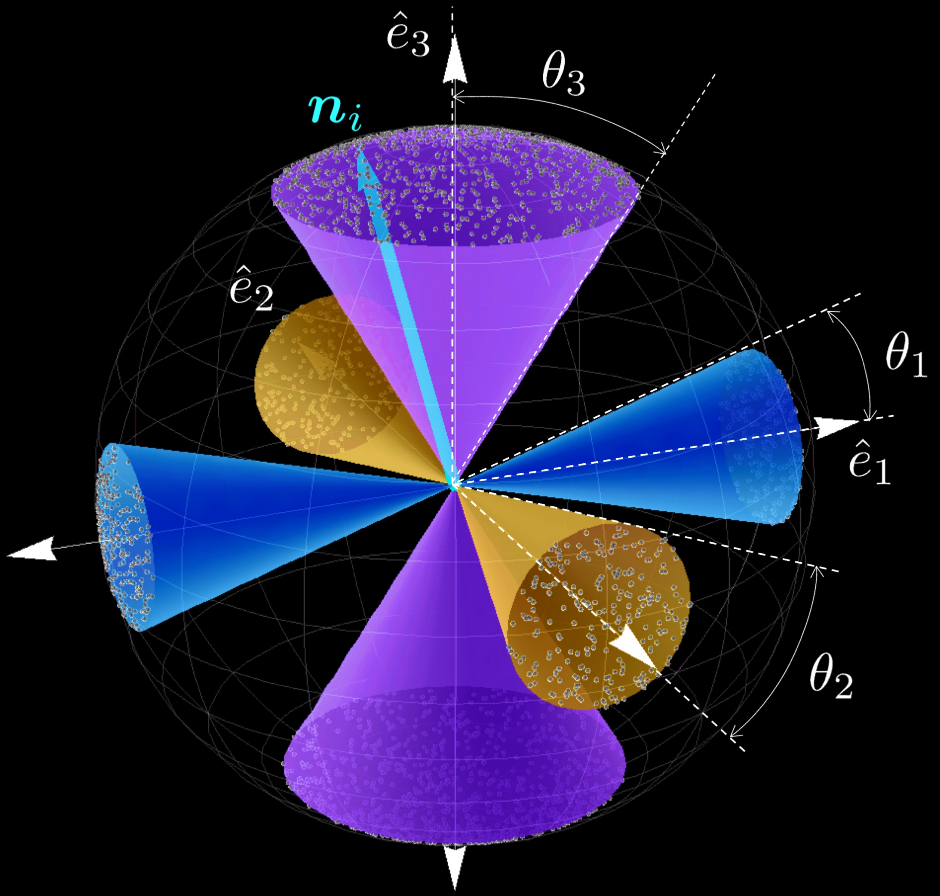
random wave vectors: $\boldsymbol{n}_i \sim \mathcal{U}(S^1)$

**Smooth bi-continuous structures which are also solutions to spinodal decomposition PDE**

# Spinodoid parameterization

Wave vector distribution:




**Gaussian random field (GRF):**

$$\varphi(\boldsymbol{x}) = \sum_{i=1}^{N \gg 1} A_i \cos(\beta \boldsymbol{n}_i \cdot \boldsymbol{x} + \alpha_i)$$

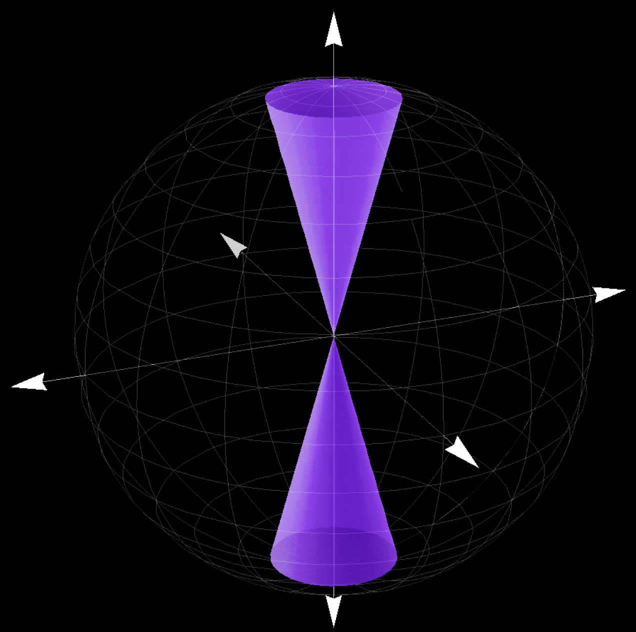
Parameterization

- $\theta_1$: Max wave vector angle along x-axis
- $\theta_2$: Max wave vector angle along y-axis
- $\theta_3$: Max wave vector angle along z-axis
- $\rho$: Relative density

$\Bigg\}$ **seamless tunability**

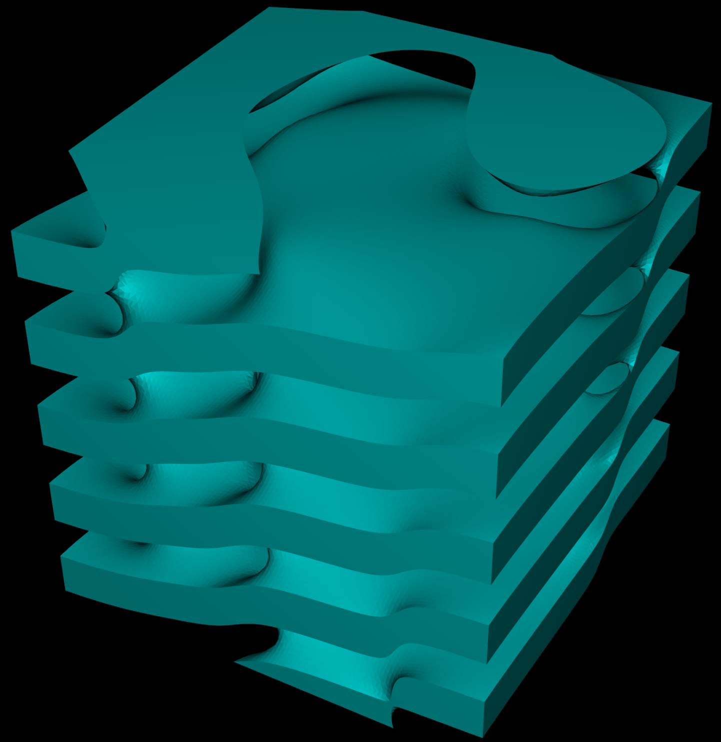
Kumar et al., Inverse-designed spinodoid metamaterials, npj Comp. Mater., 2020

# Tunable anisotropy: lamellar



Wave-vector distribution:
$\theta_1 = 0^\circ, \theta_2 = 0^\circ, \theta_3 = 15^\circ$

Relative density:
$\rho = 0.5$



Topology

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & \text{sym.} & & & C_{55} & 0 \\ & & & & & C_{66} \end{bmatrix}$$

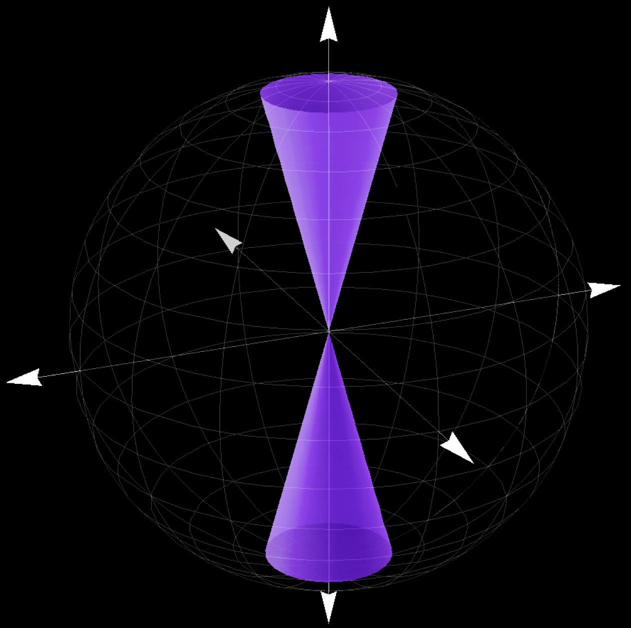
Stiffness matrix

Kumar et al., Inverse-designed spinodoid metamaterials, npj Comp. Mater., 2020

# Tunable anisotropy: lamellar

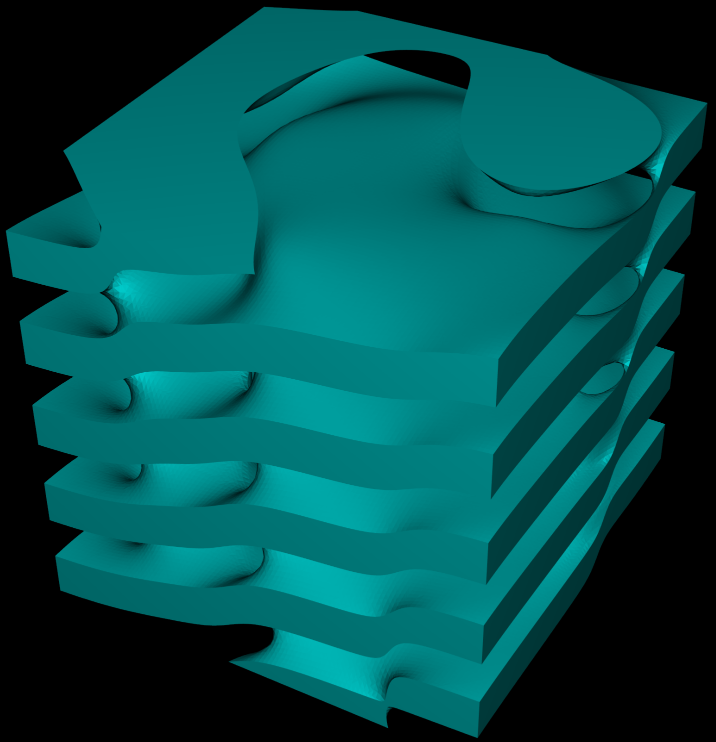
$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & \text{sym.} & & & C_{55} & 0 \\ & & & & & C_{66} \end{bmatrix}$$

Visualize

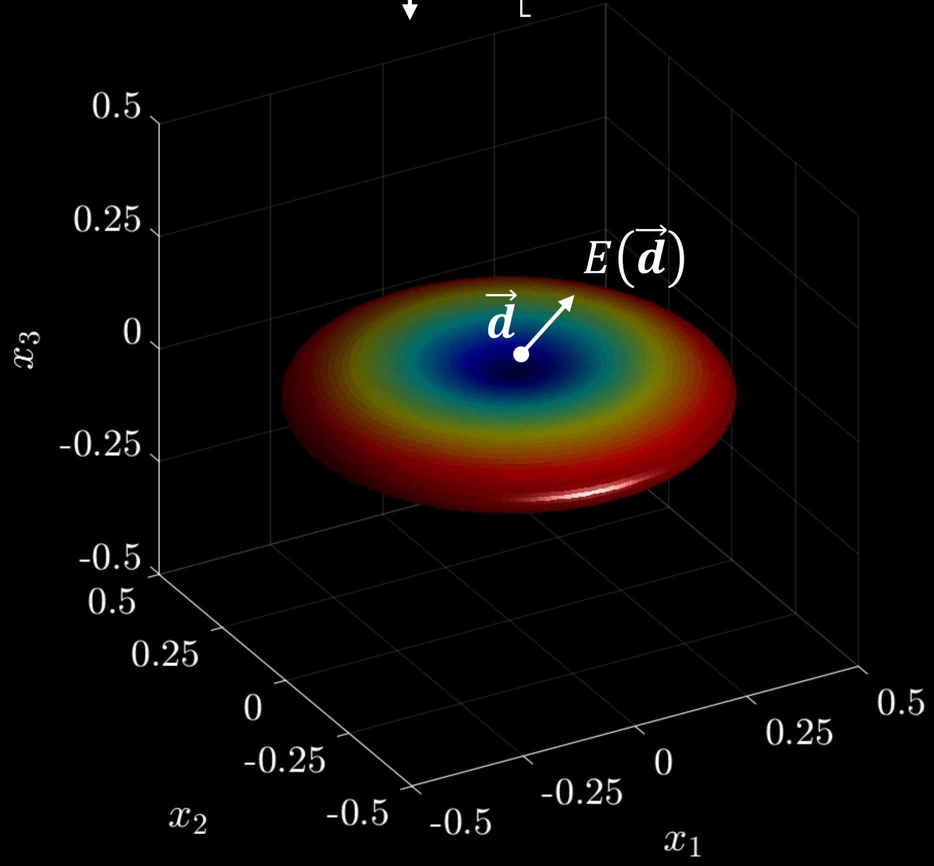


Wave-vector distribution:
$\theta_1 = 0°, \theta_2 = 0°, \theta_3 = 15°$

Relative density:
$\rho = 0.5$



Topology



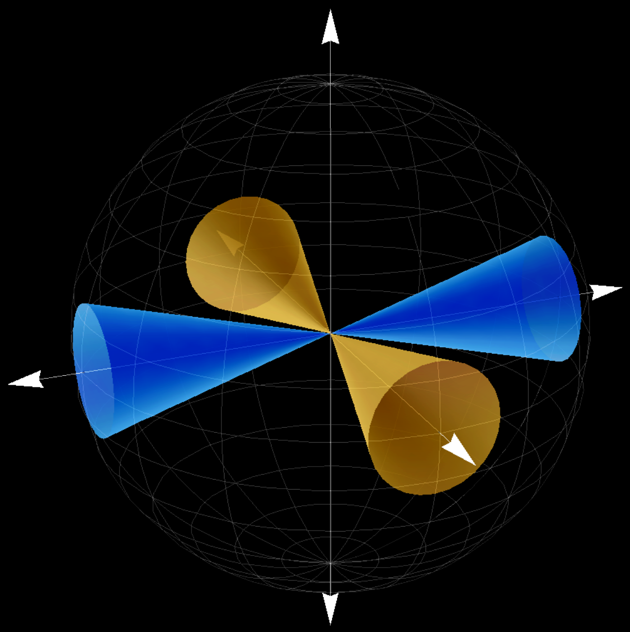

Elasticity surface

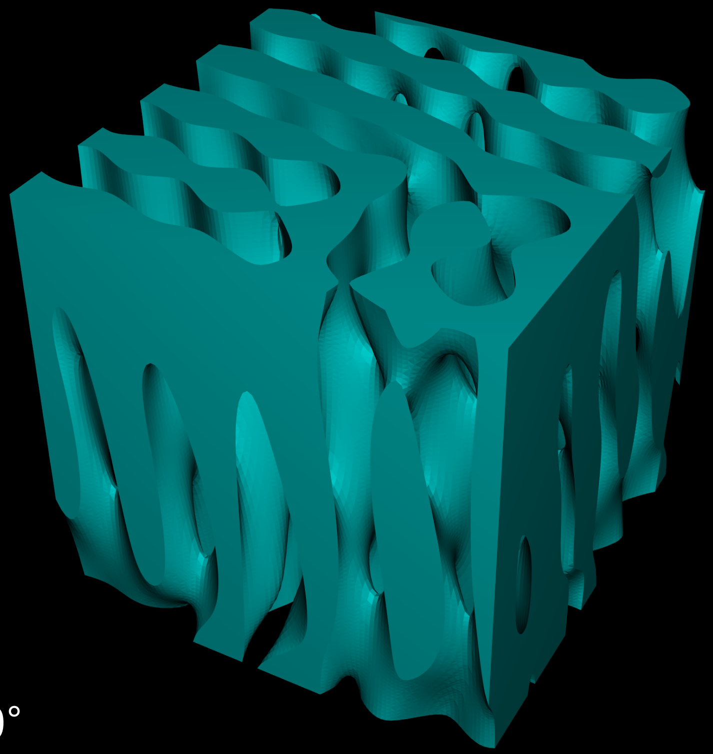
Kumar et al., Inverse-designed spinodoid metamaterials, npj Comp. Mater., 2020

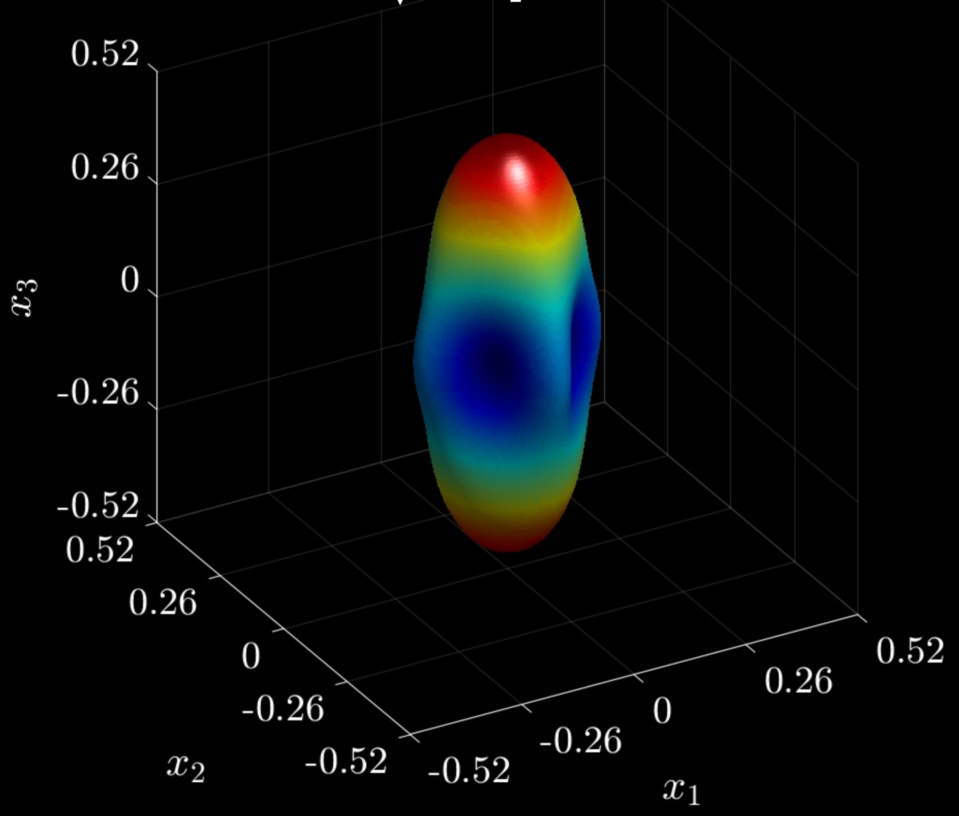
# Tunable anisotropy: Columnar

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & \text{sym.} & & & C_{55} & 0 \\ & & & & & C_{66} \end{bmatrix}$$

Visualize








Wave-vector distribution:
$\theta_1 = 15^\circ, \theta_2 = 15^\circ, \theta_3 = 0^\circ$

Relative density:
$\rho = 0.5$

Topology

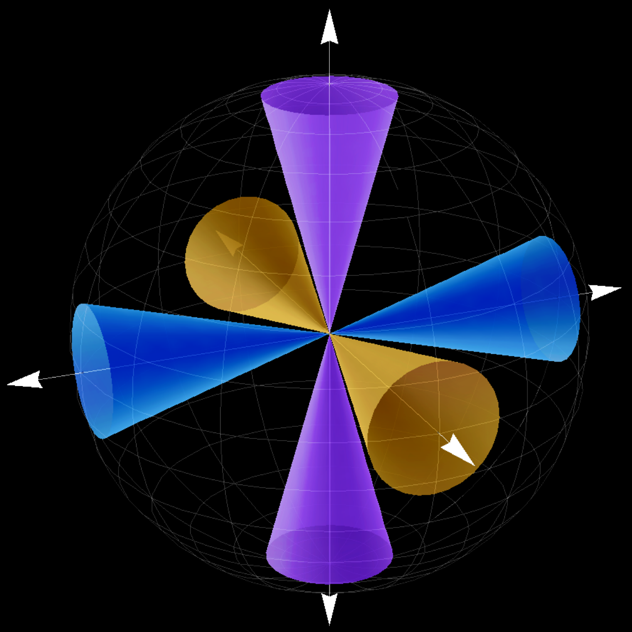
Elasticity surface

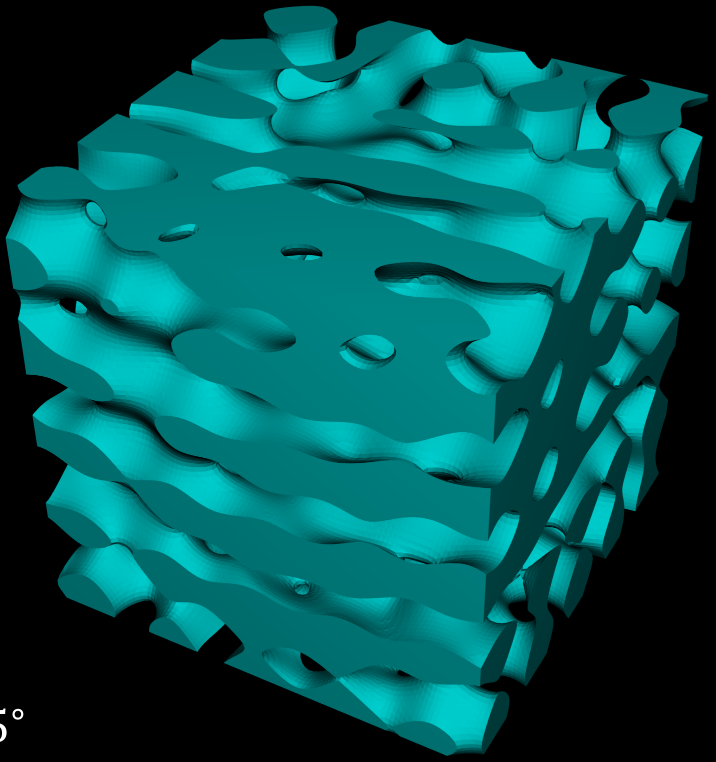
Kumar et al., Inverse-designed spinodoid metamaterials, npj Comp. Mater., 2020

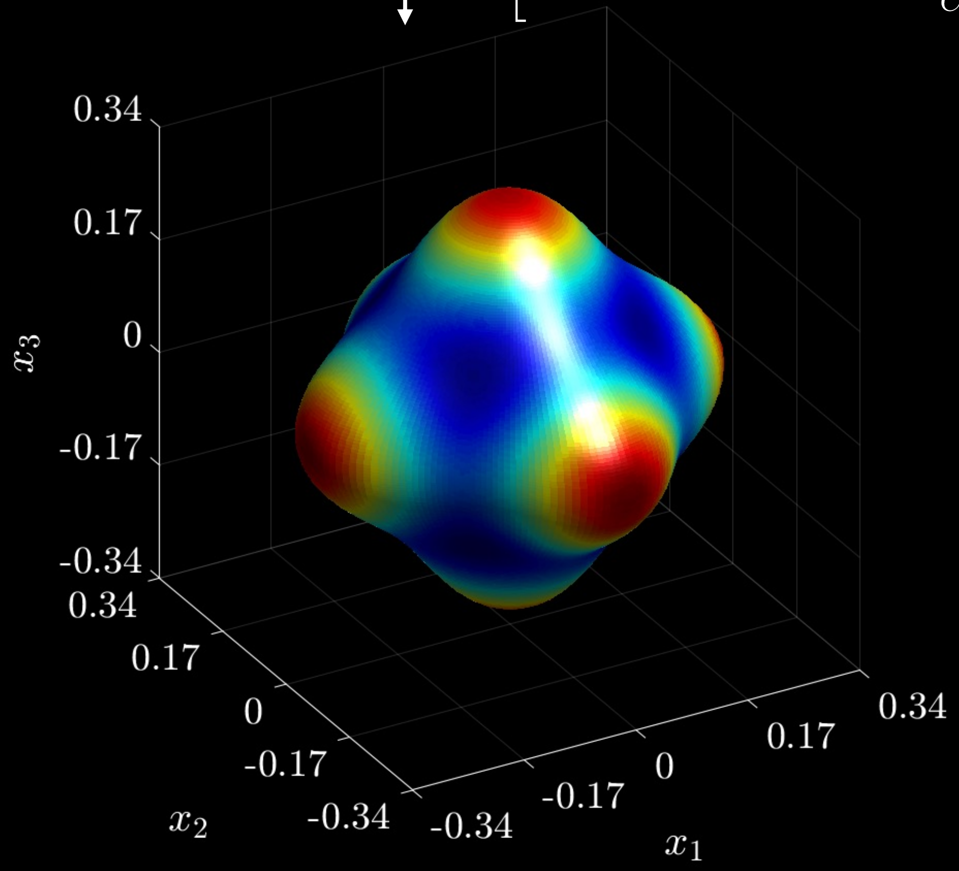
# Tunable anisotropy: cubic

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & \text{sym.} & & & C_{55} & 0 \\ & & & & & C_{66} \end{bmatrix}$$

Visualize








Wave-vector distribution:
$\theta_1 = 15°, \theta_2 = 15°, \theta_3 = 15°$

Relative density:
$\rho = 0.5$

Topology

Elasticity surface

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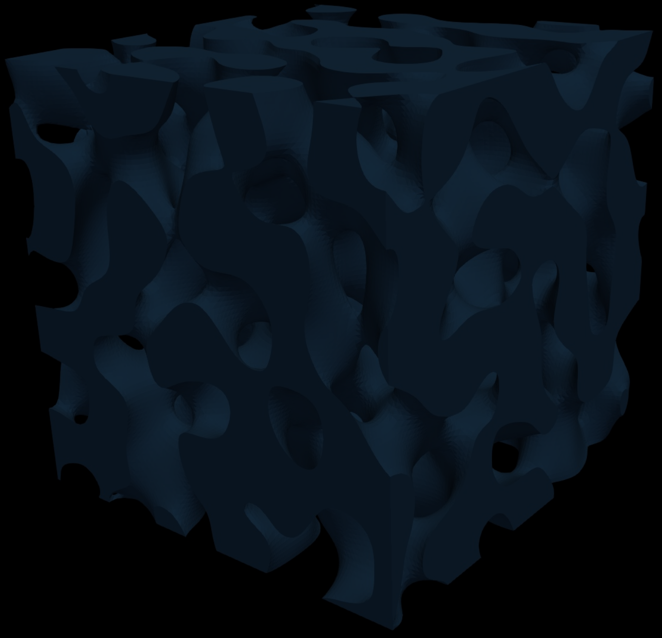
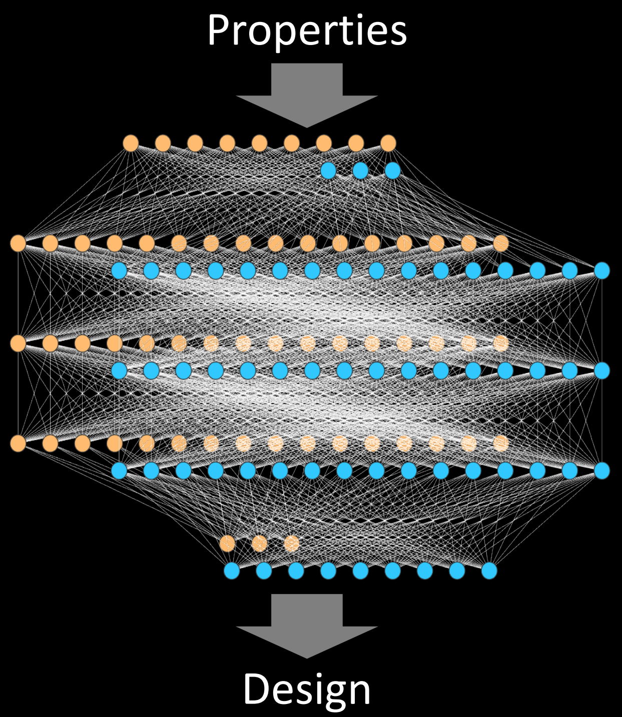
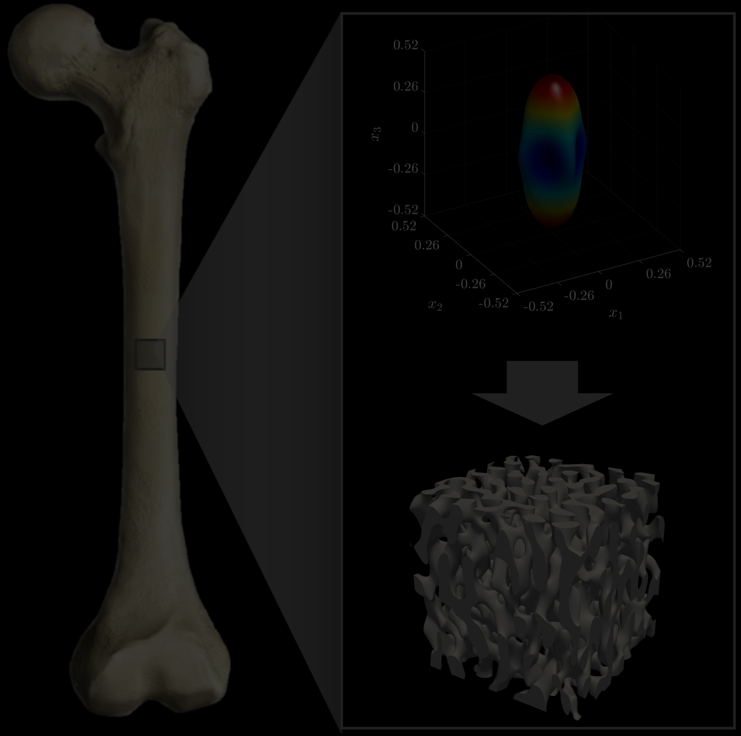
# What I will talk about





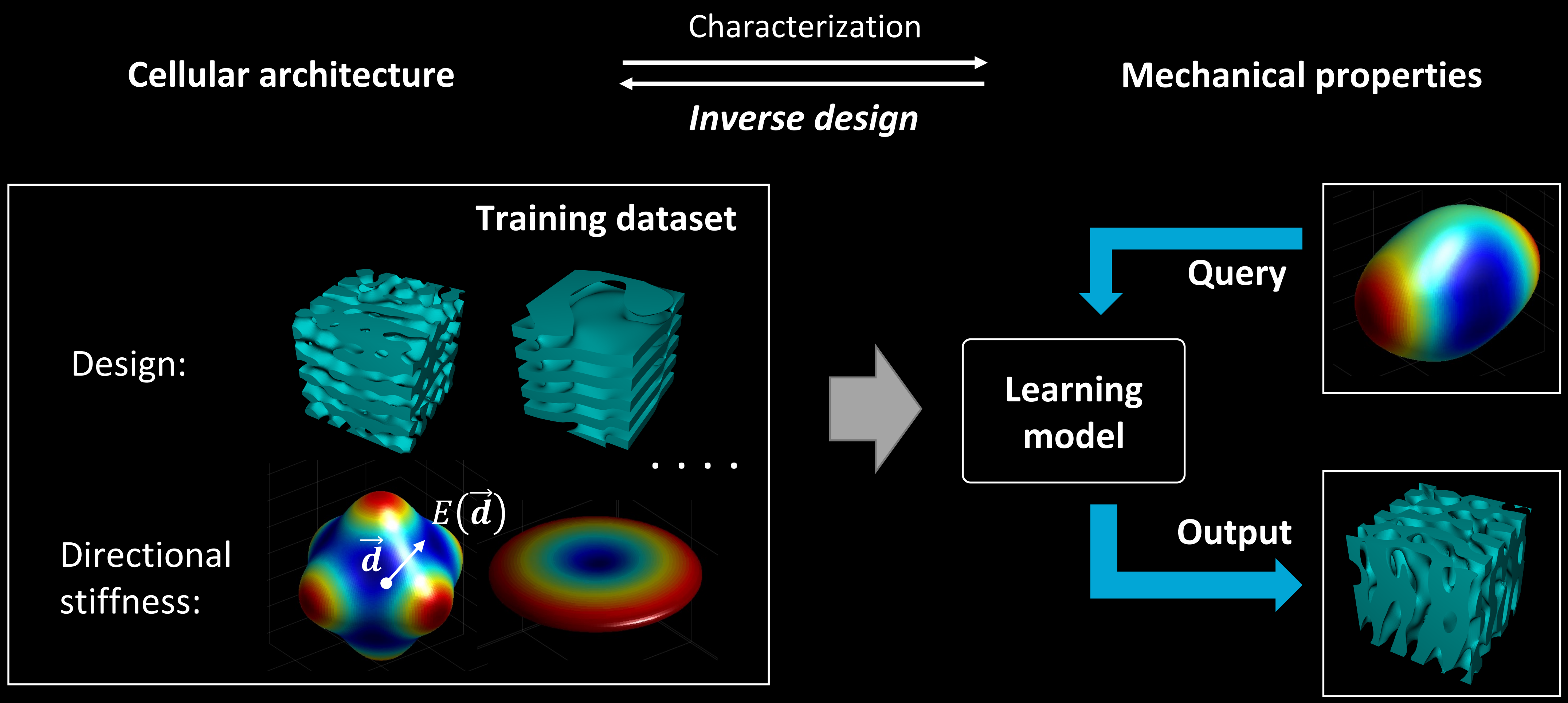



A new class of metamaterials for anisotropic tunability: **Spinodoids**

**Inverse design** using machine learning

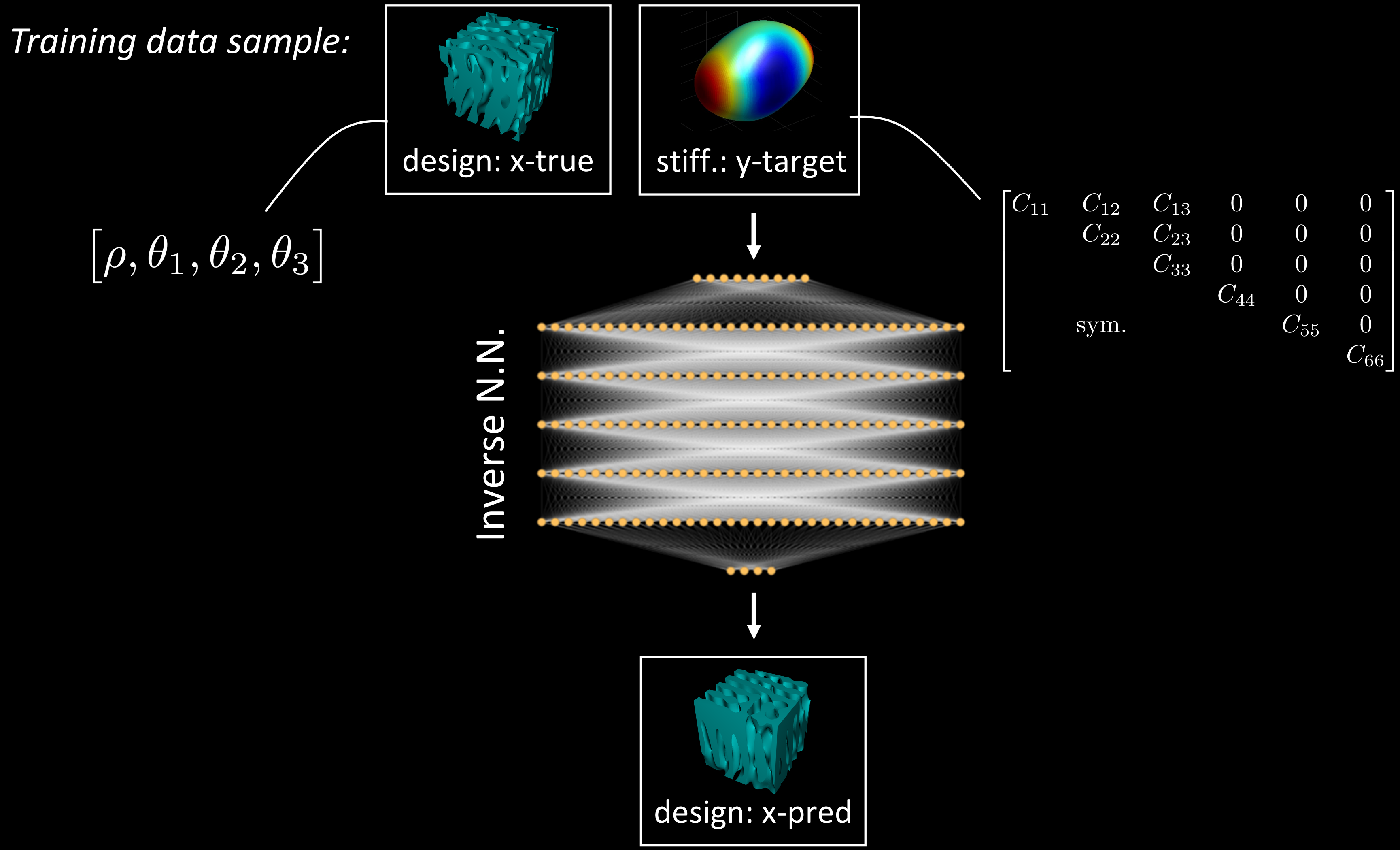
Applications to **synthetic bones** & **lightweight structures**

# Inverse-designed spinodoid metamaterials




Kumar et al., Inverse-designed spinodoid metamaterials, npj Comp. Mater., 2020

# Inverse-designed spinodoid metamaterials

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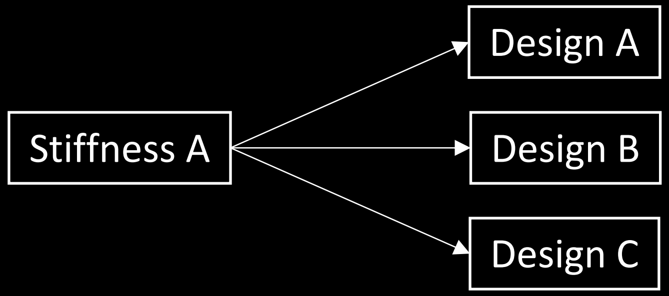
# Inverse-designed spinodoid metamaterials

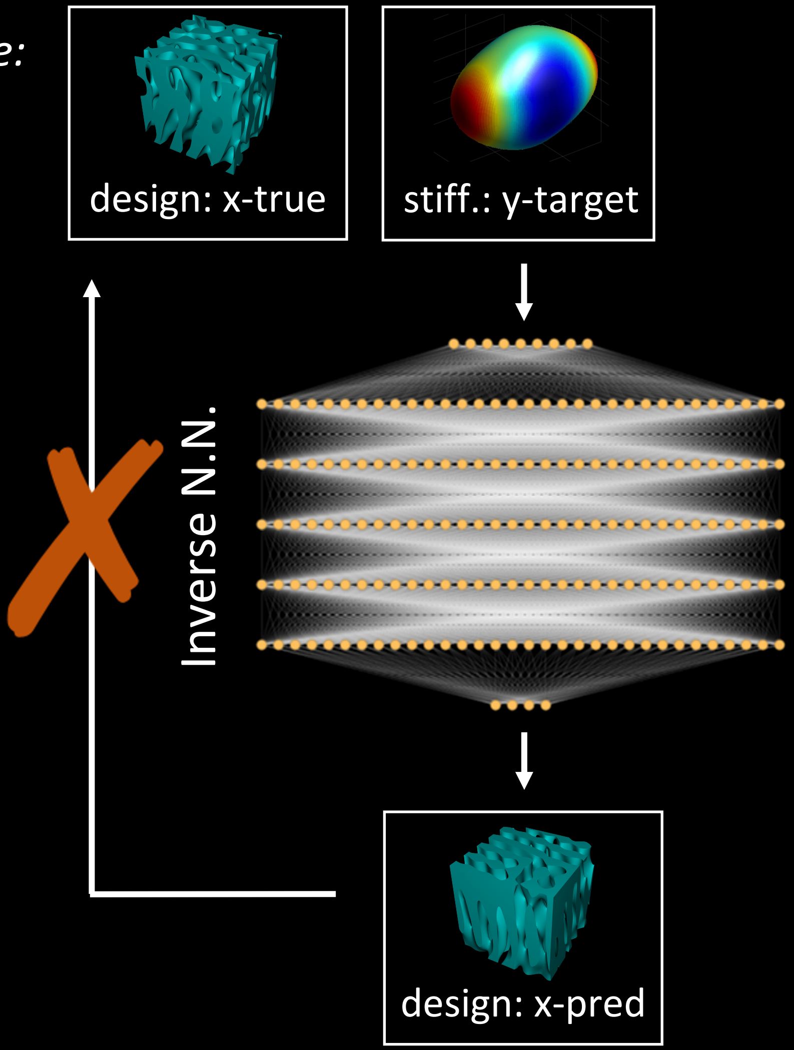
*Training data sample:*

**Challenge**: multiple designs can have same/similar stiffness

**Inverse problem:**




ill-posed!

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# Inverse-designed spinodoid metamaterials

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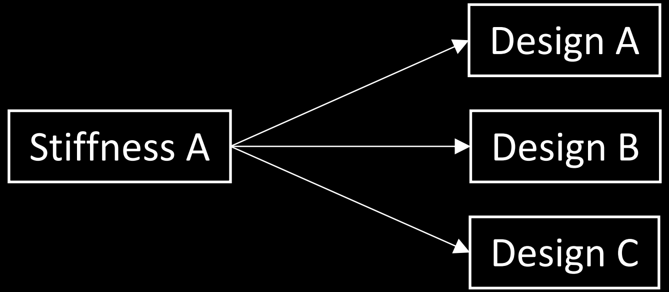


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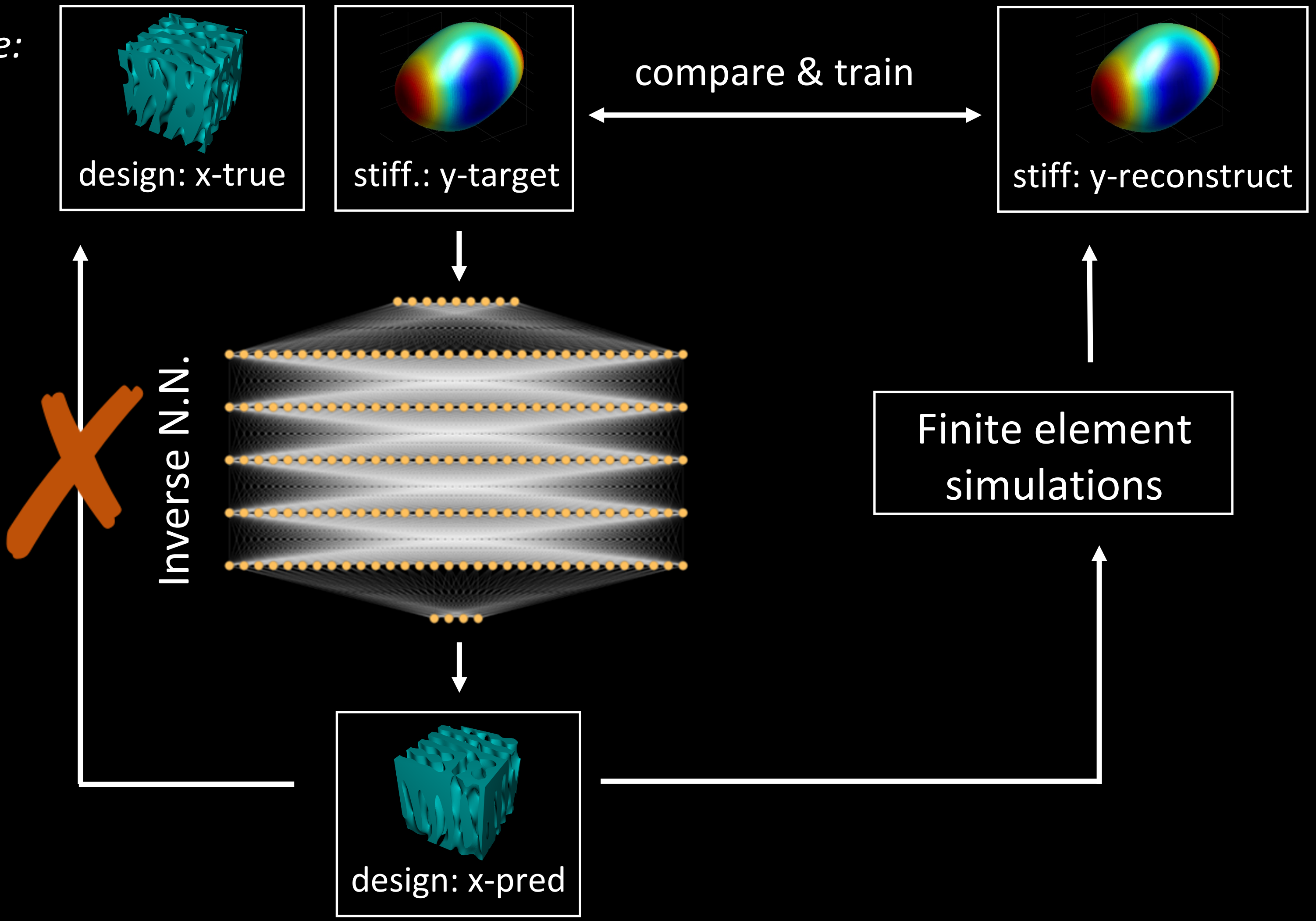
*Training data sample:*

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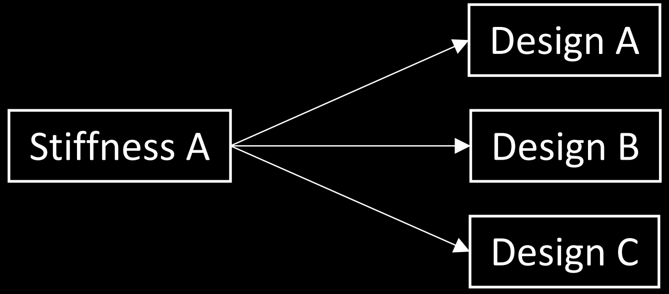
# Inverse-designed spinodoid metamaterials

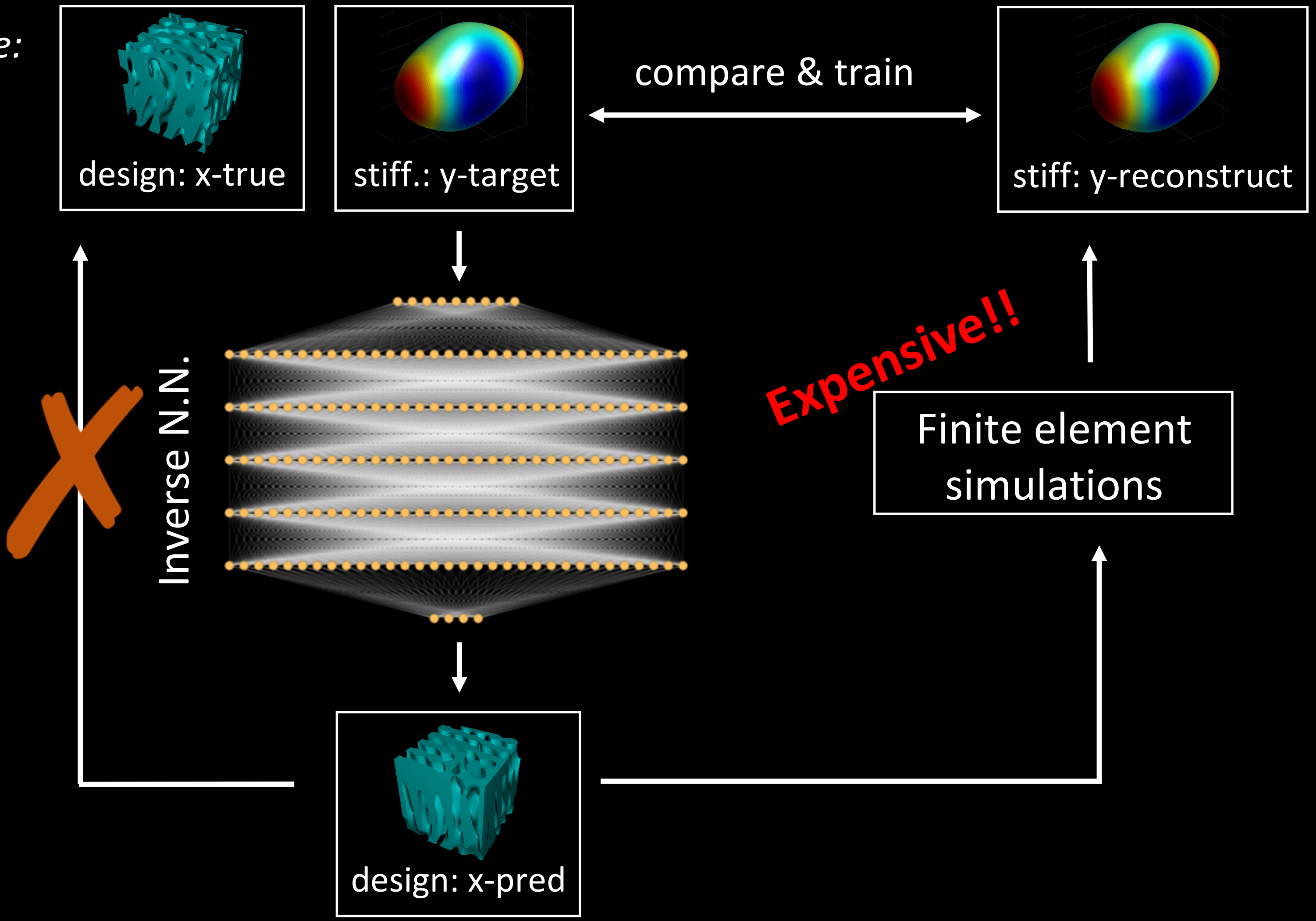
**Challenge**: multiple designs
can have same/similar stiffness

**Inverse problem:**




ill-posed!

*Training data sample:*

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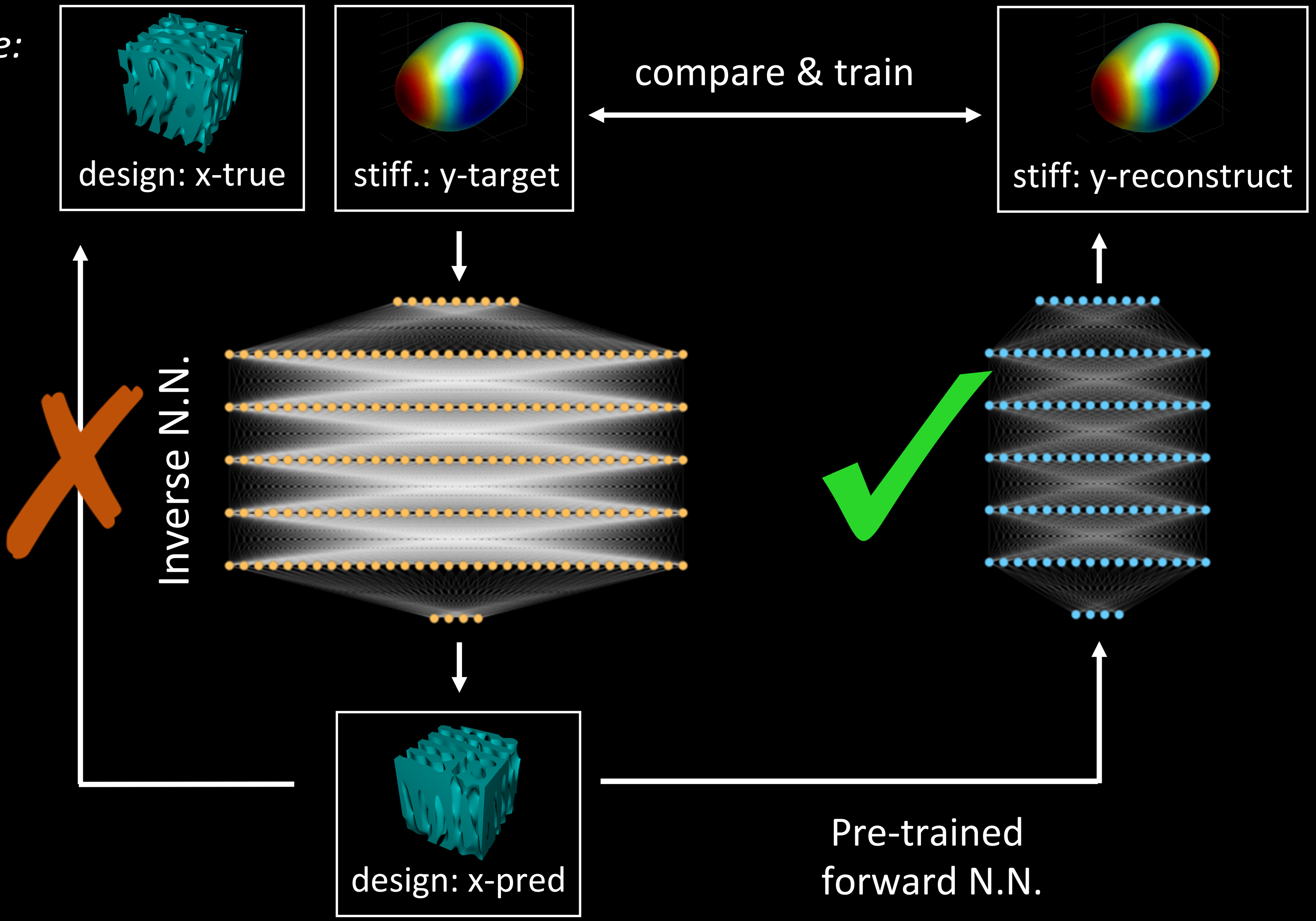
# Inverse-designed spinodoid metamaterials

*Training data sample:*




**Challenge**: multiple designs can have same/similar stiffness

**Inverse problem:**

Stiffness A → Design A
Stiffness A → Design B
Stiffness A → Design C

ill-posed!

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# Training scheme

**Forward N.N.** $\boldsymbol{y} = \mathbf{fwd}(\boldsymbol{x})$

- Input | design vector: $x$
- Output | stiffness vector: $y$
- Training:

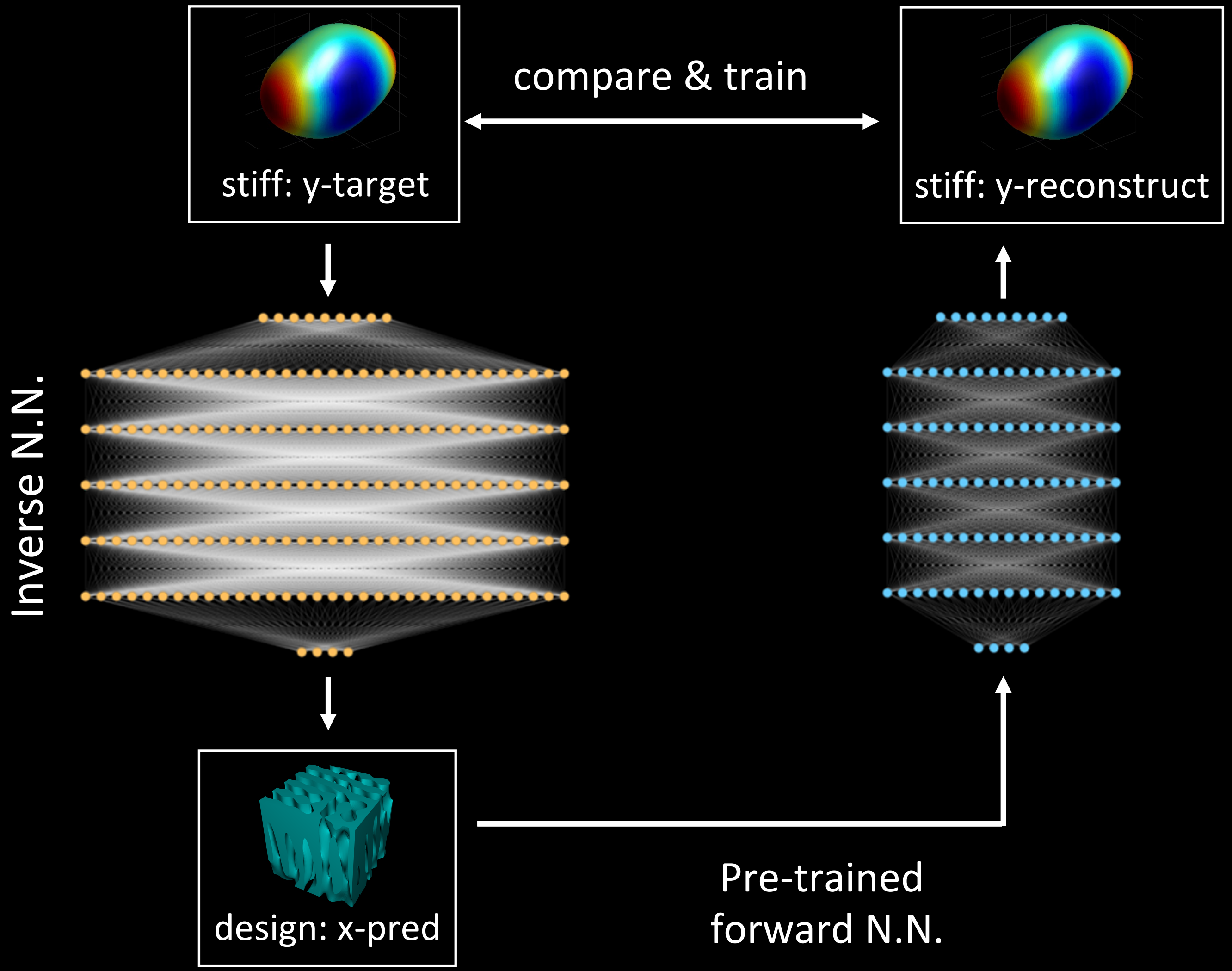
$$\min \ \|\mathrm{fwd}(x) - y_{\mathrm{true}}\|^2 \ \checkmark$$

**Inverse N.N.** $\boldsymbol{x} = \mathbf{inv}(\boldsymbol{y})$

- Input | stiffness vector: $y$
- Output | design vector: $x$
- fwd: treat as fixed, do NOT optimize
- Training:

$$\min \ \|\mathrm{inv}(y_{\mathrm{target}}) - x_{\mathrm{true}}\|^2 \ \times$$

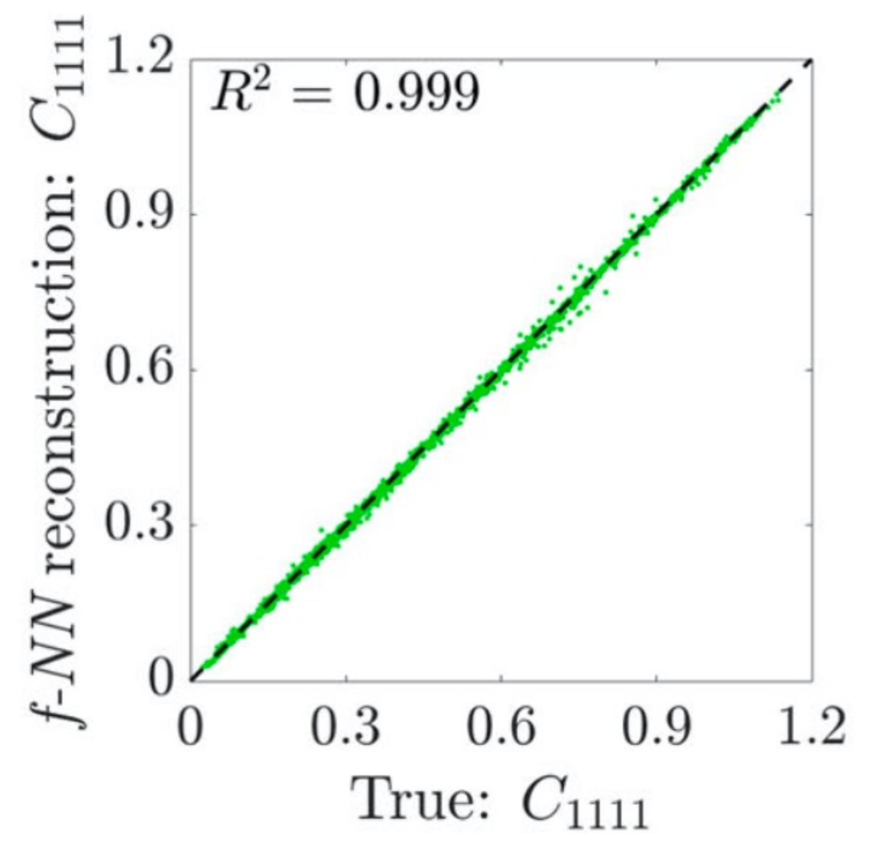
$$\min \ \|\mathrm{fwd}[\mathrm{inv}(y_{\mathrm{target}})] - y_{\mathrm{target}}\|^2 \ \checkmark$$



# Results

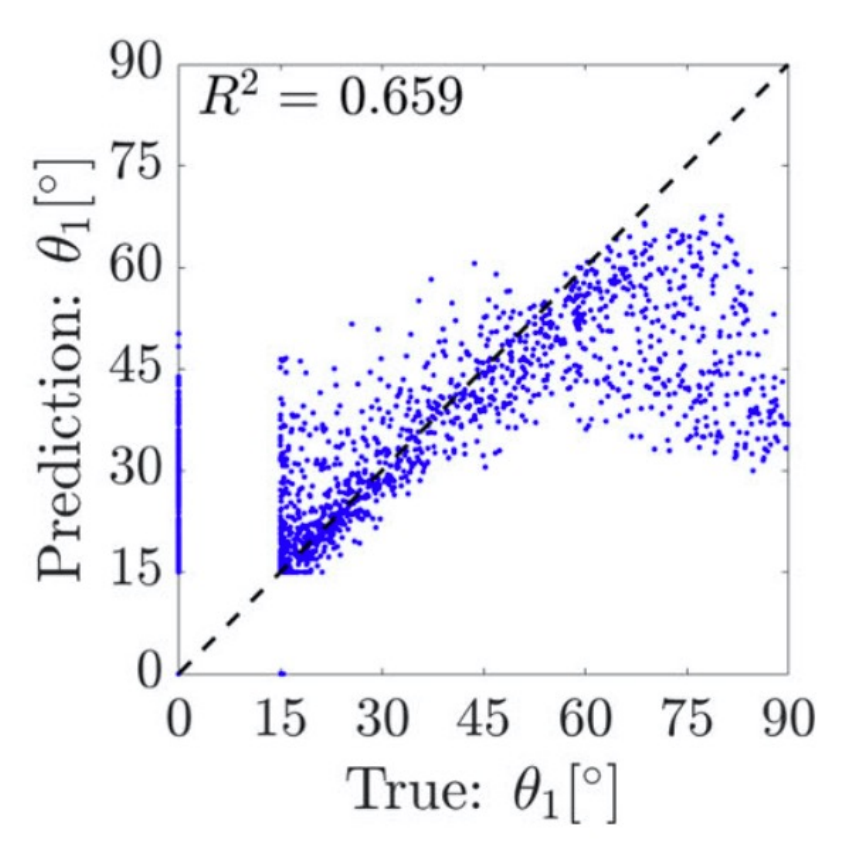
Expected to be bad! ☺
➔ confirms the existence of multiple designs

Stiffness: y-reconstruction



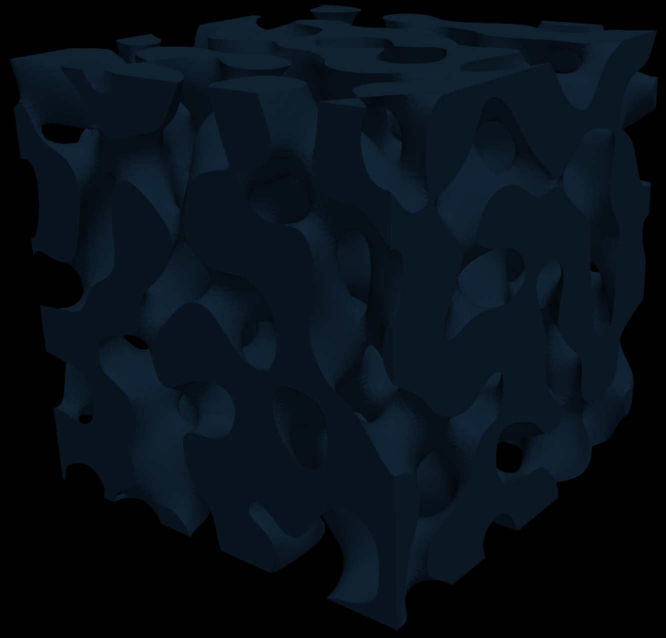

Stiffness: y-target

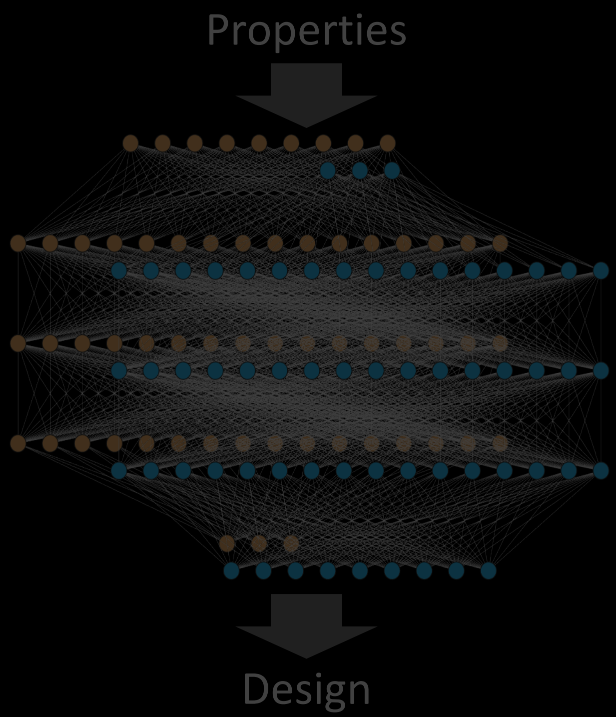
Design: x-prediction

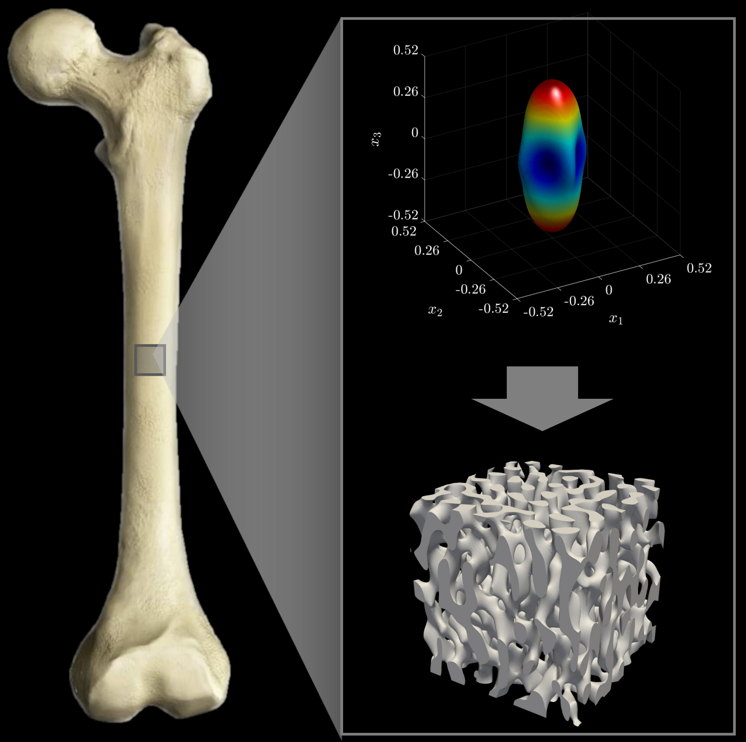



Design: x-true

# What we will talk about



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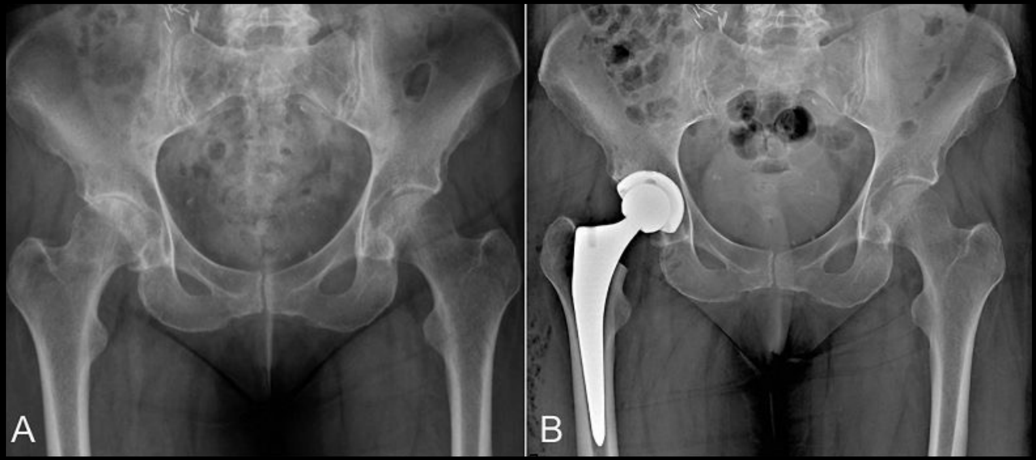
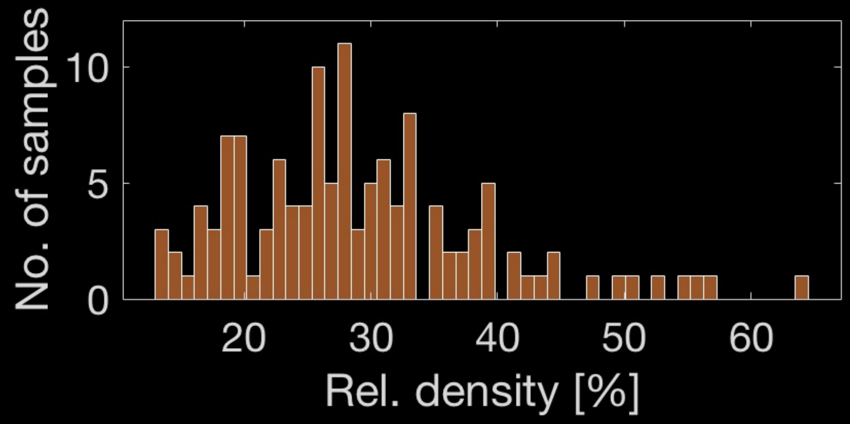
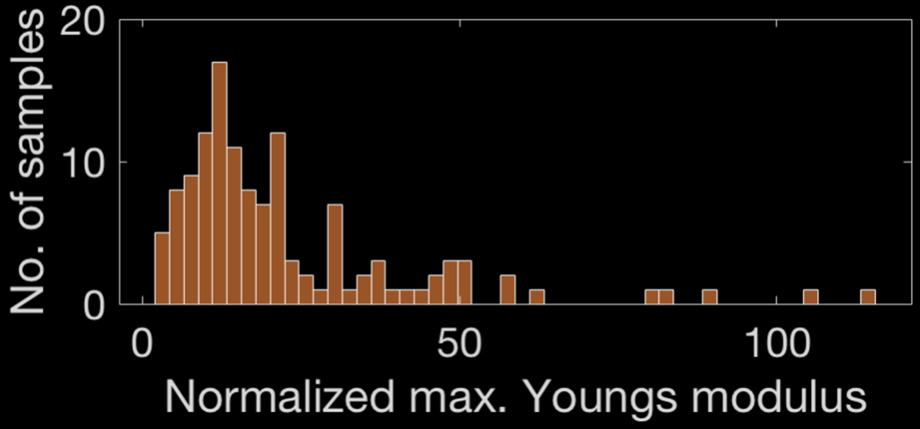
# Applications: synthetic bones




http://www.opnews.com/wp-content/uploads/2017/12/OPN-PSI-Figure-4-800x500_c.jpg

- Implants usually made from Ti or steel
- Stress shielding causes stiffness mismatch and bone atrophy
- Variability of bone density and stiffness



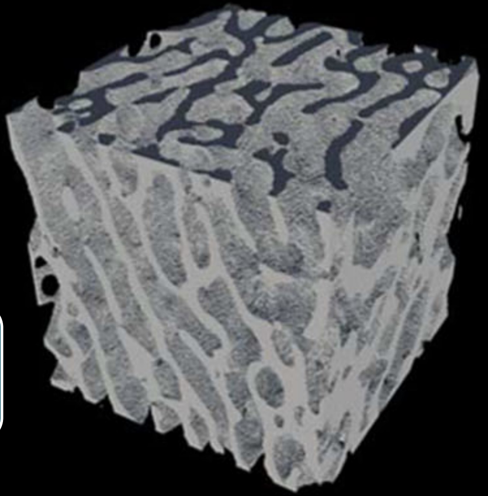




*(Data extracted from micro-CT scans of femurs by Marangalou et al., 2013)*

# Patient- & site-specific implants

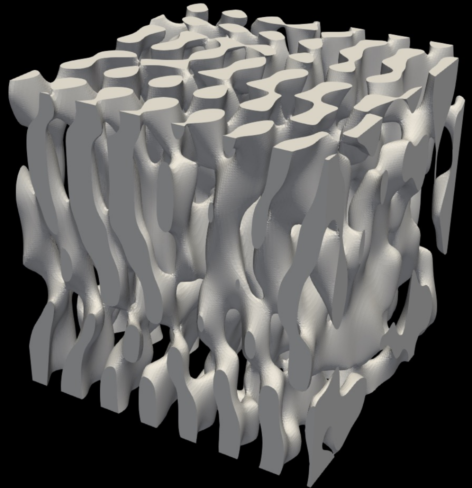
Bone micro-CT from Colabella et al, 2017

($\rho = 0.38$)



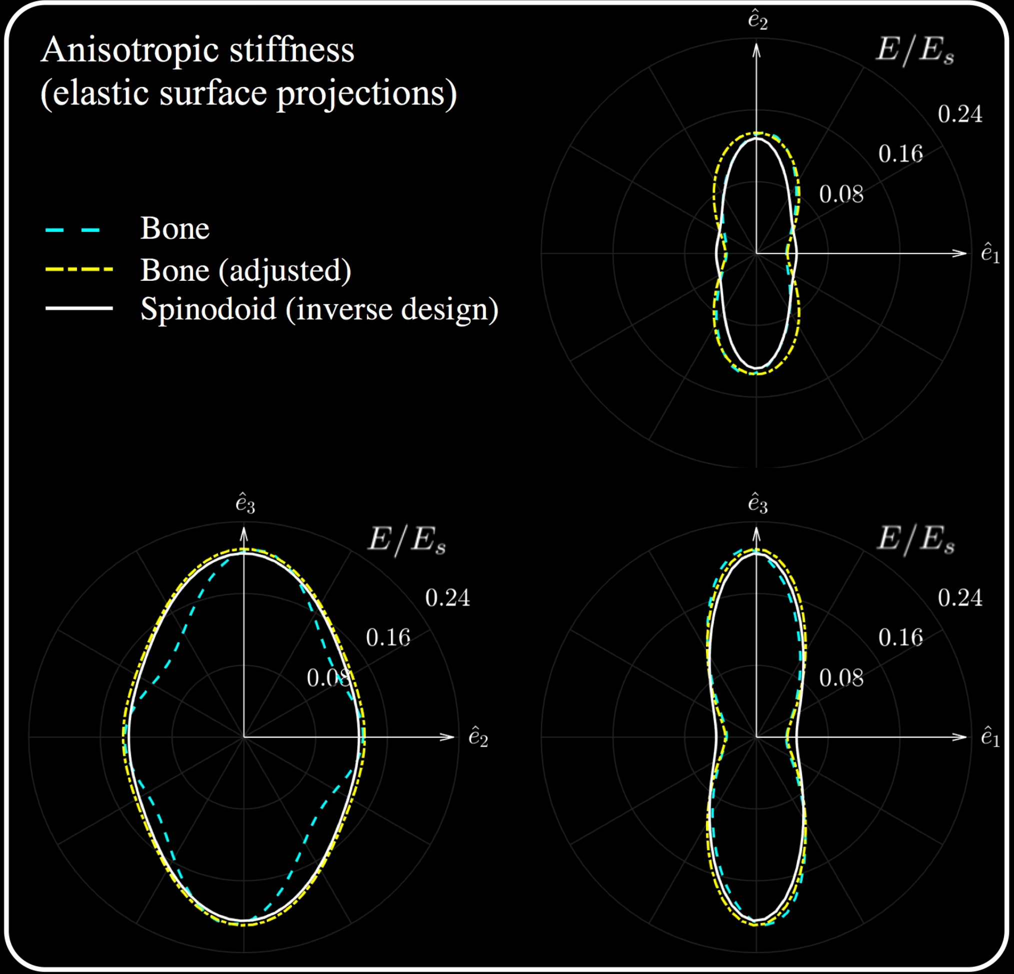
No bone data during training

Geometric and topological similarity



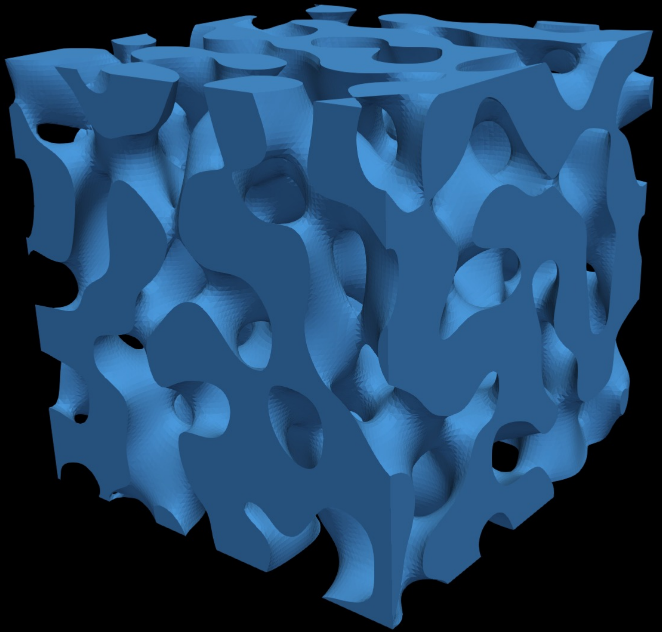
Predicted synthetic bone topology

($\rho = 0.34$)

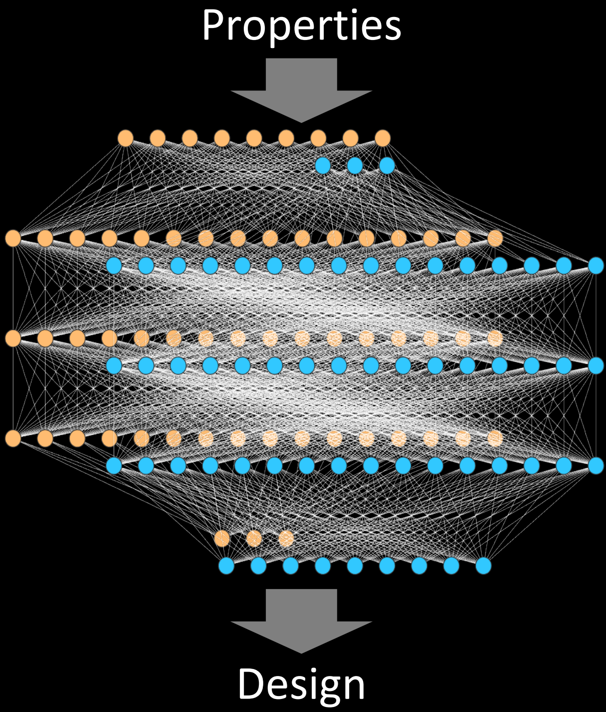



Kumar et al., Inverse-designed spinodoid metamaterials, npj Comp. Mater., 2020

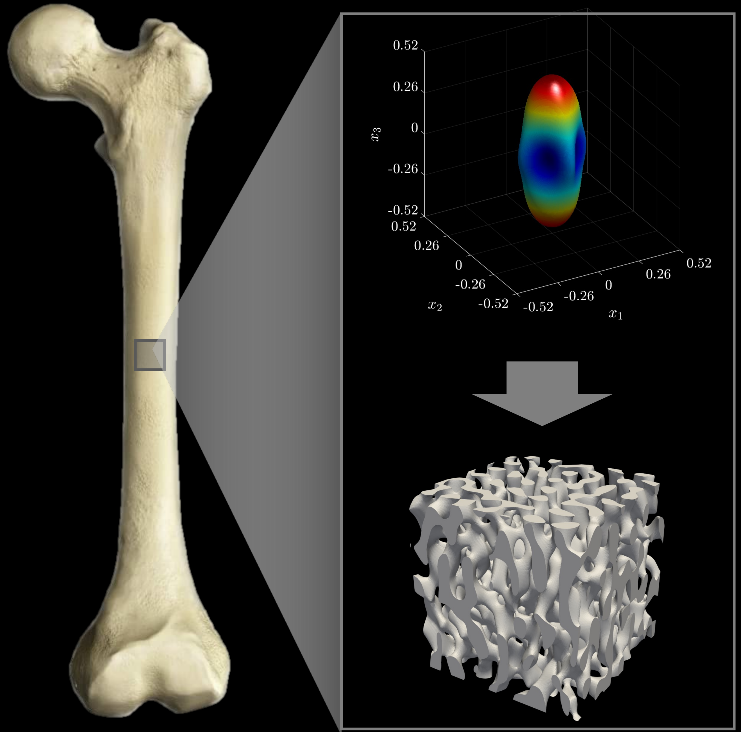
# What we talked about



A new class of metamaterials for anisotropic tunability: **Spinodoids**

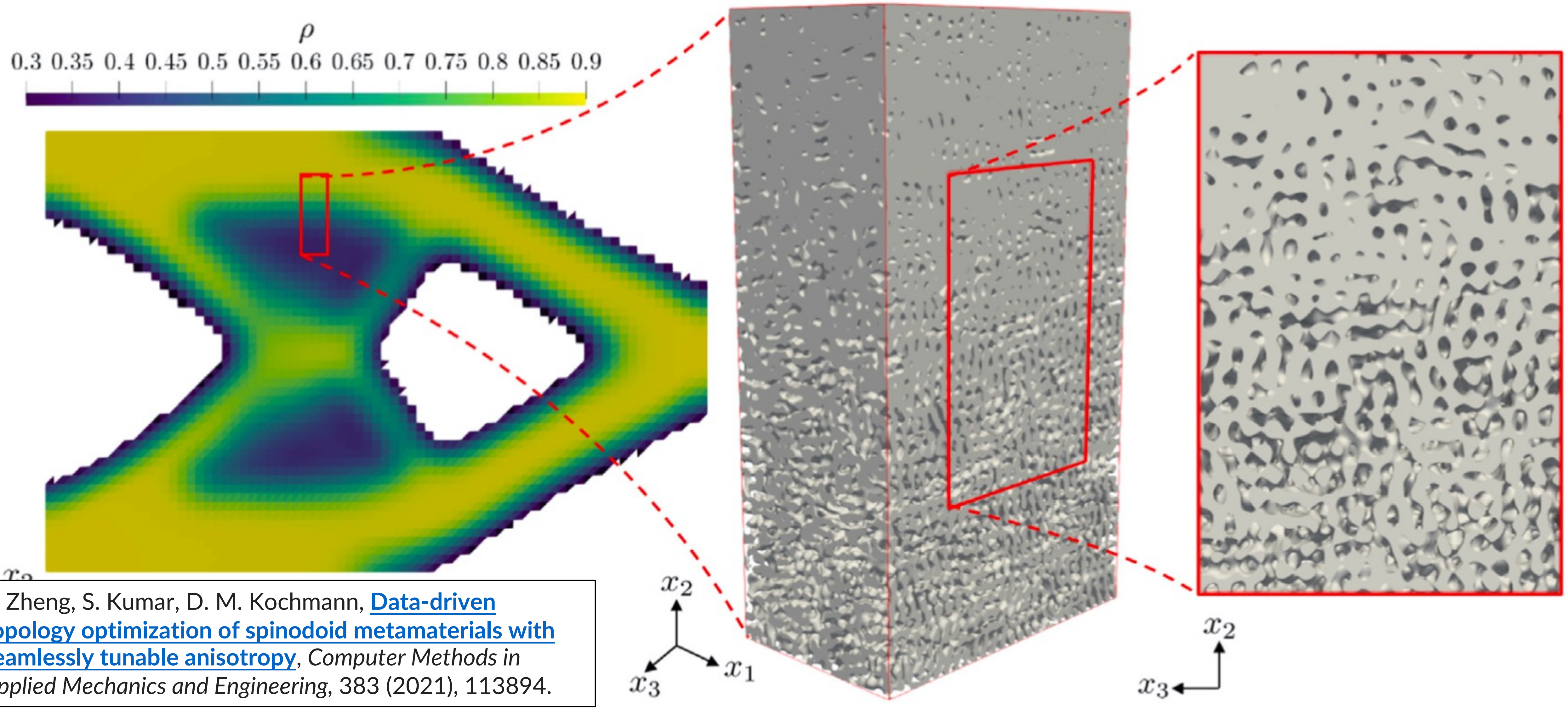



**Inverse design** using machine learning



Applications to **synthetic bones** & **lightweight structures**

# Topology optimization with spinodoid metamaterials




L. Zheng, S. Kumar, D. M. Kochmann, [Data-driven topology optimization of spinodoid metamaterials with seamlessly tunable anisotropy](), *Computer Methods in Applied Mechanics and Engineering*, 383 (2021), 113894.

# Questions & comments . . .

**Project based on:**

- **Inverse-designed spinodoid metamaterials**, *npj Computational Materials*, 6 (2020), 73.

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## Inverse-designed spinodoid metamaterials

Siddhant Kumar[1], Stephanie Tan[2], Li Zheng[1] and Dennis M. Kochmann[1,3]

After a decade of periodic truss-, plate-, and shell-based architectures having dominated the design of metamaterials, we introduce the non-periodic class of spinodoid topologies. Inspired by natural self-assembly processes, spinodoid metamaterials are a close approximation of microstructures observed during spinodal phase separation. Their theoretical parametrization is so intriguingly simple that one can bypass costly phase-field simulations and obtain a rich and seamlessly tunable property space. Counter-intuitively, breaking with the periodicity of classical metamaterials is the enabling factor to the large property space and the ability to introduce seamless functional grading. We introduce an efficient and robust machine learning technique for the inverse design of (meta-)materials which, when applied to spinodoid topologies, enables us to generate uniform and functionally graded cellular mechanical metamaterials with tailored direction-dependent (anisotropic) stiffness and density. We specifically present biomimetic artificial bone architectures that not only reproduce the properties of trabecular bone accurately but also even geometrically resemble natural bone.

*npj Computational Materials* (2020)6:73 ; https://doi.org/10.1038/s41524-020-0341-6