# Inverse Design Metamaterials –
## From Trusses and Spinodoids to General Architectures

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joint work with (primarily):

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**Jan-Hendrik Bastek**

**Sid Kumar**
(TU Delft)

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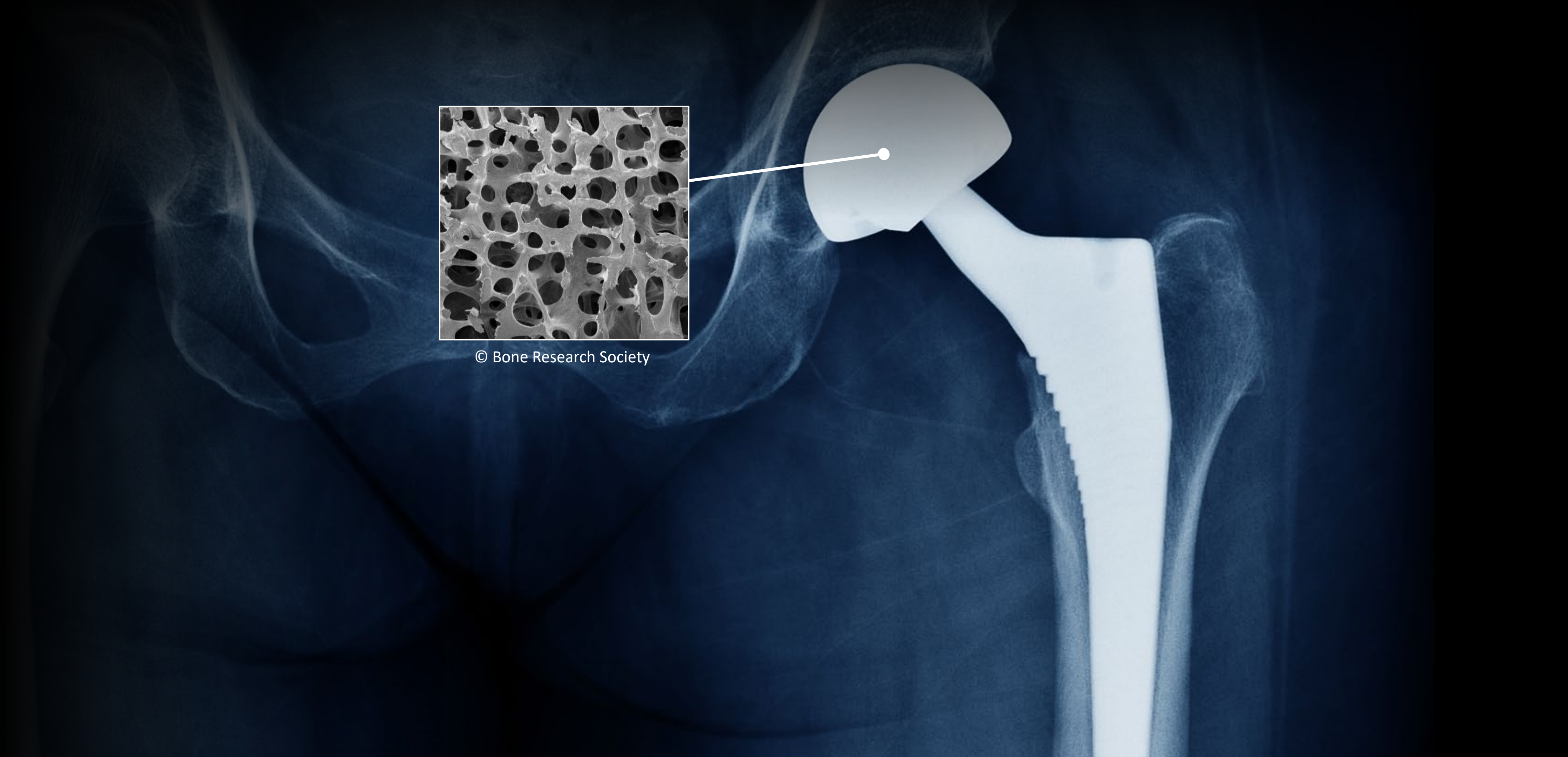
# **Architected Materials** or **Metamaterials** *



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* *To me these two mean the same; it's a matter of semantics.*

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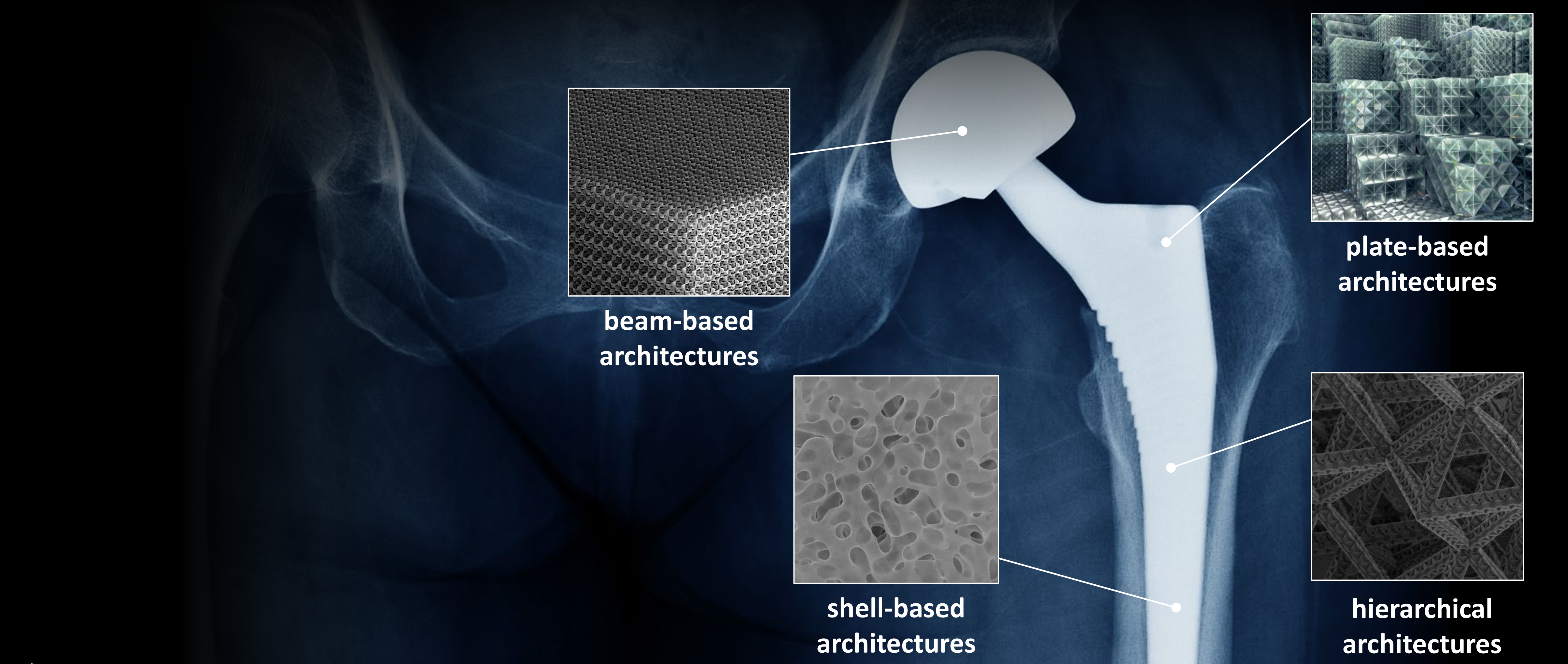
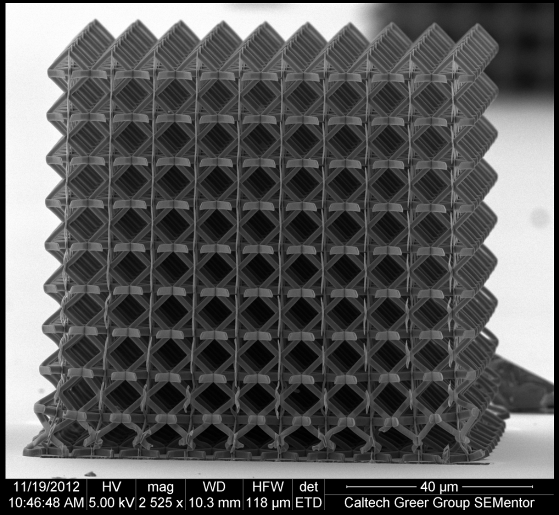
# Architected Materials or Metamaterials *

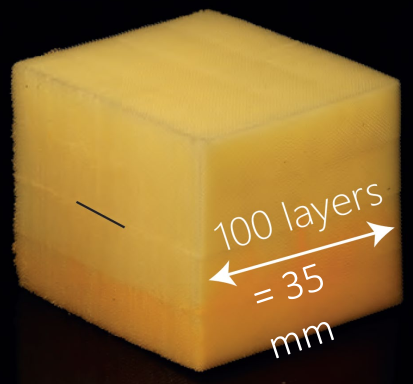



* *To me these two mean the same; it's a matter of semantics.*

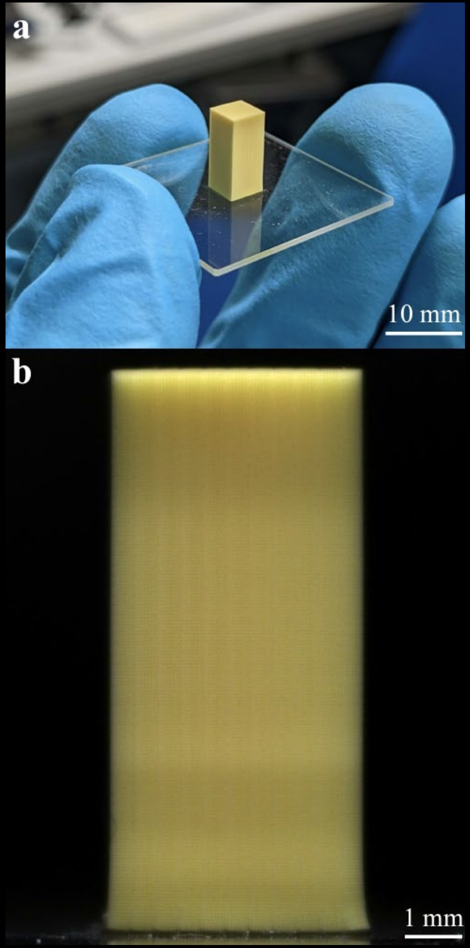
# Miniaturization & Applications




*(Julia R. Greer, Caltech)*

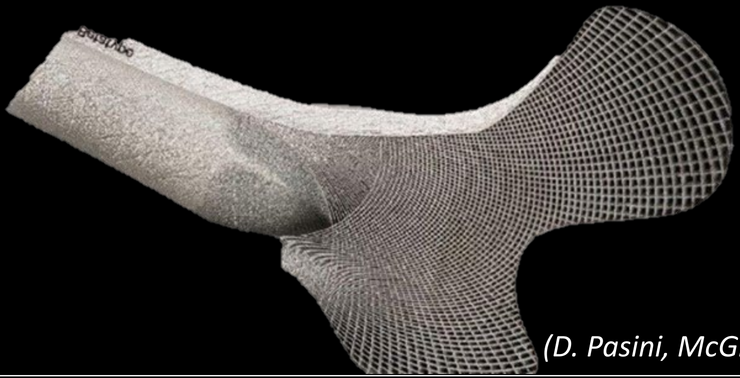



*(Shaikeea et al., Nature Mater. 2022)*



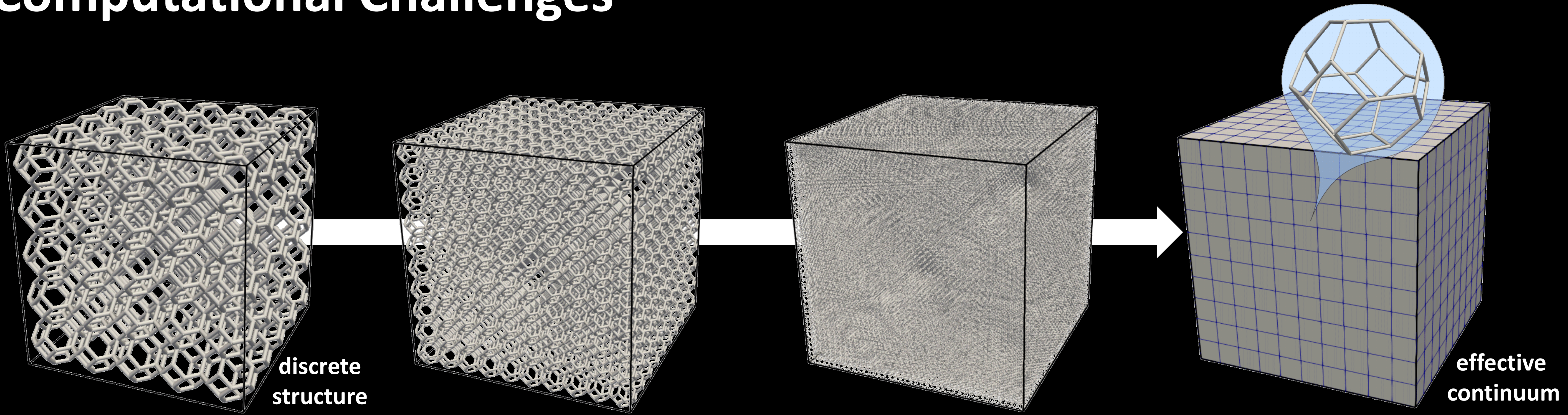

*(Kiefer et al., Light: Adv. Manuf. 2024)*
*cf. talk by Martin Wegener*

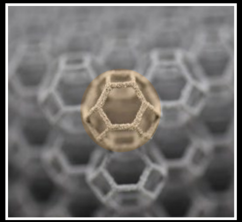
*(adidas; https://www.3dnatives.com/en/3d-printed-bicycle-helmet-voronoi-190820204)*

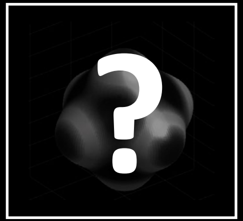


*(D. Pasini, McGill)*

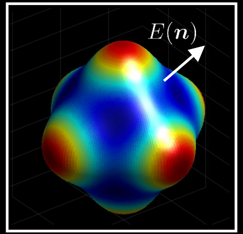
# Computational Challenges



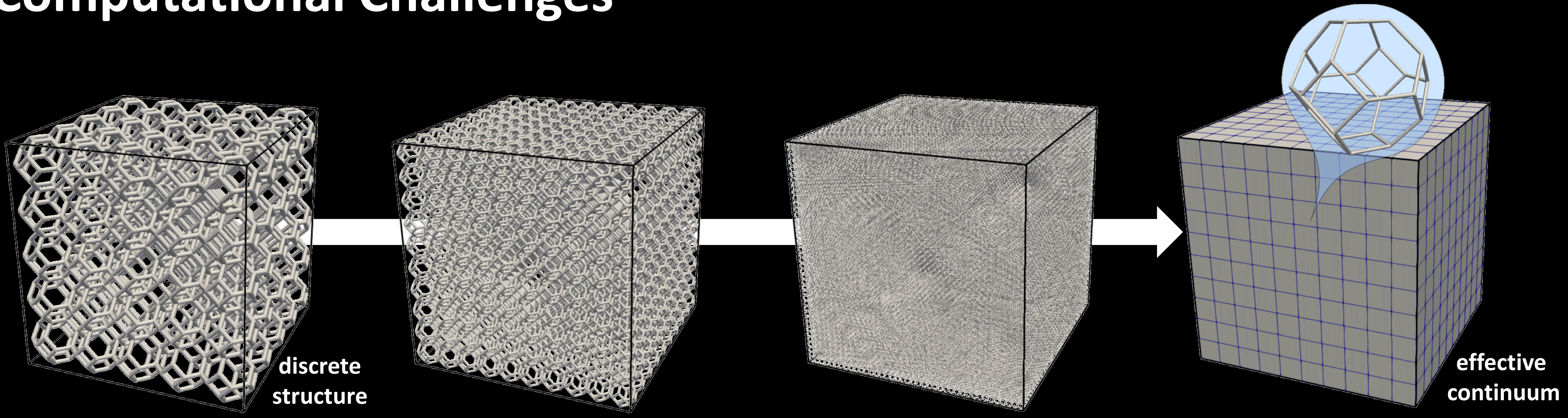


**Forward challenge: predicting effective properties**
(stiffness, strength, toughness, wave dispersion, …)



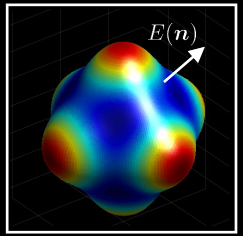

**Inverse challenge: predicting structures having target properties**
(trusses, plates, shells, non-periodic designs, composites, …)

# Computational Challenges

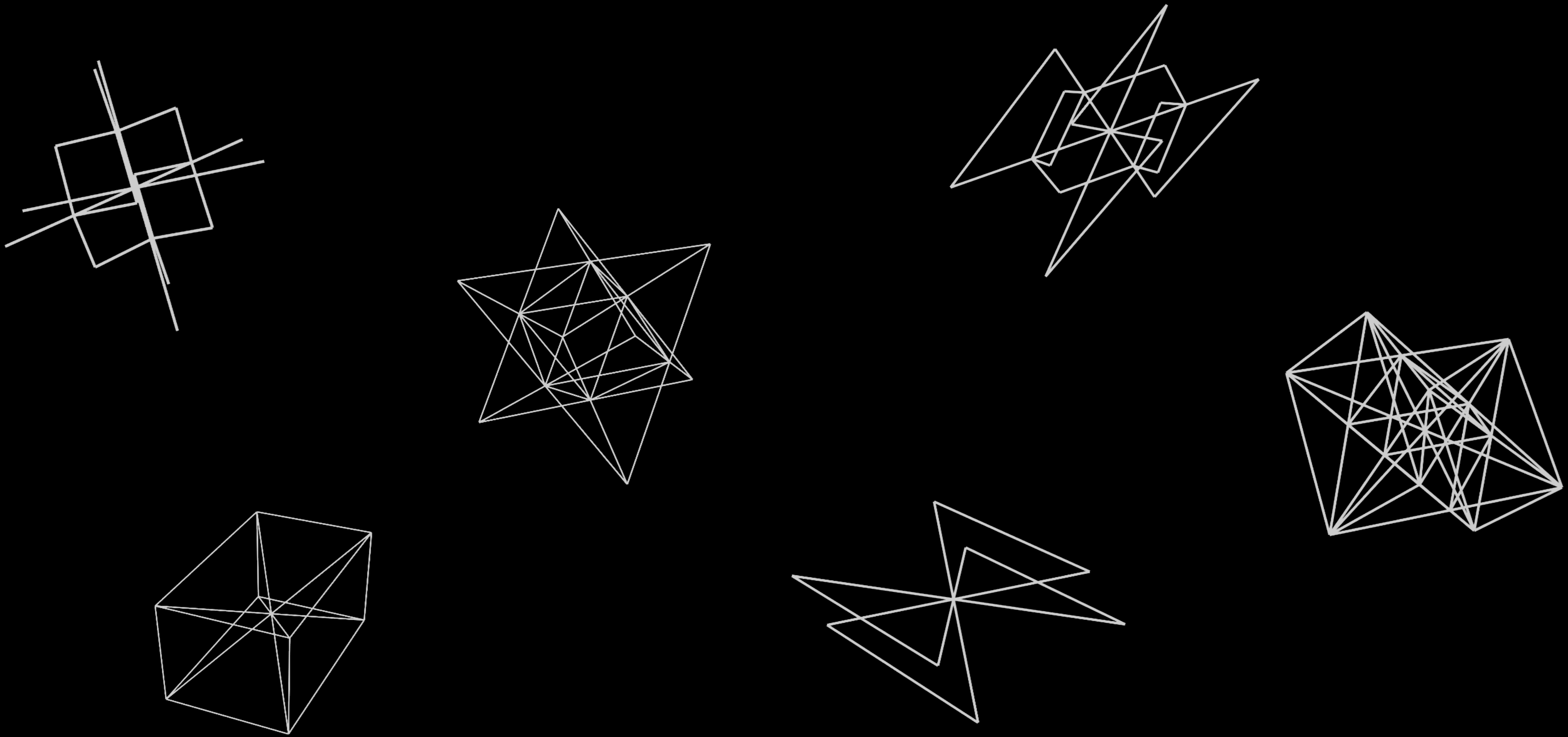



**<u>Inverse challenge</u>: predicting structures having target properties**

(trusses, plates, shells, non-periodic designs, composites, …)

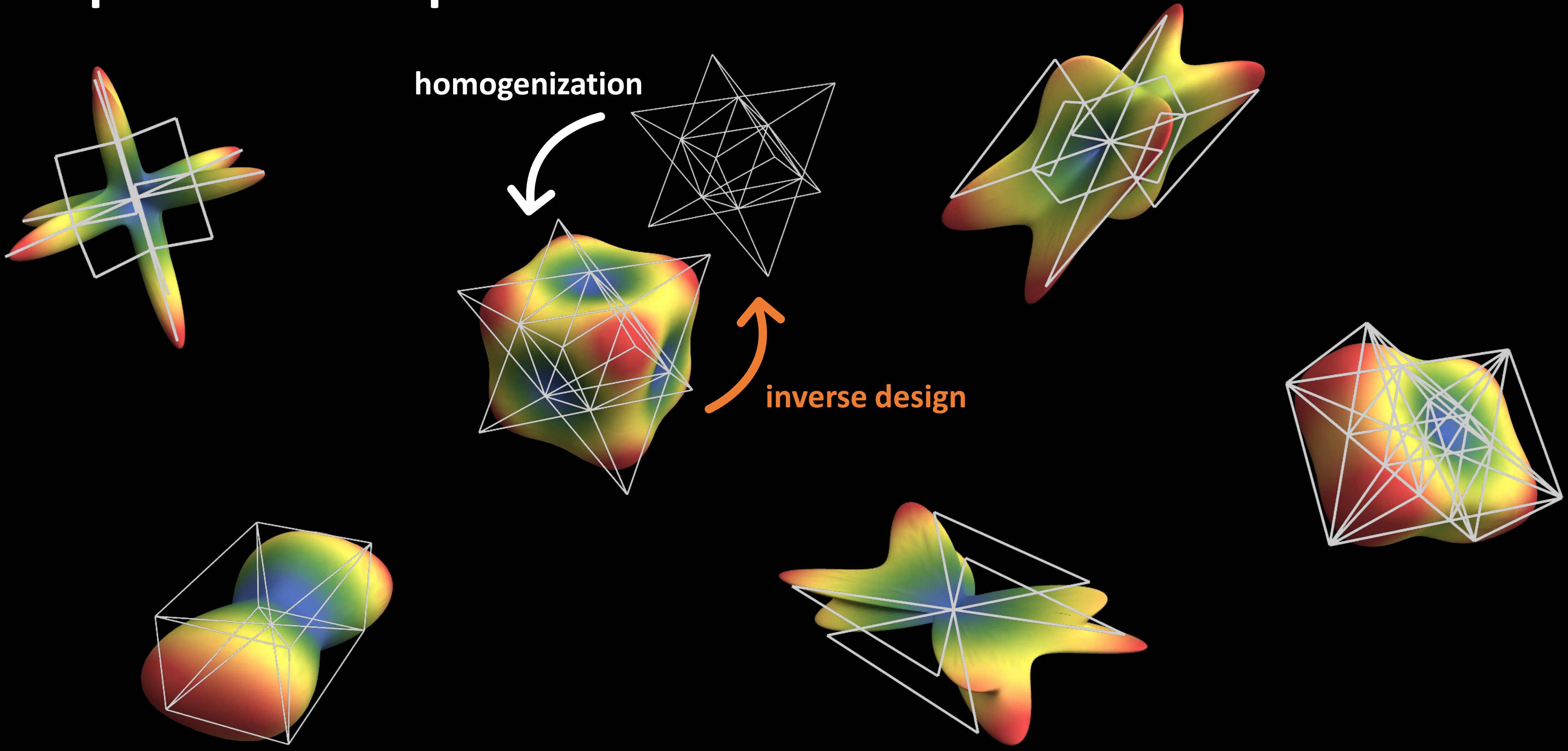


# Example: Anisotropic Unit Cells in 3D



(Bastek et al., PNAS 2022)

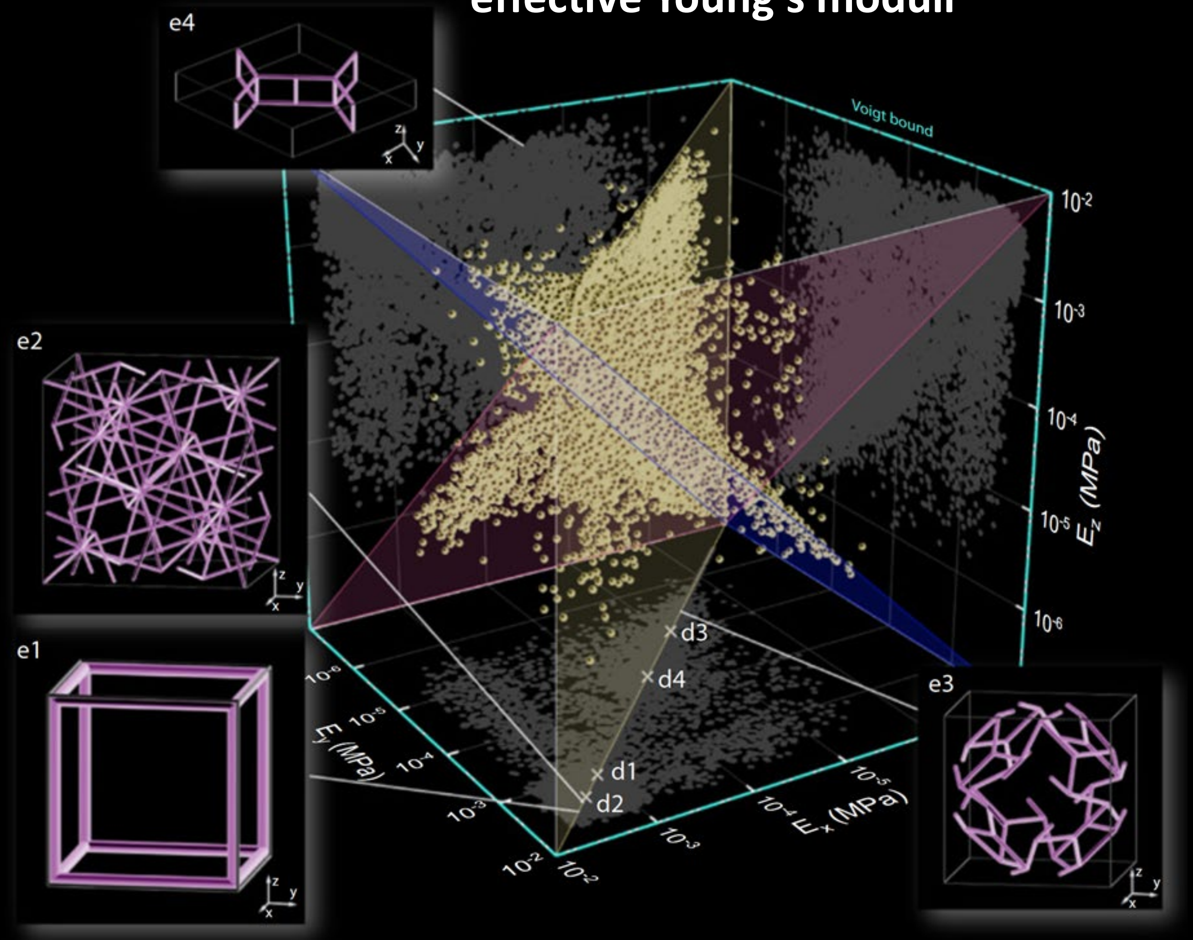
# Example: Anisotropic Unit Cells in 3D



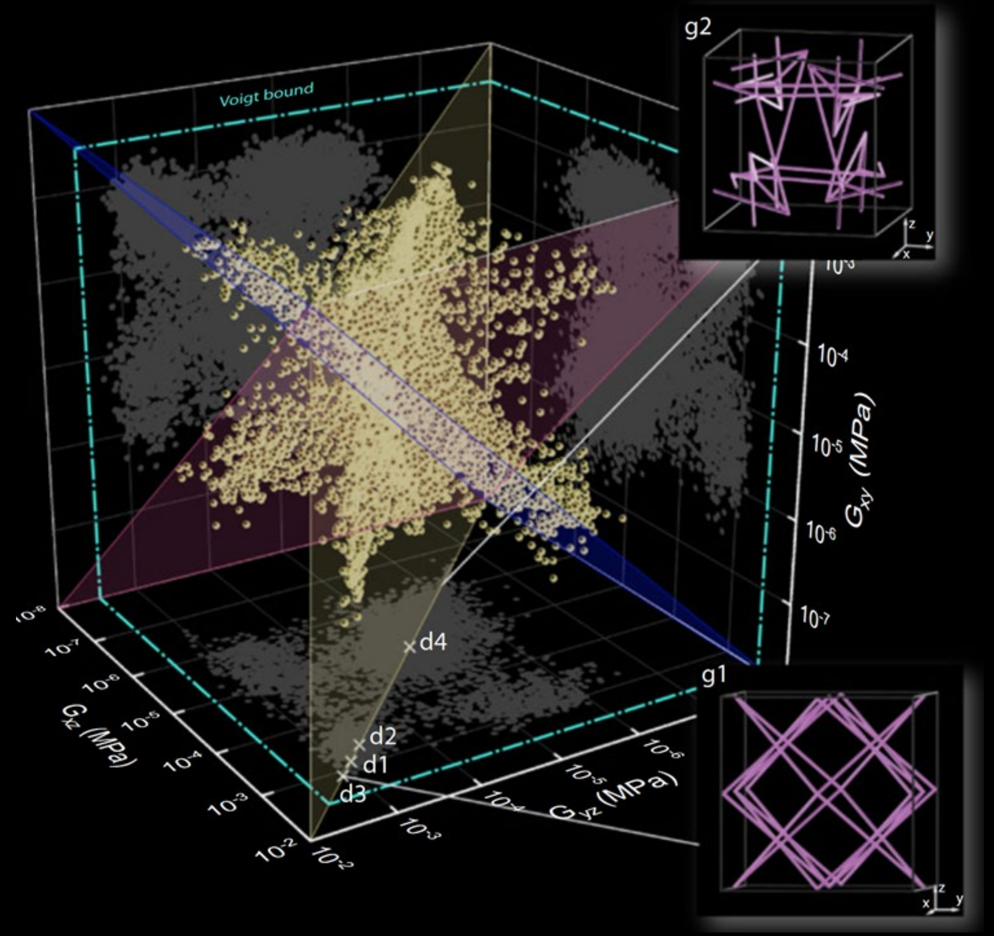

(Bastek et al., PNAS 2022)

# Example: Anisotropic Stiffness Space of Trusses

**effective Young's moduli**

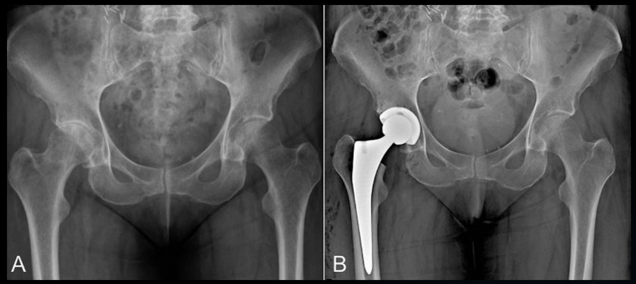


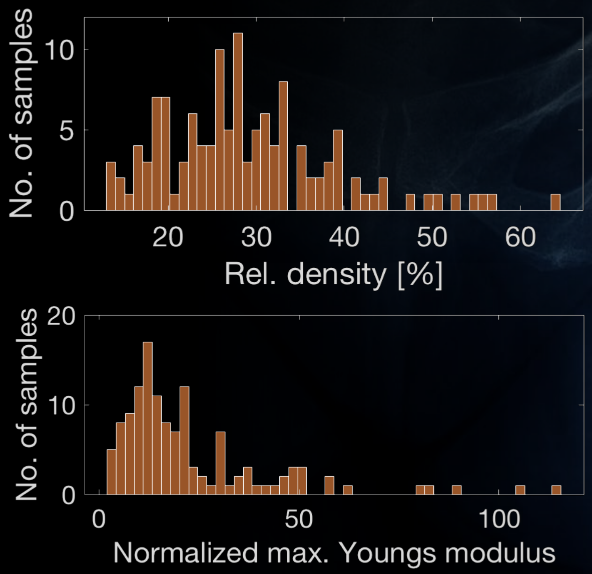

**effective shear moduli**



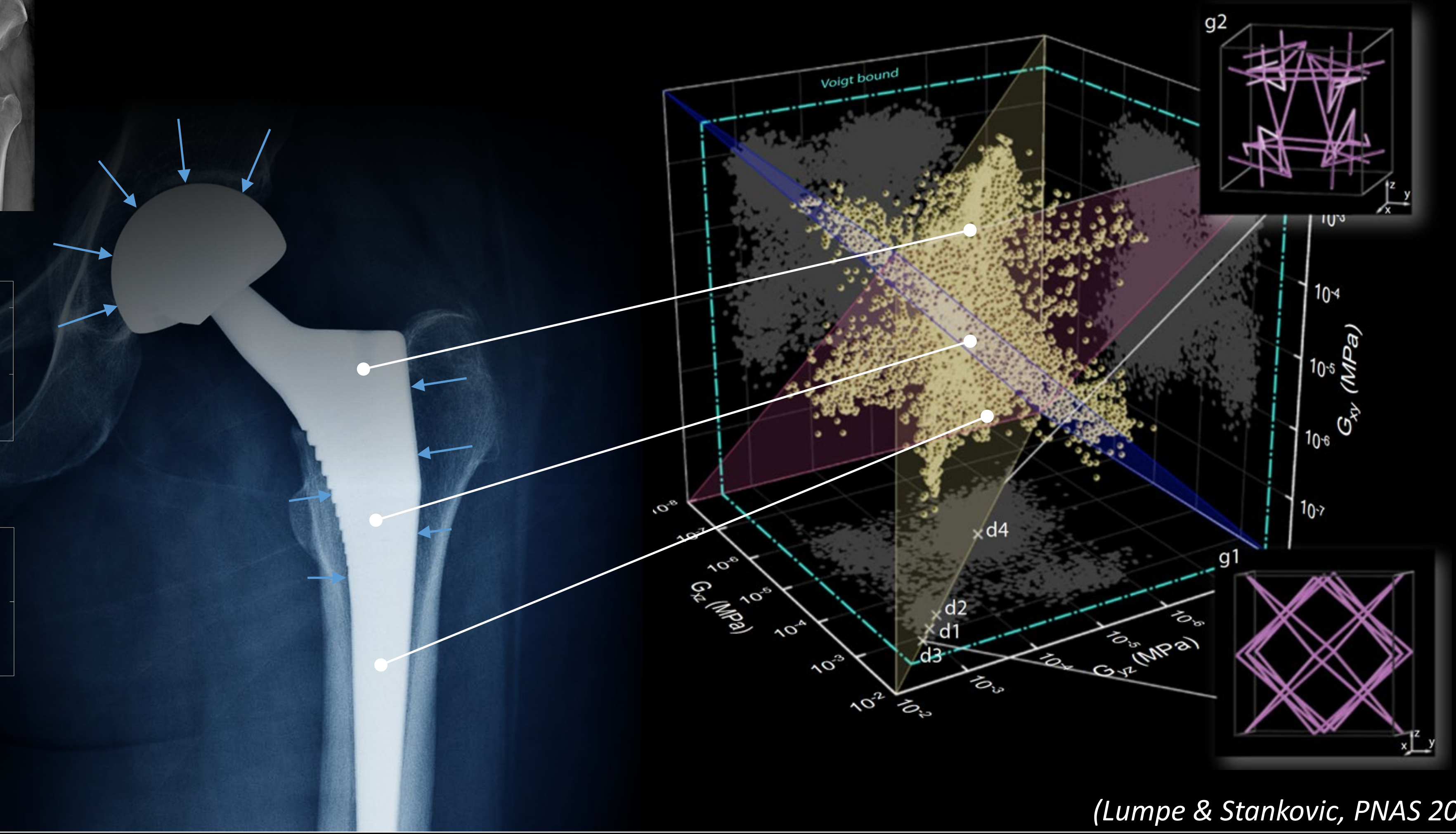

*(Lumpe & Stankovic, PNAS 2021)*

# Multiscale Design of Advanced Materials & Structures




effective shear moduli




(Marangalou et al., 2013; image: ChooChin/Shutterstock)

(Lumpe & Stankovic, PNAS 2021)

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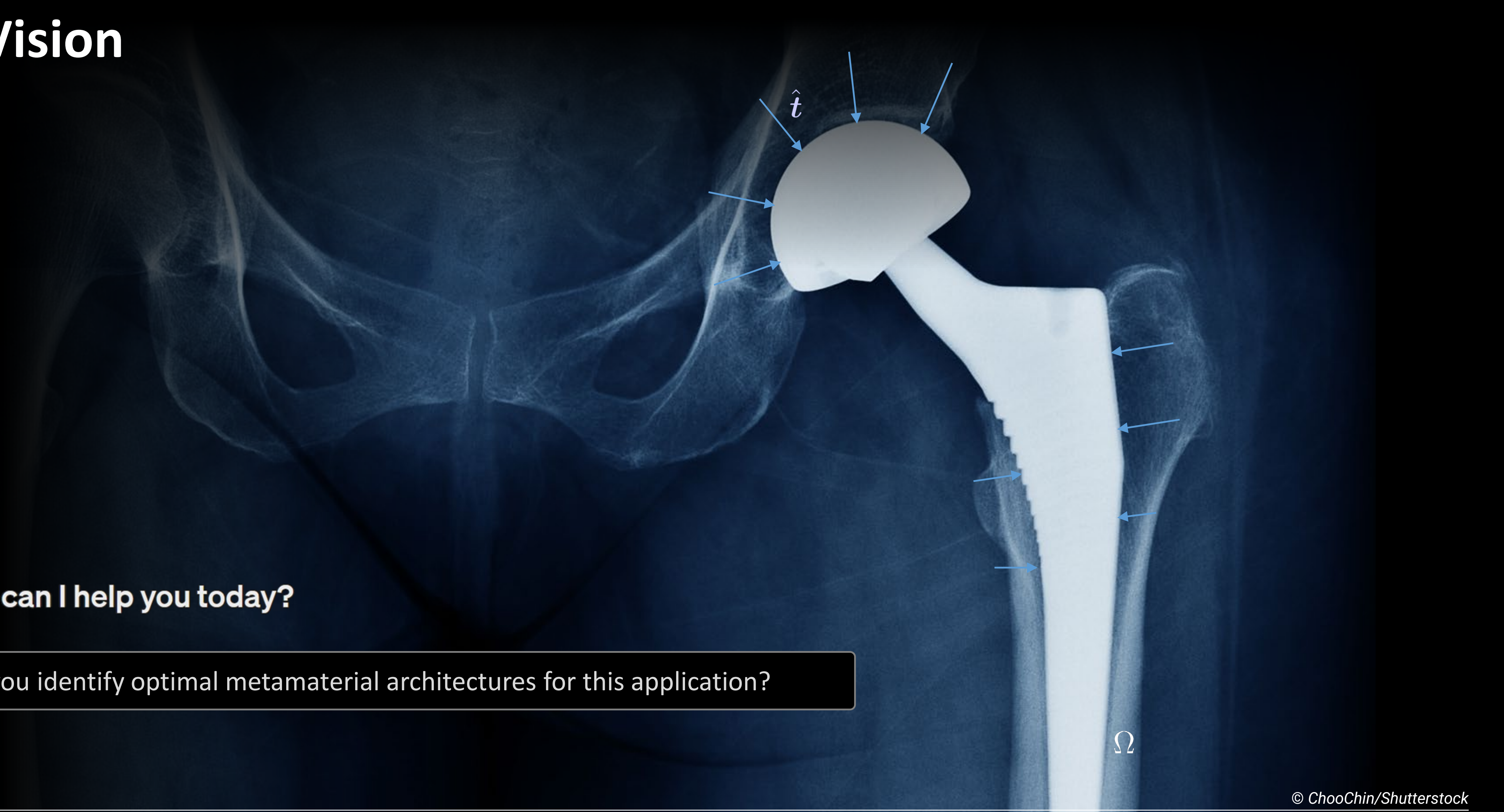
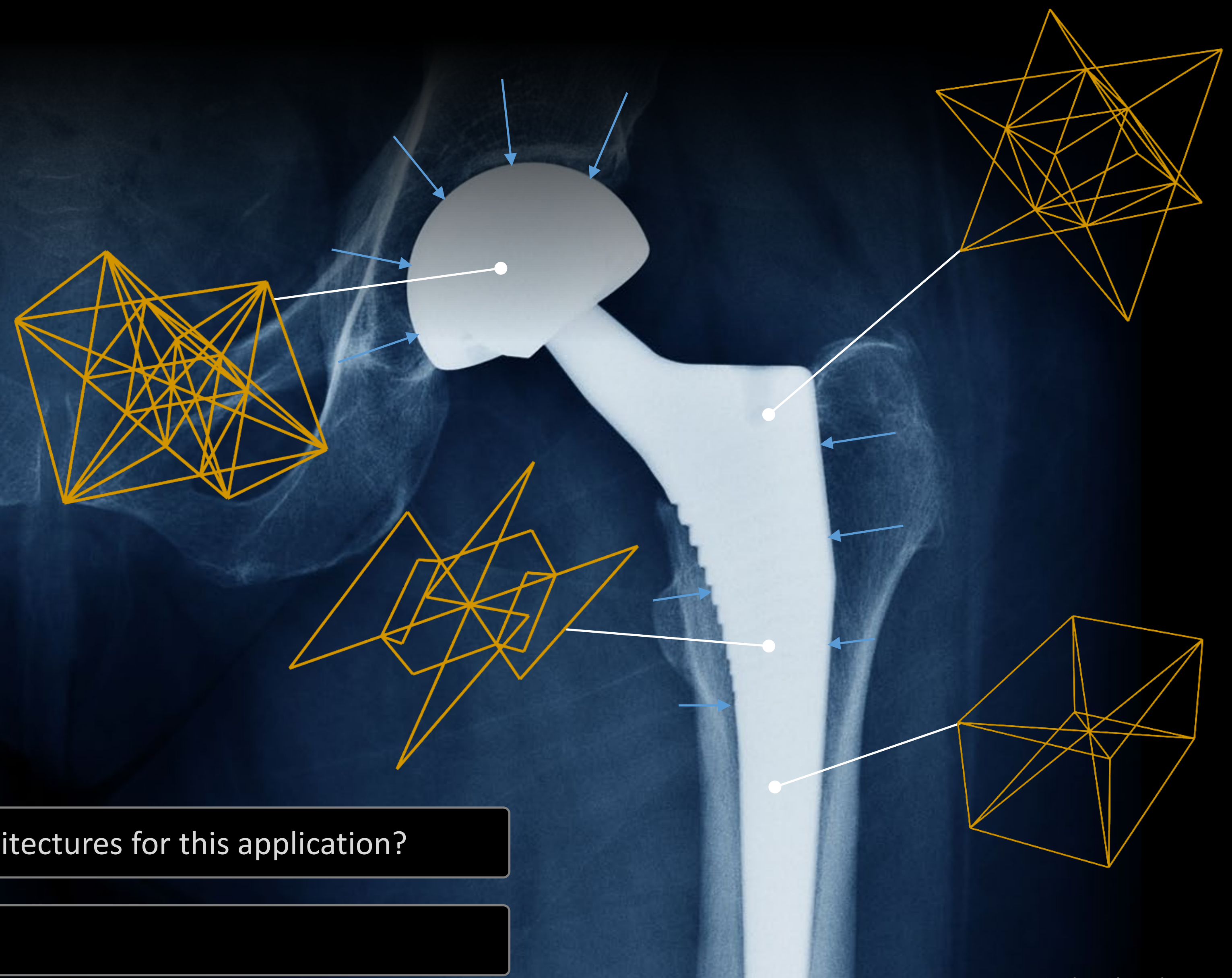
# The Vision




How can I help you today?

DK Can you identify optimal metamaterial architectures for this application?

# The Vision



How can I help you today?

DK Can you identify optimal metamaterial architectures for this application?

Of course, here you go.

# Multiscale Topology Optimization

*(recall also the presentation by Anthony Gravouil)*

## example: linear elastic compliance minimization

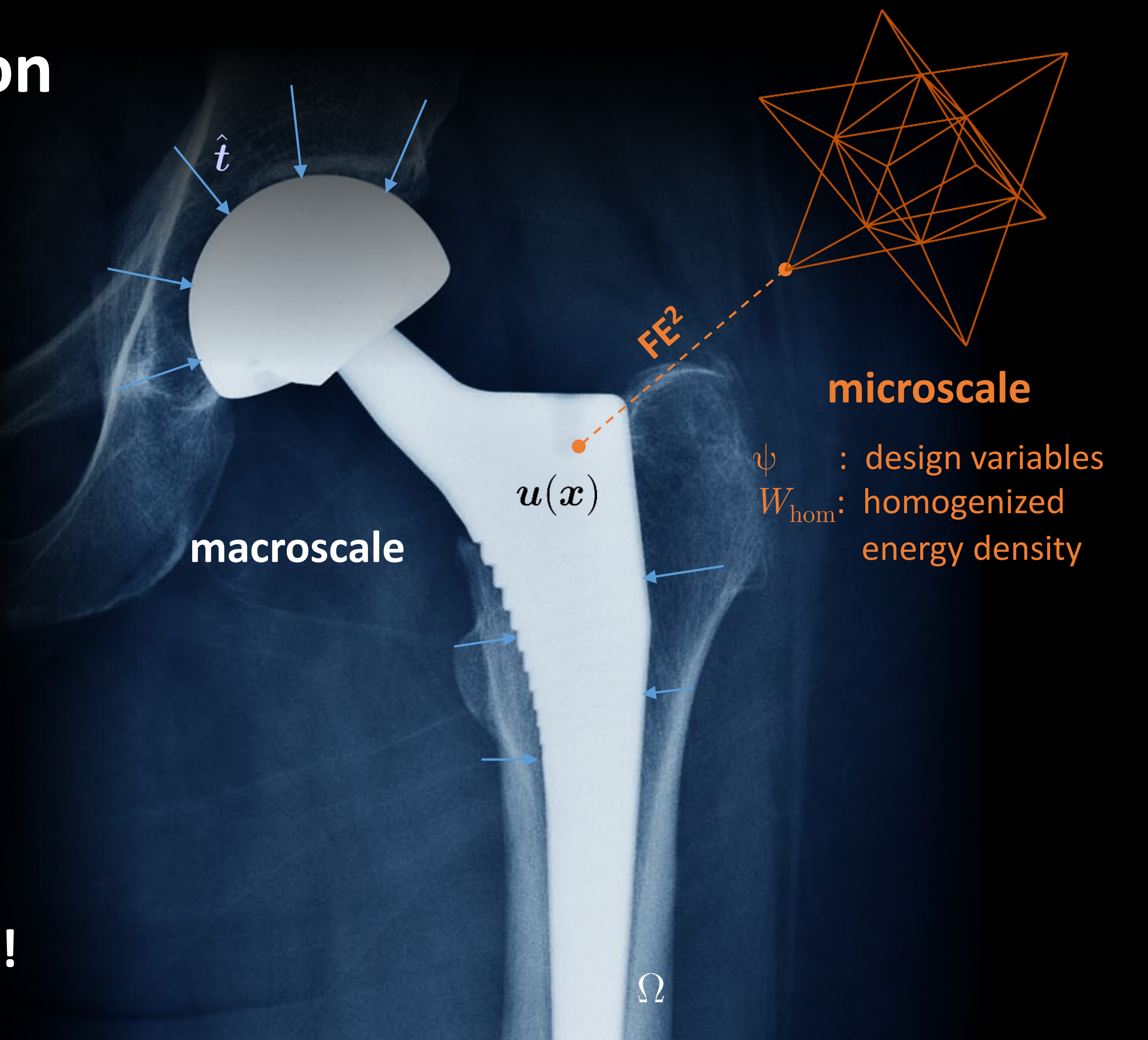
$$\min_{\psi(\boldsymbol{x})} \; : \; \mathcal{I}[\boldsymbol{u};\psi] = \int_\Omega \left( W_{\text{hom}}(\nabla \boldsymbol{u};\psi) + c||\nabla\psi||_p \right) \mathrm{d}V$$

$$\text{s.t.} \; : \; \int_\Omega W_{\text{hom}}(\nabla \boldsymbol{u};\psi)\,\mathrm{d}V = \int_{\partial\Omega_N} \hat{\boldsymbol{t}}\cdot\boldsymbol{u}\,\mathrm{d}S$$

$$: \; \int_\Omega \rho(\psi)\,\mathrm{d}V \le V_{\max}$$

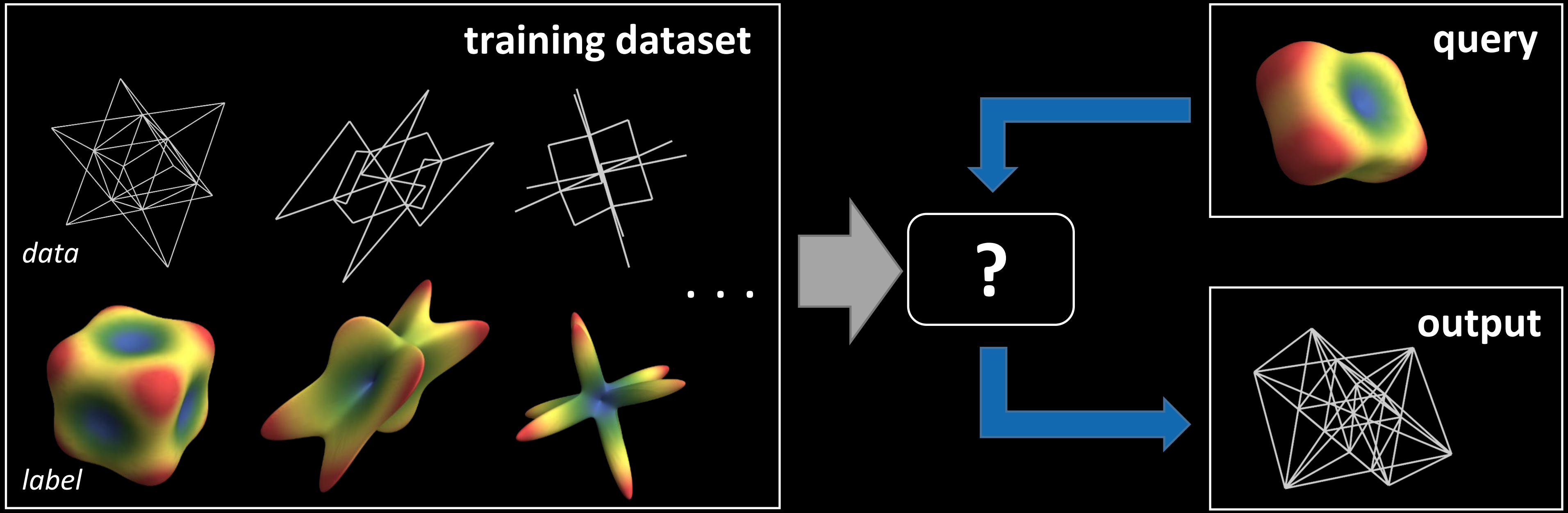
$$: \; \text{geometric/topological constraints}$$

**This is the classical approach (based on HI)!**



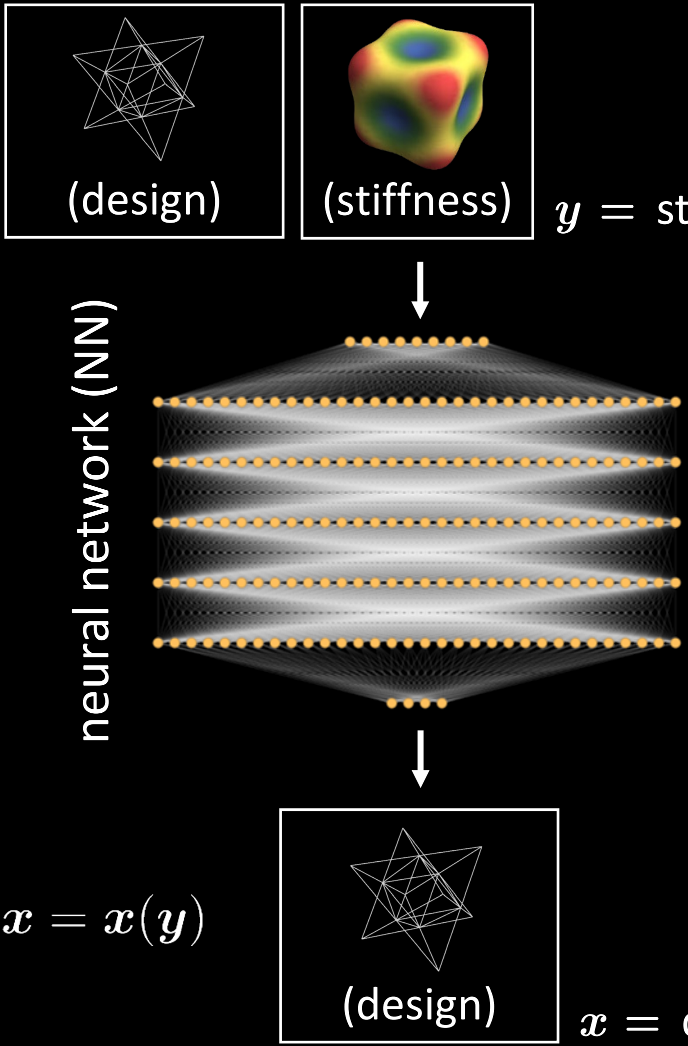

*(Telgen et al., J. Appl. Mech. 2022; Glaesener et al., IJSS 2019/2020 & JMPS 2021)*

# A Data-Driven Perspective (Based on AI)



# ML for the Inverse Design Challenge

$x'$




$y =$ stiffness

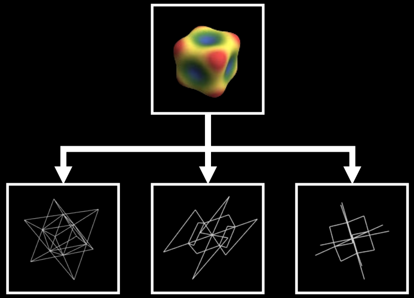
$$||x(y) - x'|| \rightarrow \min$$

**find:** $x = x(y)$

$x =$ design parameters (ODF)

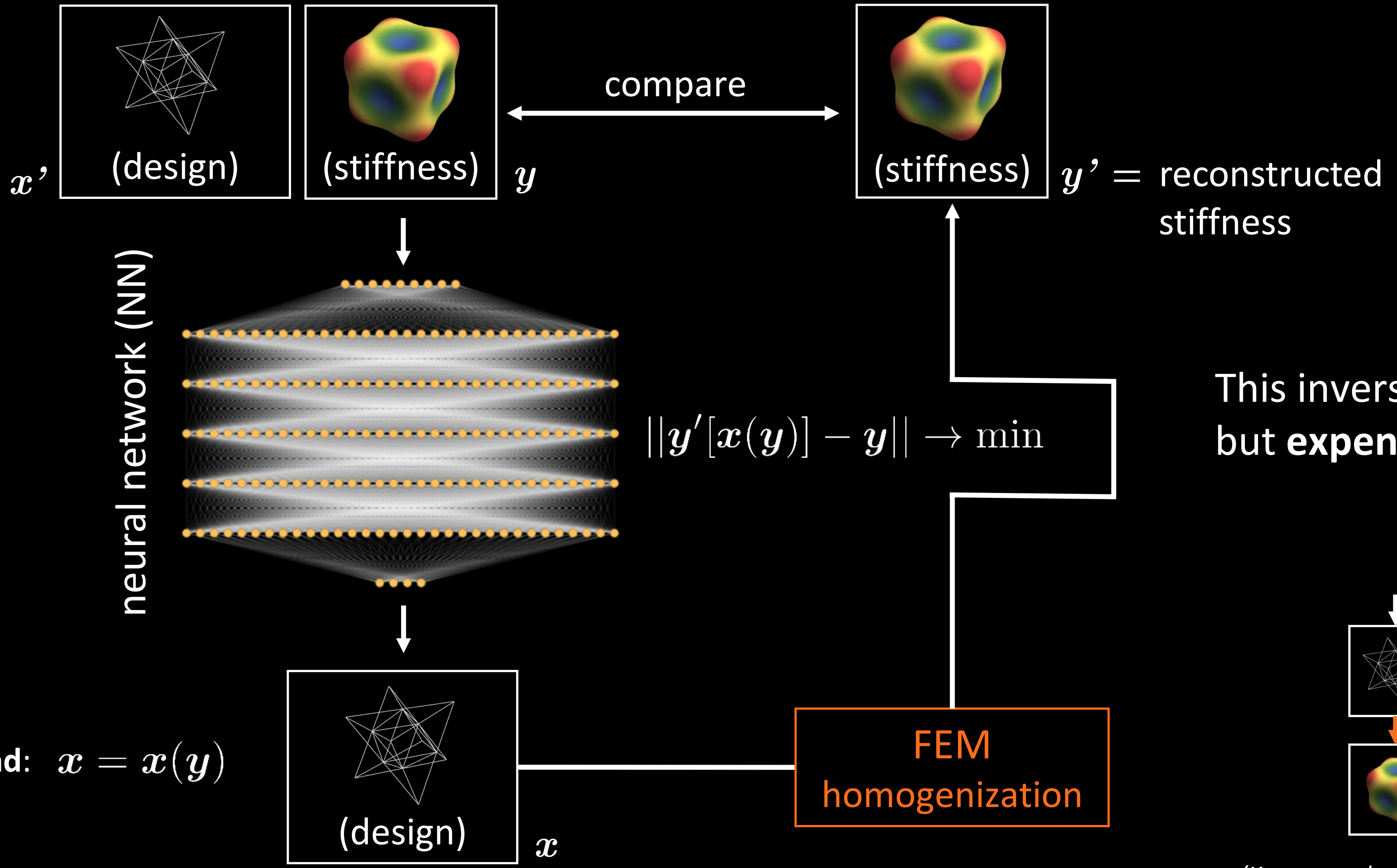
This inverse problem is **ill-posed**.

**Why?** Multiple topologies may have the same/similar stiffness

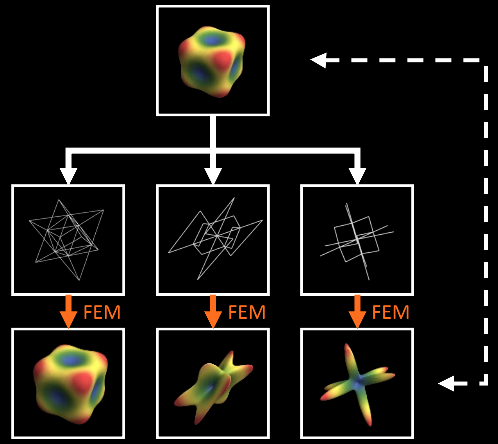


*(Kumar et al., npj Comput. Mater. 2020; Bastek et al., PNAS 2022)*

# ML for the Inverse Design Challenge

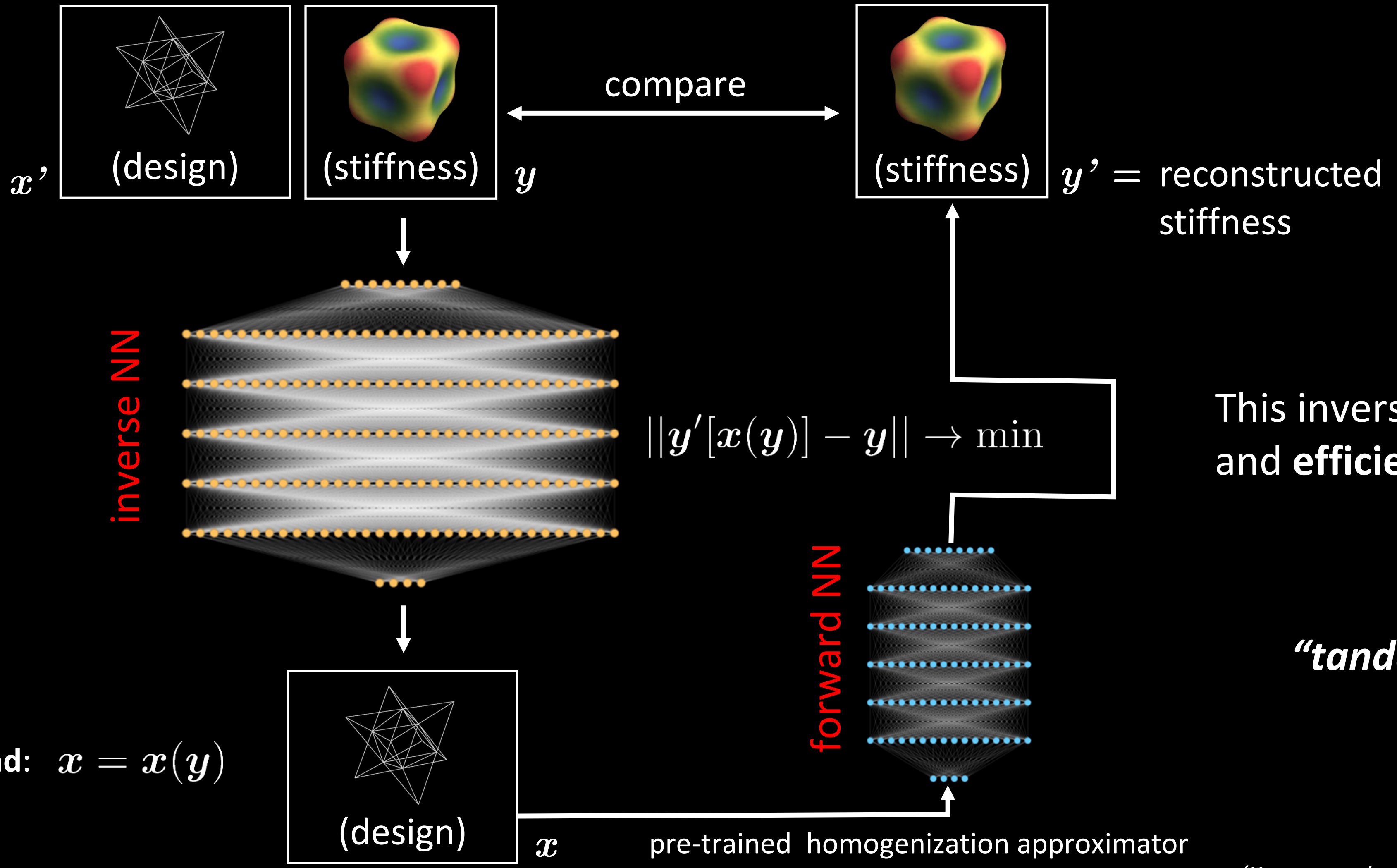



This inverse problem is **well-posed** but **expensive**.




(Kumar et al., *npj Comput. Mater.* 2020; Bastek et al., *PNAS* 2022)

# ML for the Inverse Design Challenge

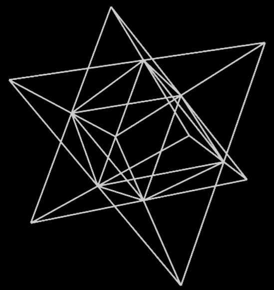



This inverse problem is **well-posed** and **efficient**.

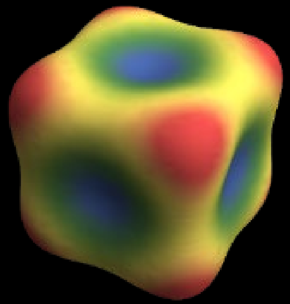
***"tandem neural network" approach***

*(Kumar et al., npj Comput. Mater. 2020; Bastek et al., PNAS 2022)*

# ML for the Inverse Design Challenge



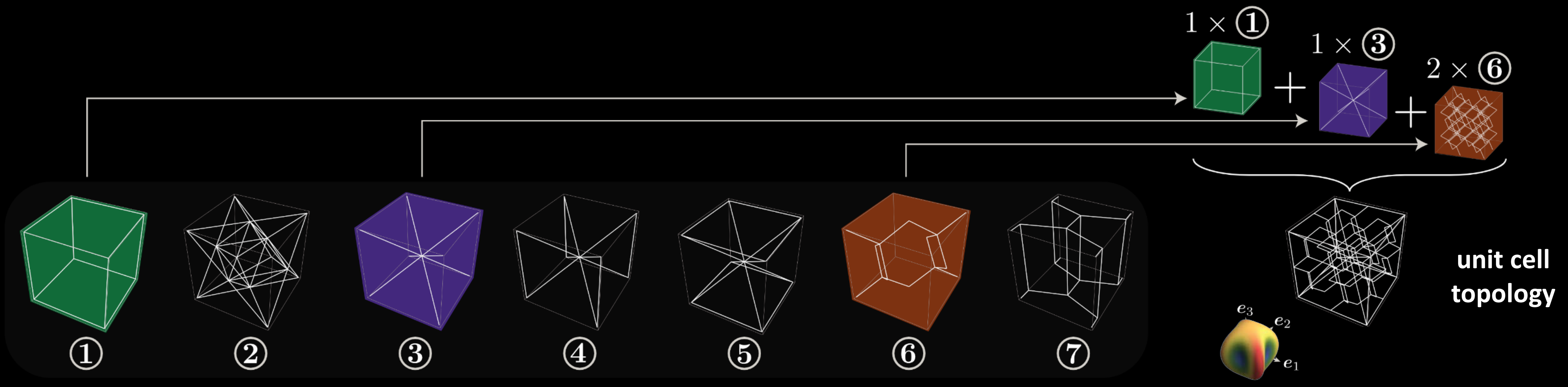
design space



property space

**Required is an *efficient* parameterization of the design space**
(geometry, topology, etc.).

# Parameterization Example #1: Beam-Based Unit Cells




**design variables:** elementary topologies + rotations + stretches

*(Bastek et al., PNAS 2022)*

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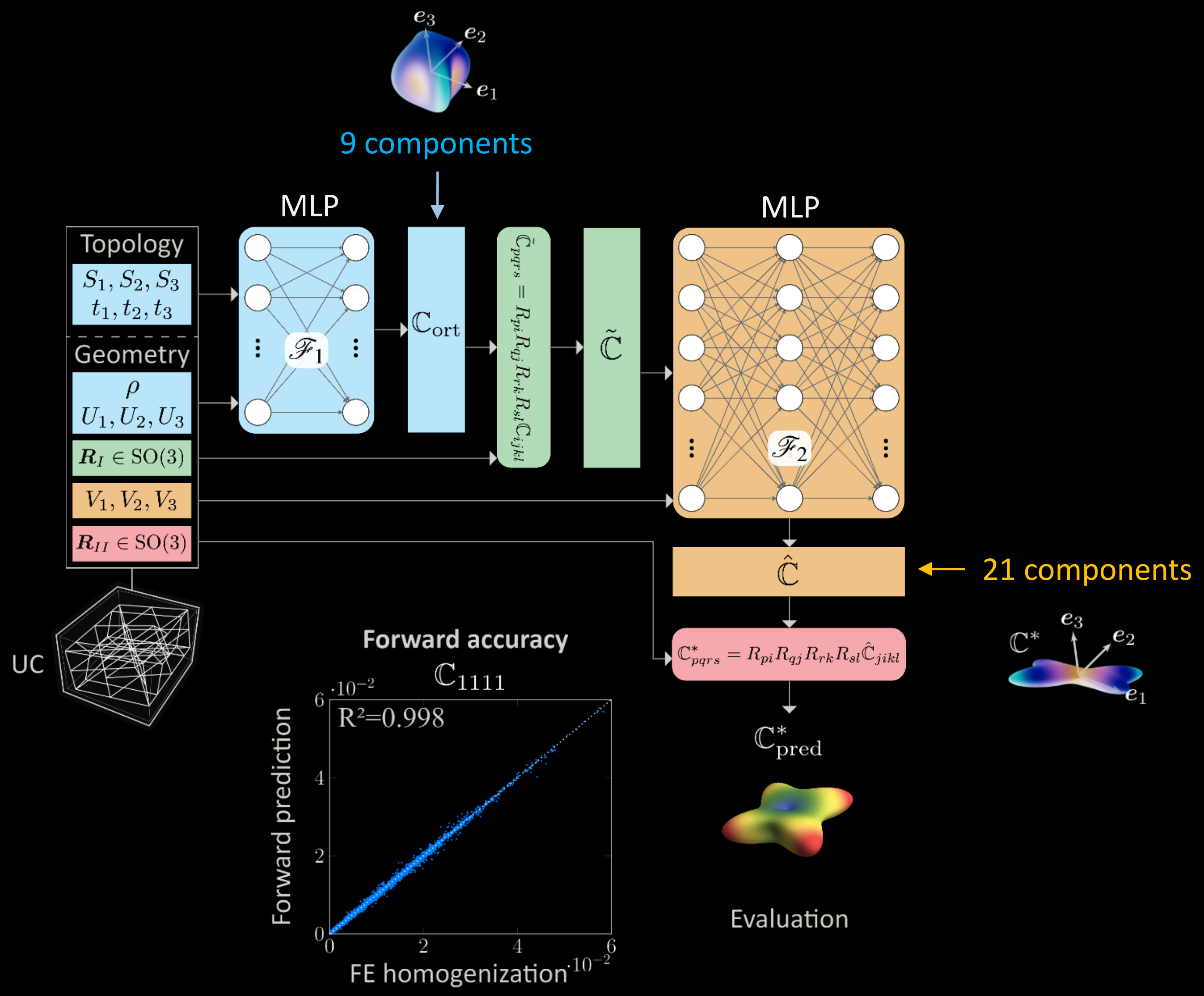
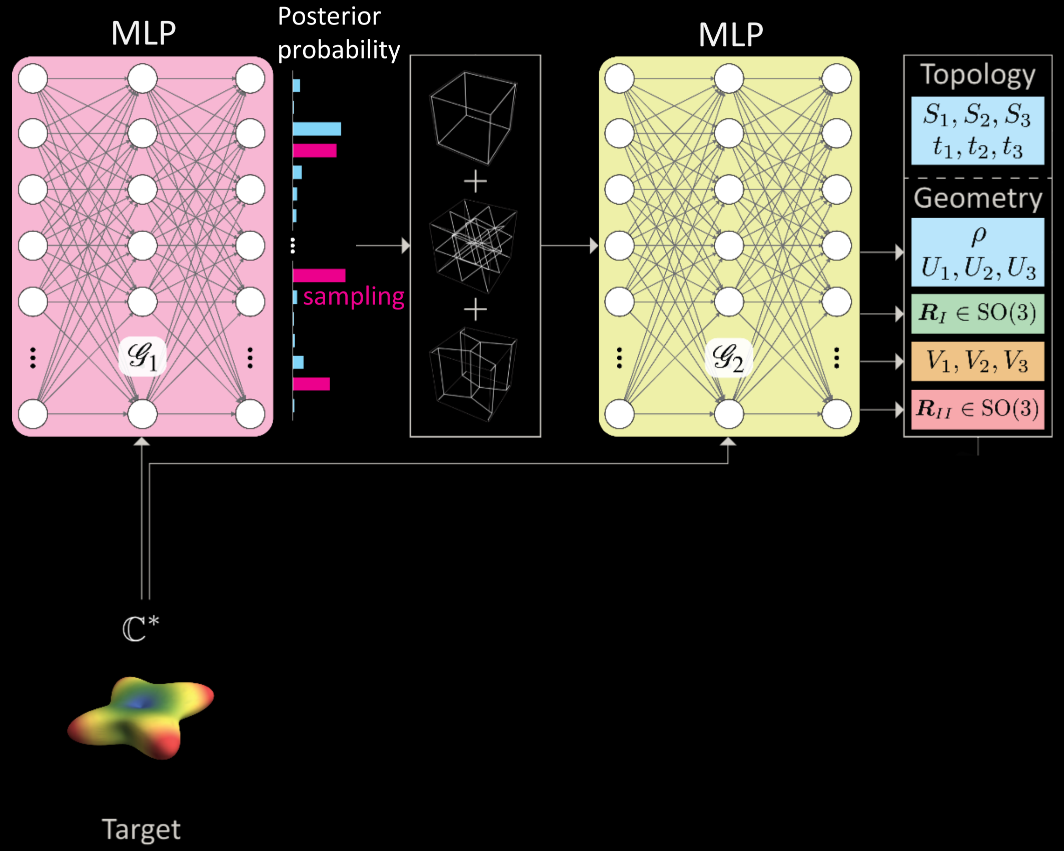
# The Forward Model



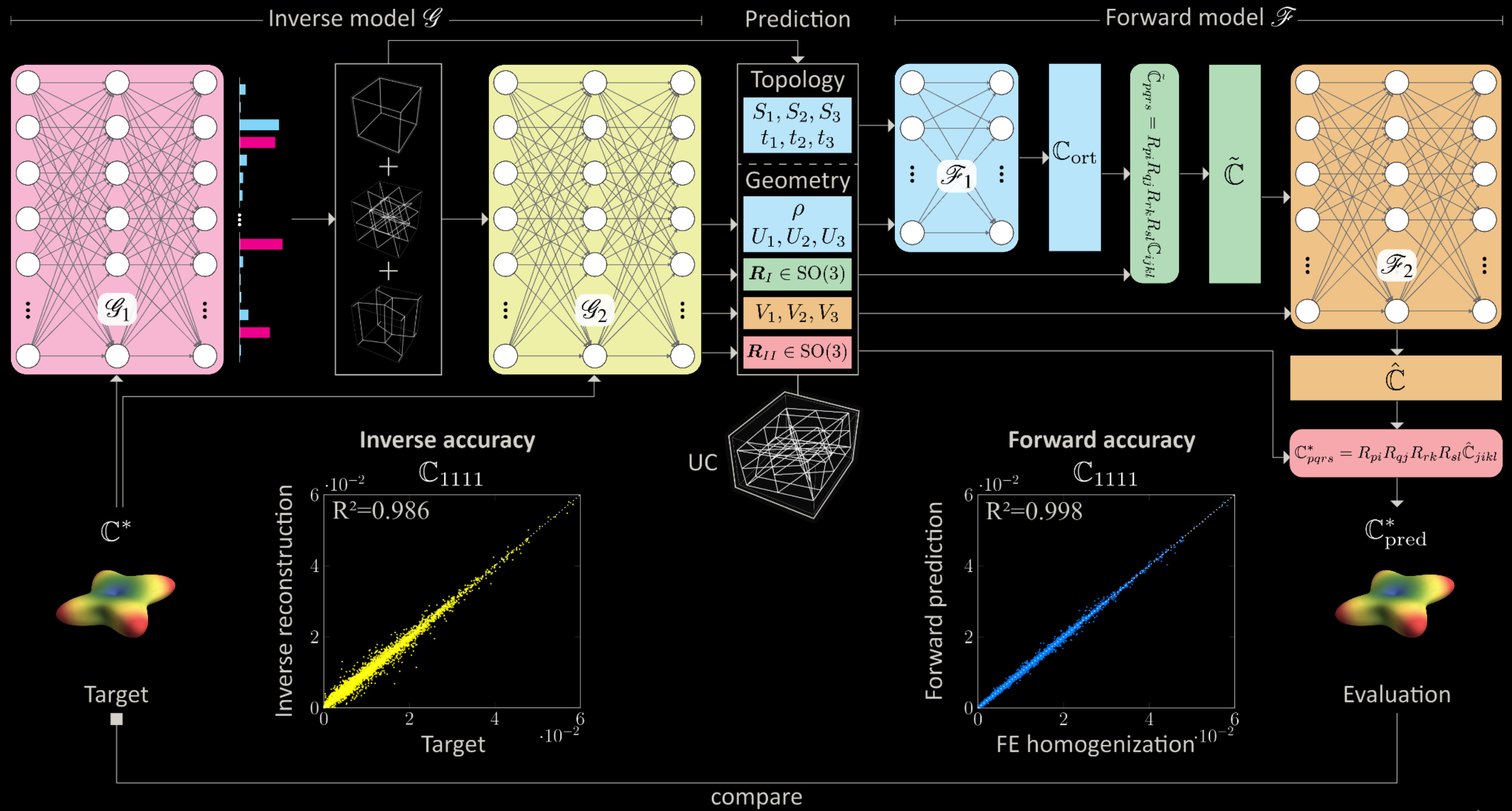

(Bastek et al., PNAS 2022)

# The Inverse Model




(Bastek et al., PNAS 2022)

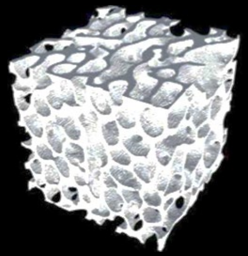
# The Full Model



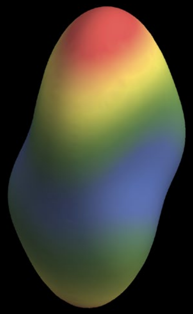

(Bastek et al., PNAS 2022)

# Application to Bone Implants

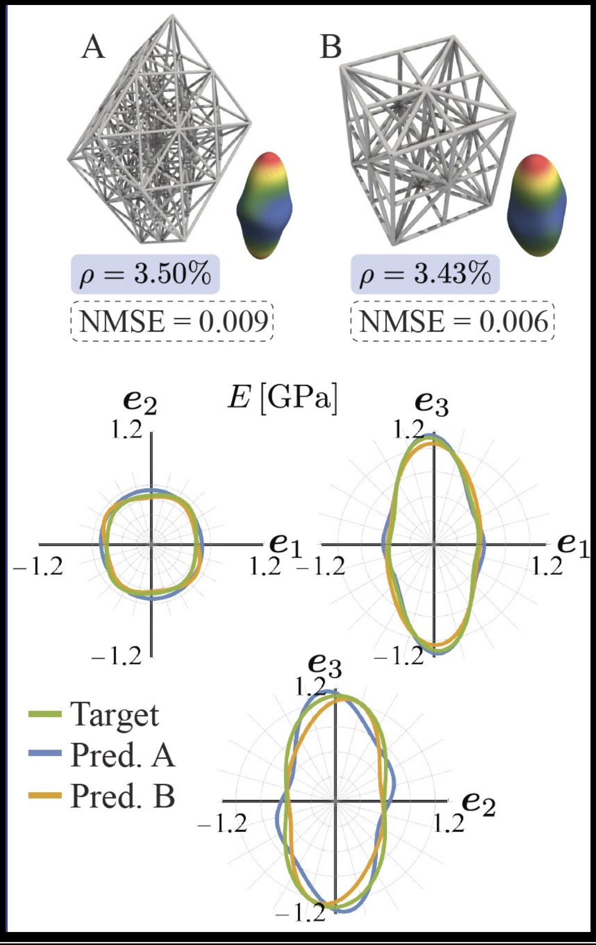
**Input:**



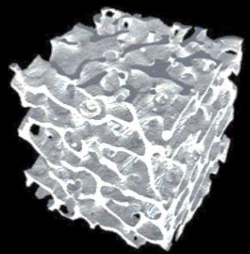
**Trabecular bone topology**
(Colabella et al., 2017, sample #3)



**Predictions:**

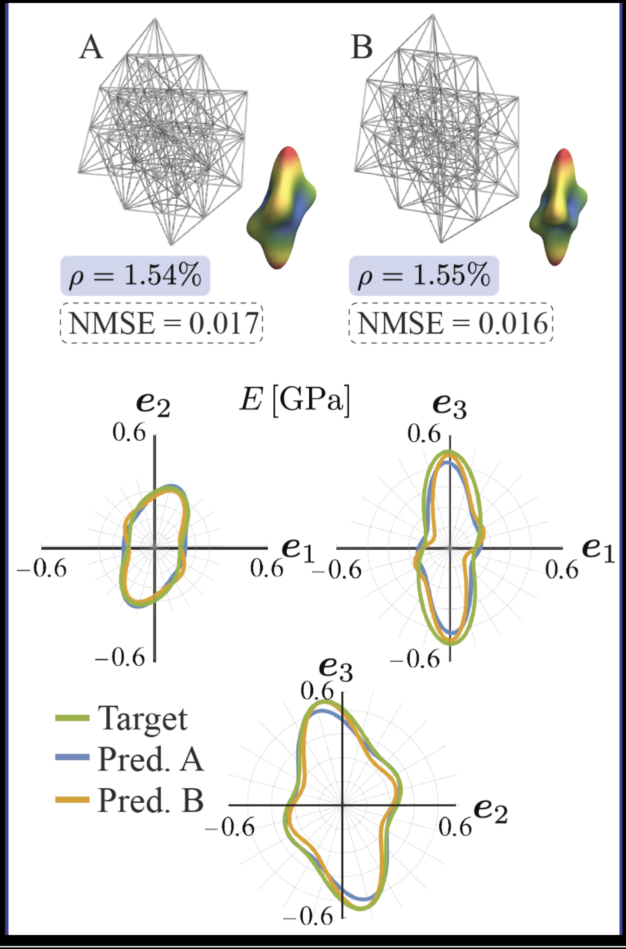



**Input:**



**Trabecular bone topology**
(Colabella et al., 2017, sample #4)

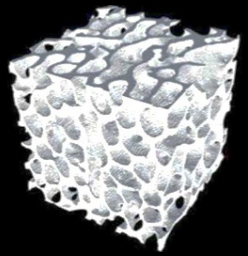
**Predictions:**




*(Bastek et al., PNAS 2022)*

# Application to Bone Implants

**Input:**



**Trabecular bone topology**
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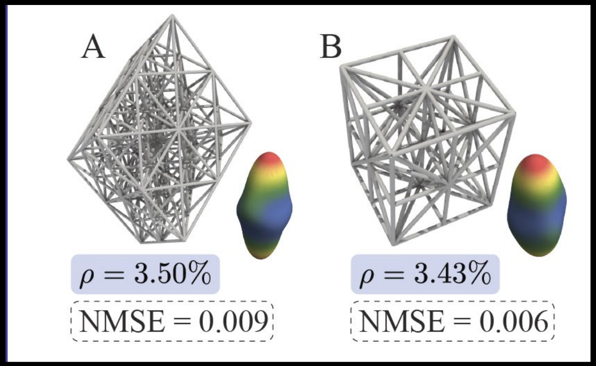
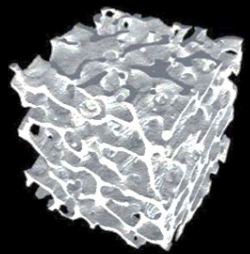
**Predictions:**




**Input:**



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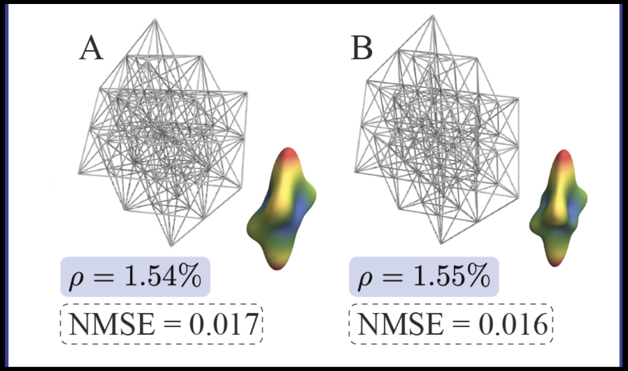
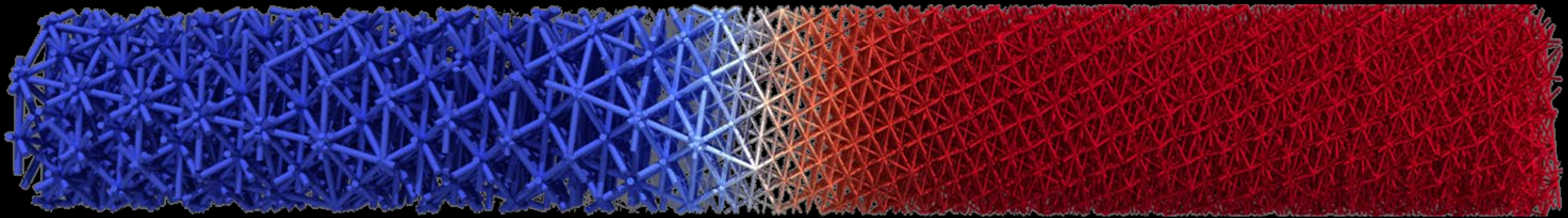
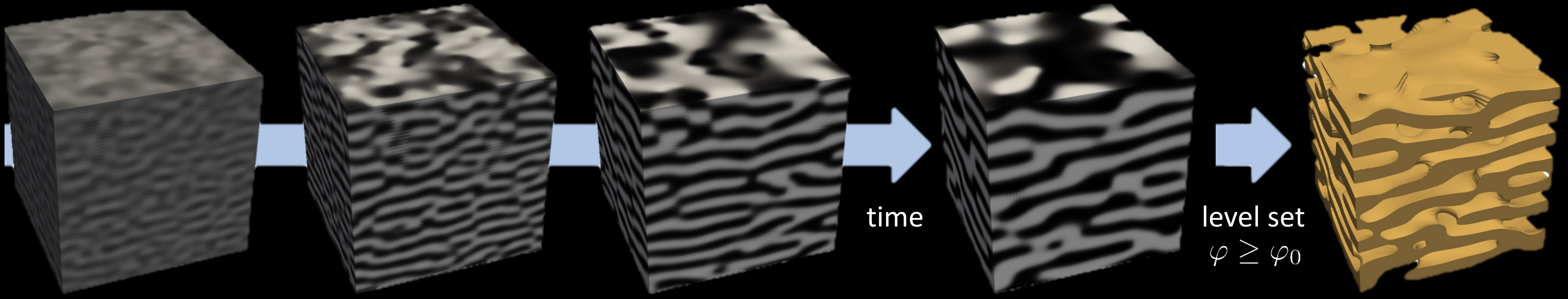


**What about designs that go beyond beams?**

*(Bastek et al., PNAS 2022)*

# Diffusion-Driven Phase Separation




Cahn-Hilliard equation
(linear Fourier expansion)

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

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

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

level set

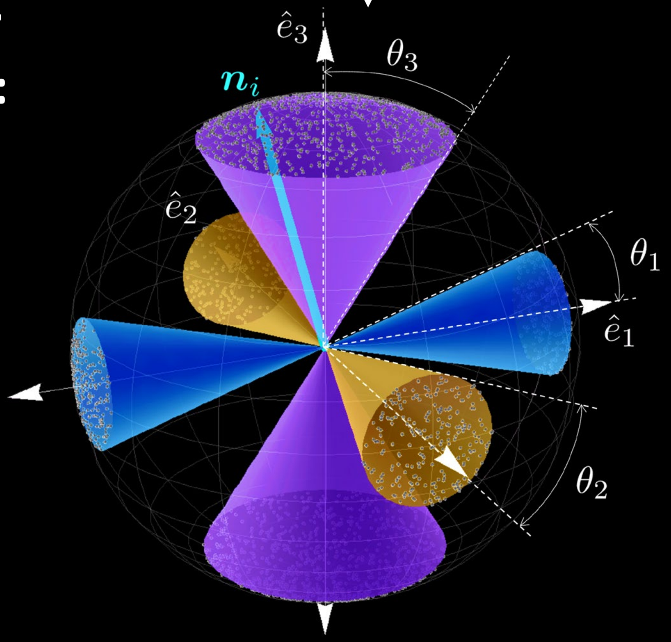
*(Cahn, J. Chem. Phys. 1965; Soyarslan et al., Acta Mater 2018)*

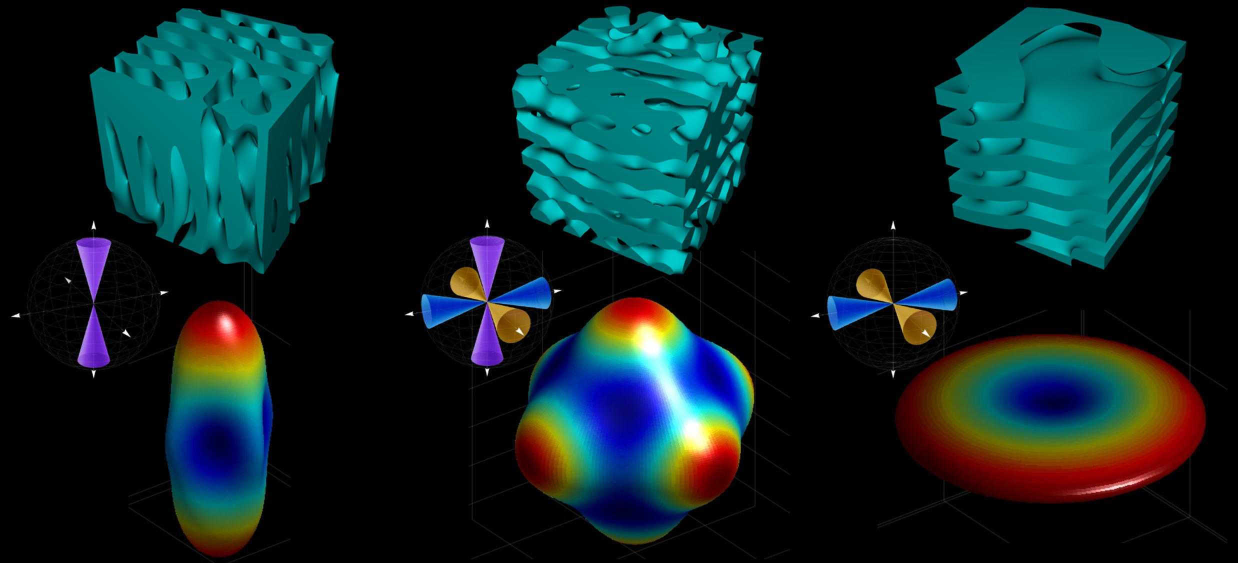
# Parameterization Example #2: Spinodoid Architectures

**anisotropic Gaussian random field (GRF):**

$$\varphi(\boldsymbol{x}) = \sqrt{\frac{2}{N}} \sum_{i=1}^{N} \cos\left(\boldsymbol{n}_i \cdot \boldsymbol{x} - \gamma_i\right) \geq \varphi_0$$

**wave vector distribution:**



columnar | cubic | lamellar

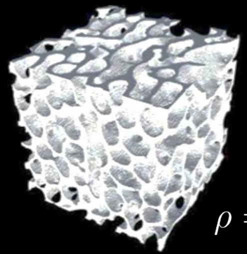
**design parametrization:**

- $\theta_1$: half-angle of cone about $x$-axis
- $\theta_2$: half-angle of cone along $y$-axis
- $\theta_3$: half-angle of cone along $z$-axis
- $\varphi_0$: relative density

*(Kumar et al., npj Comput. Mater. 2020)*

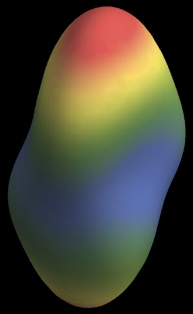
# Bone Implants (Revisited)

**Input:**



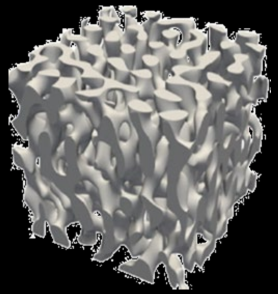
$\rho = 30\%$

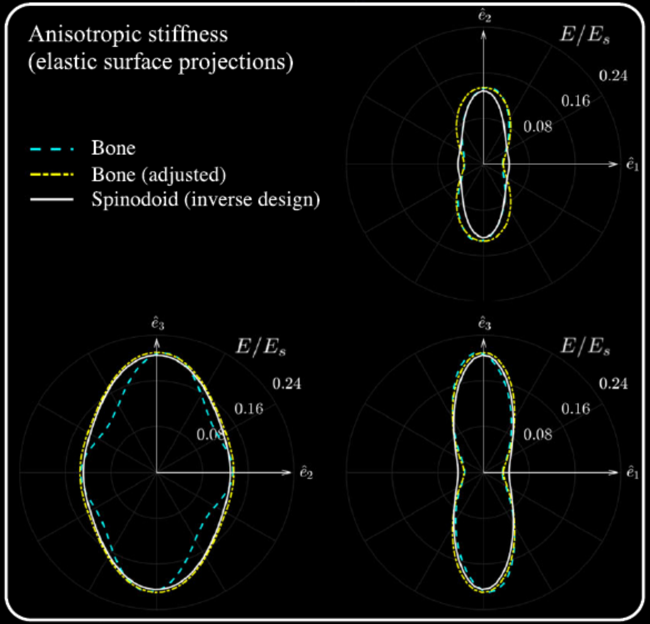
**Trabecular bone topology**
(Colabella et al., 2017, sample #3)



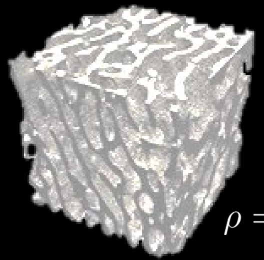
**Prediction:**

$$\rho = 31\%$$
$$\theta_1 = 51.4^\circ$$
$$\theta_2 = 44.1^\circ$$
$$\theta_3 = 0^\circ$$



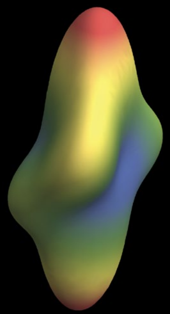



**Input:**



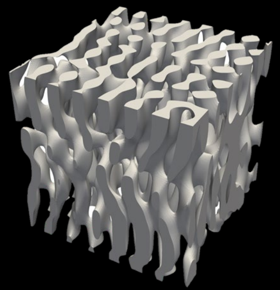
$\rho = 38\%$

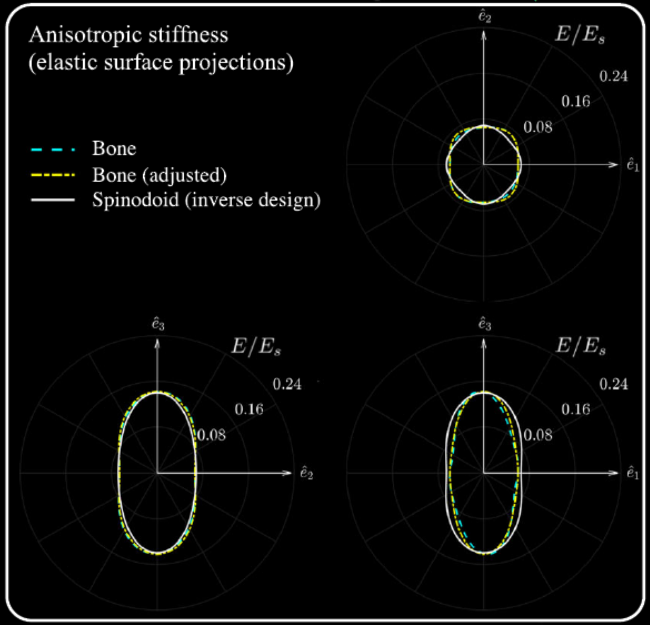
**Trabecular bone topology**
(Colabella et al., 2017, sample #4)



**Prediction:**

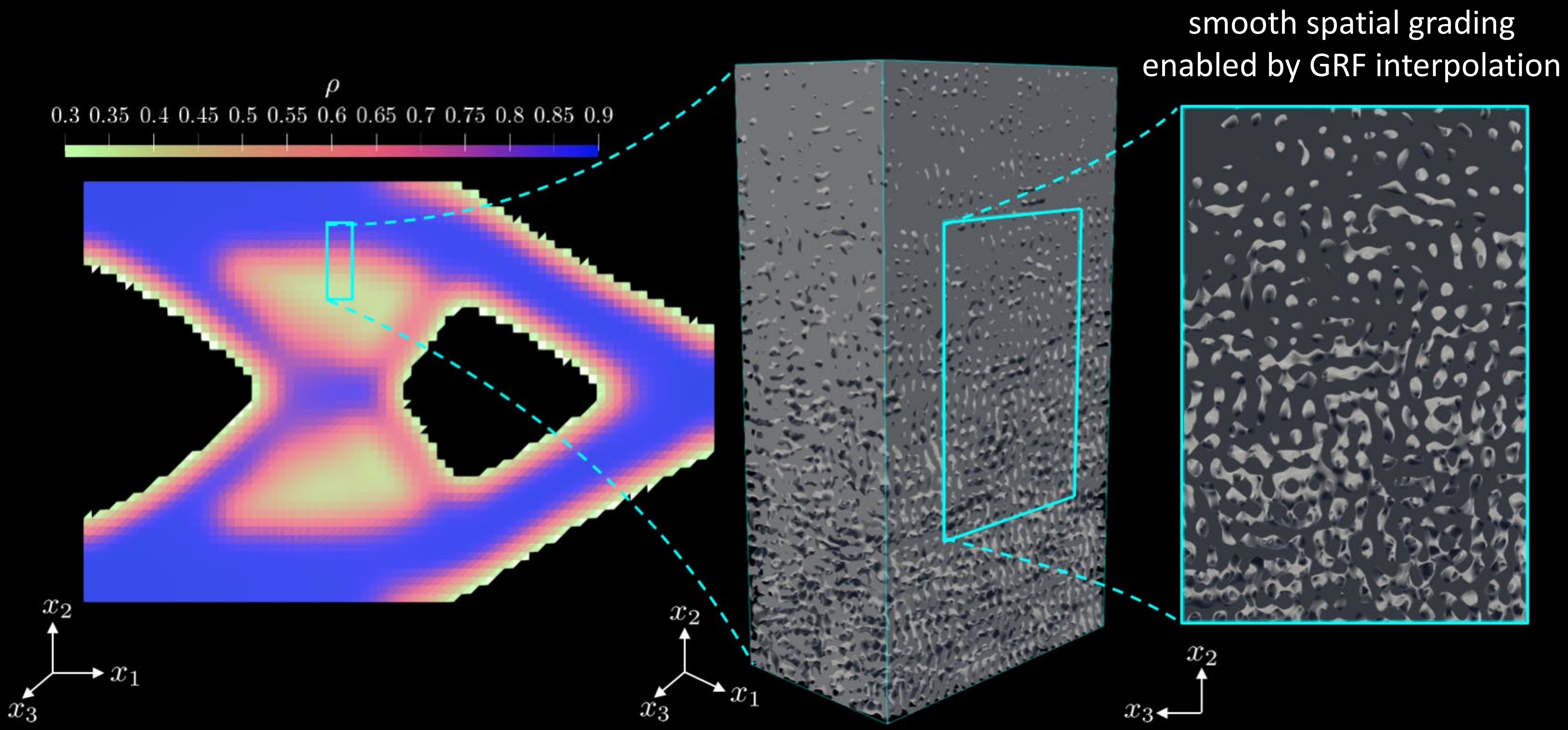
$$\rho = 34\%$$
$$\theta_1 = 36.8^\circ$$
$$\theta_2 = 15.0^\circ$$
$$\theta_3 = 0^\circ$$






*(Kumar et al., npj Comput. Mater. 2020)*

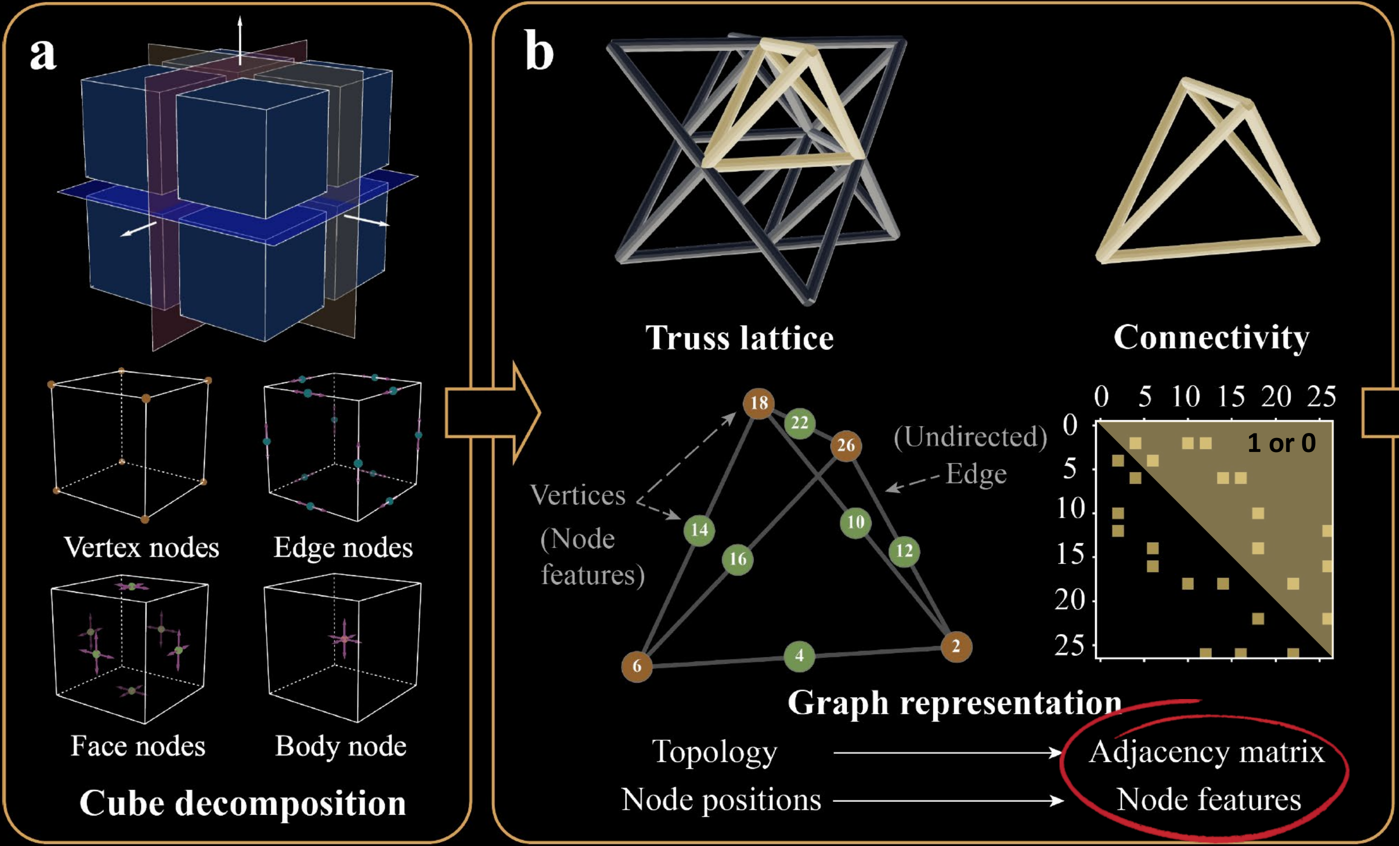
# Application to Multiscale Topology Optimization




(Li et al., CMAME 2021)

# What about generative design?

# Parameterization Example #3: General Beam Networks




**dataset generation:**

- start with classical designs (octet, bcc, …)
- **perturbations** of node positions within their admissible face/edge/volume
- **inserting and removing nodes** (and adding/removing connections)

$\Rightarrow$ 965,736 unique structures (fixed density)

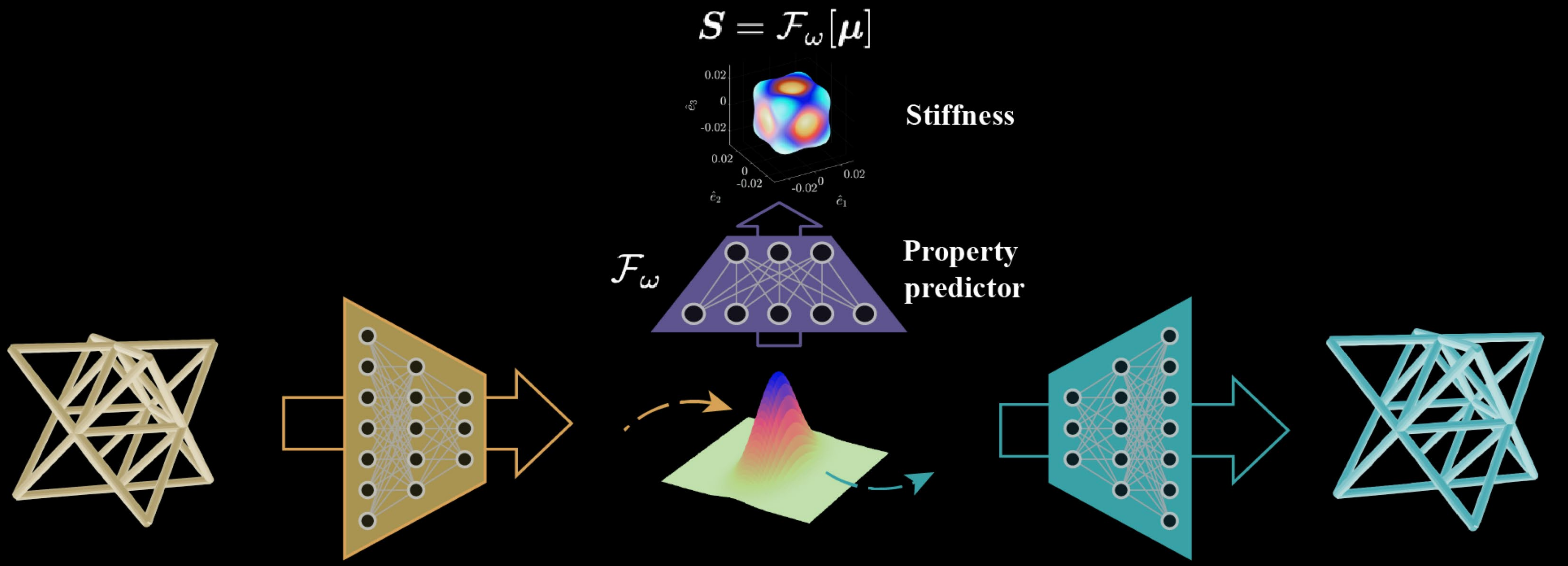
**challenges:**

- **high-dimensional** design space
- **discrete combinatorial** space

**design parameterization**: node positions $x$, adjacency matrix $A$

(Zheng et al., Nat. Comm. 2023)

# Variational Autoencoder for Beam Networks




**input** lattice:

$\boldsymbol{G} = (\boldsymbol{x}, \boldsymbol{A}) \in \mathbb{R}^N$

**encoding**

**latent distribution:**

$\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{G}}, \boldsymbol{\sigma}_{\boldsymbol{G}})$

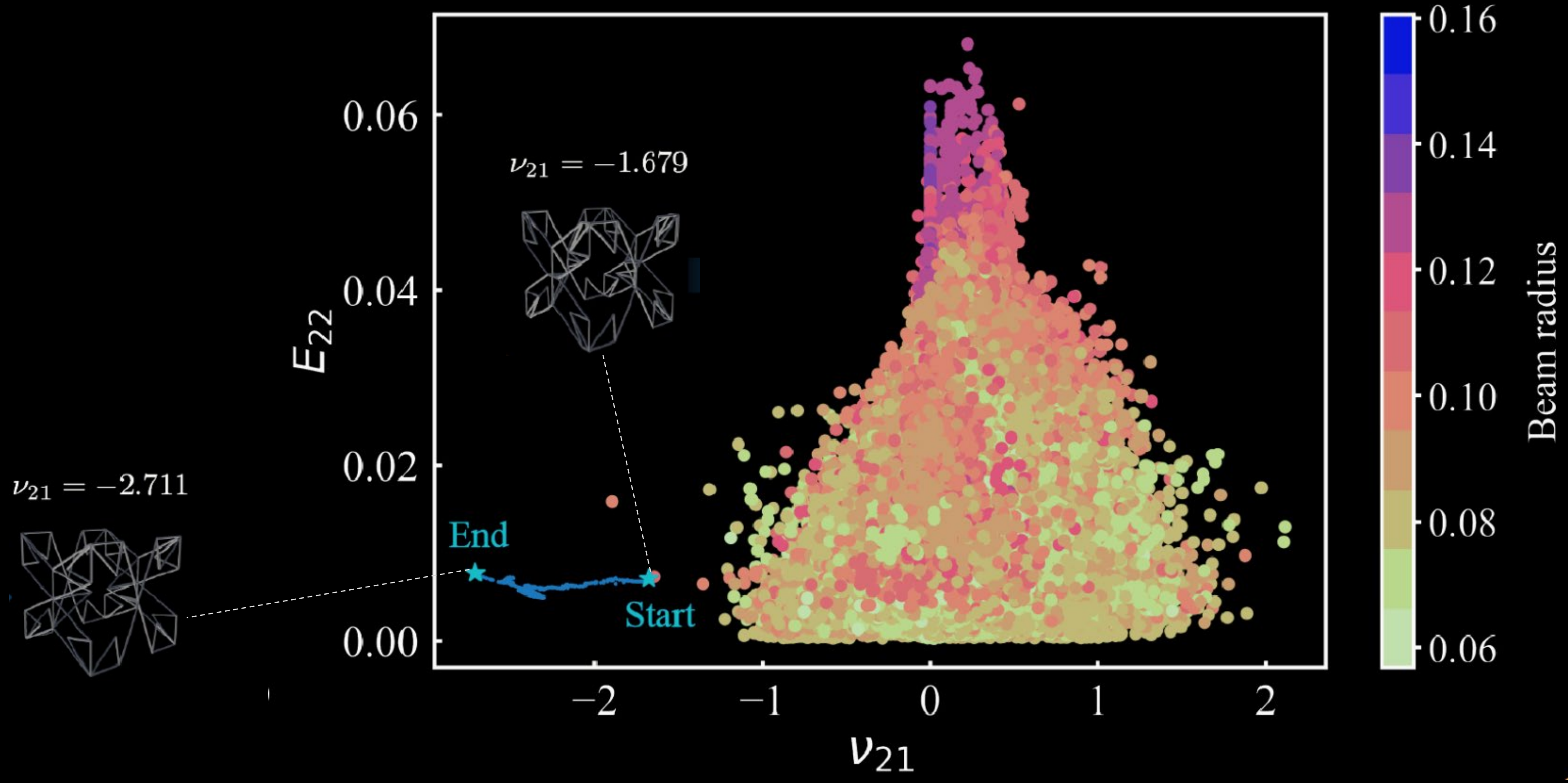
**sampling + decoding**

**reconstructed** lattice:

$\boldsymbol{G}' = (\boldsymbol{x}', \boldsymbol{A}') \in \mathbb{R}^N$

*(Zheng et al., Nat. Comm. 2023)*

# Property Optimization by Variational Autoencoders



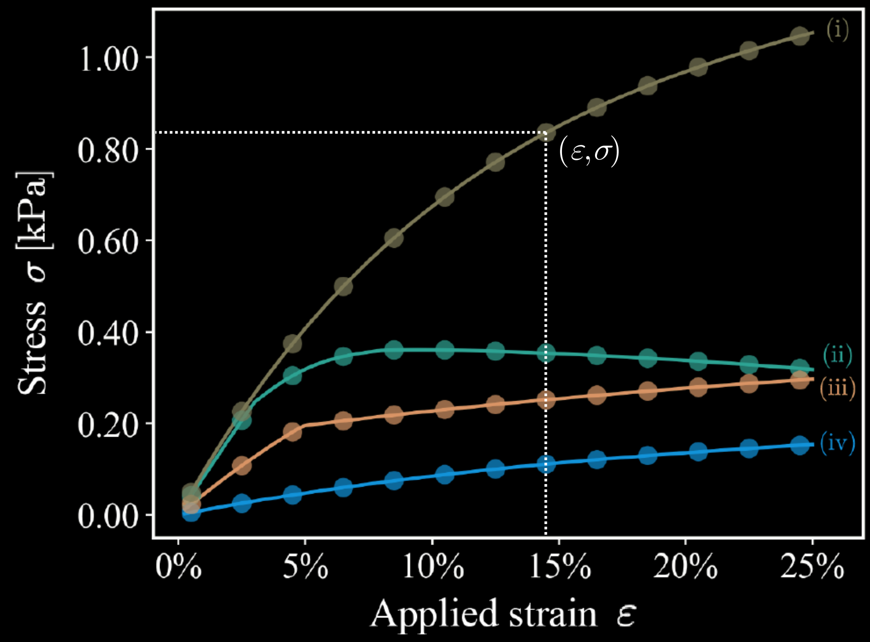

**Optimizing for auxeticity (negative Poisson's ratio): going significantly beyond the properties of the training set**

*(Zheng et al., Nat. Comm. 2023)*

# Nonlinear Stress-Strain Data

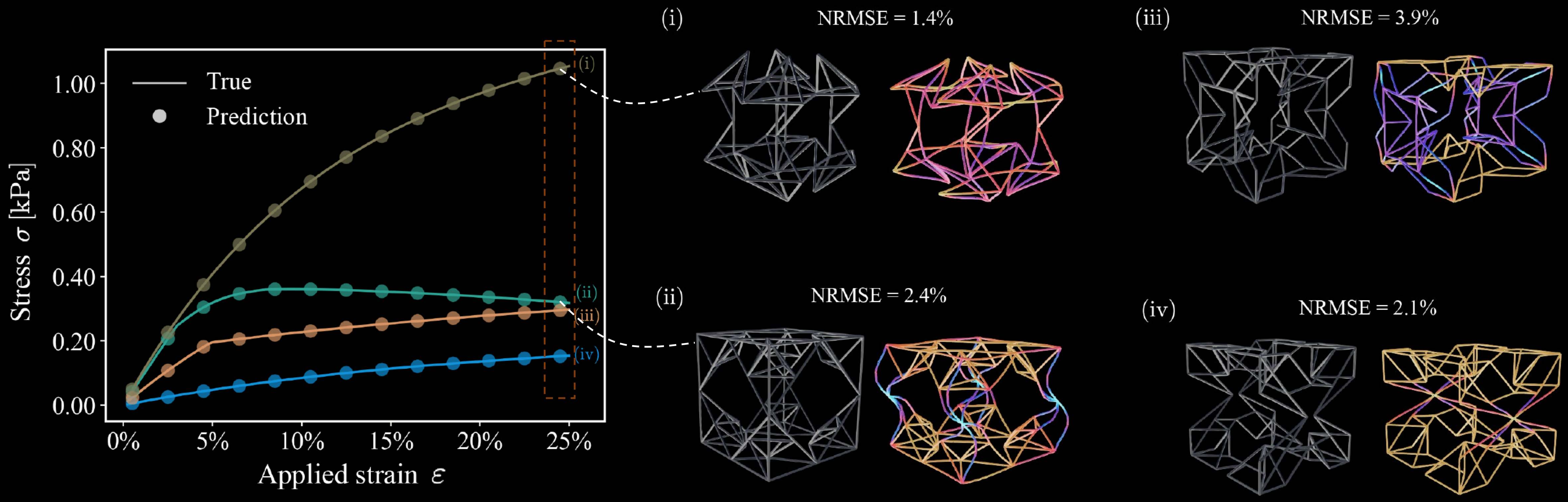
**dataset generation:**

- take a subset of the training dataset (383,729 structures)
- simulate the stress-strain response (uniaxial vertical compression up to 25%, periodic boundary conditions)
- nonlinear elastic-plastic material model
- learning labels: stress-strain curve described by $n$ discrete $(\varepsilon,\sigma)$-points




*(Zheng et al., Nat. Comm. 2023)*

# Nonlinear Stress-Strain Data – Forward Prediction




(Zheng et al., Nat. Comm. 2023)

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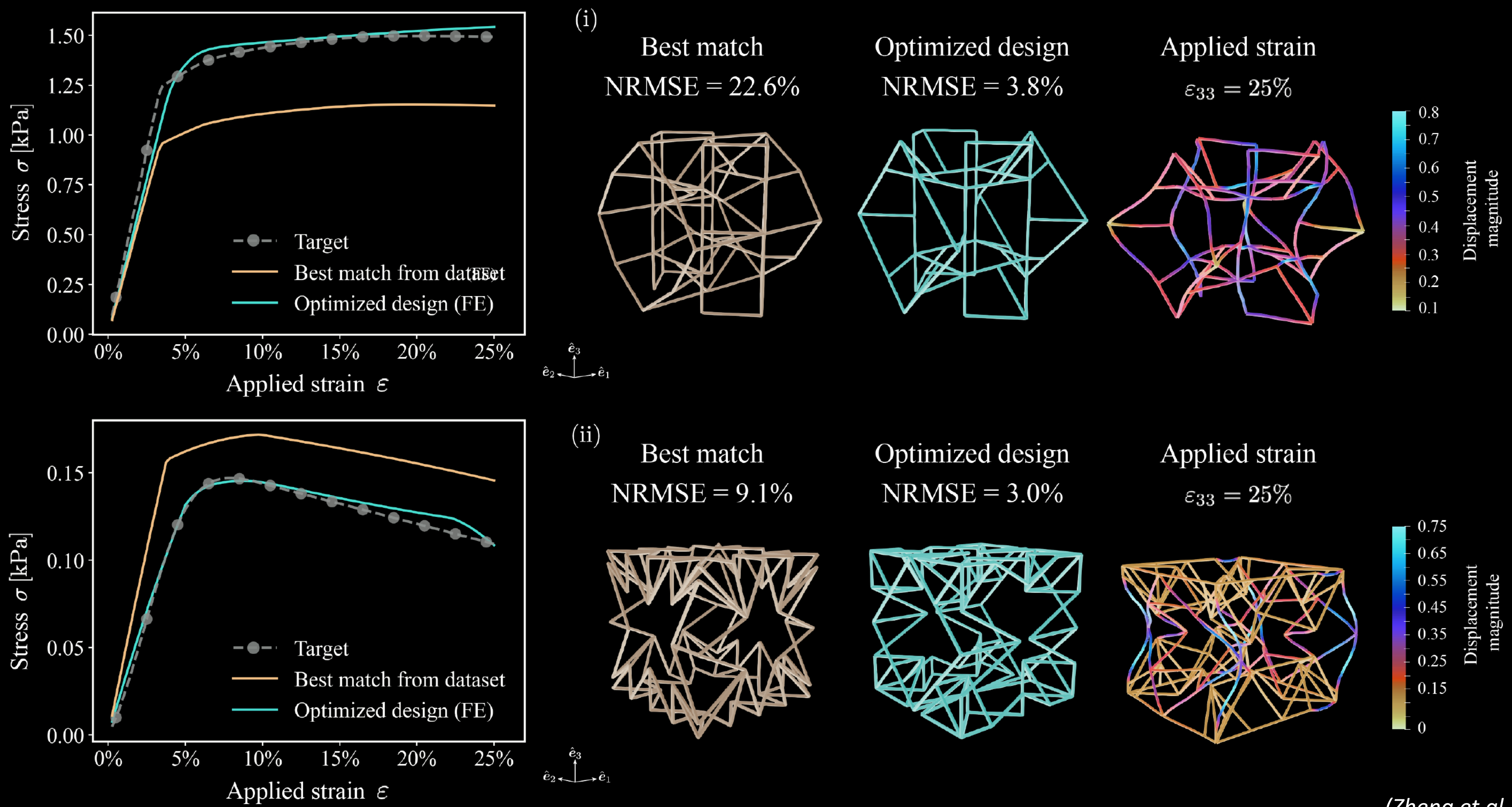
# Nonlinear Stress-Strain Data – Inverse Design




(Zheng et al., Nat. Comm. 2023)

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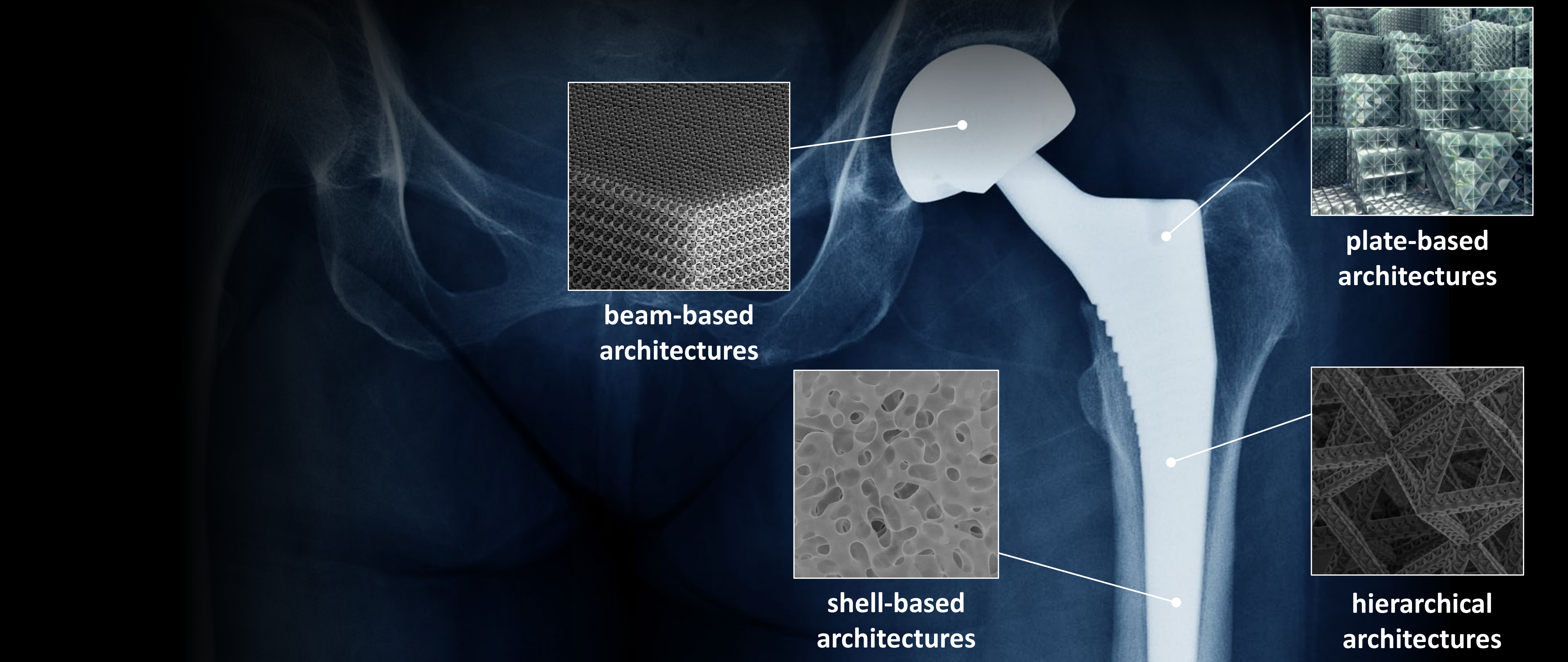
# How about an even more general design?

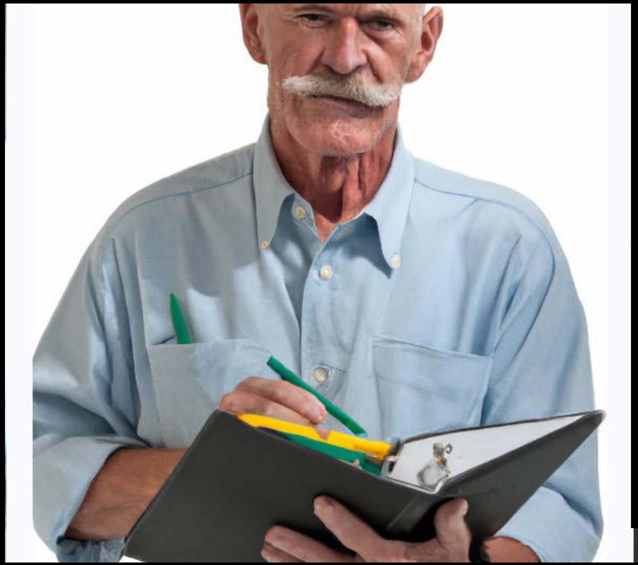
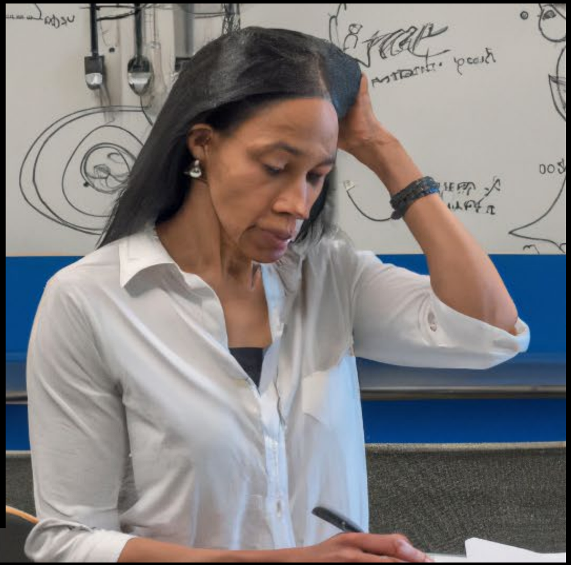
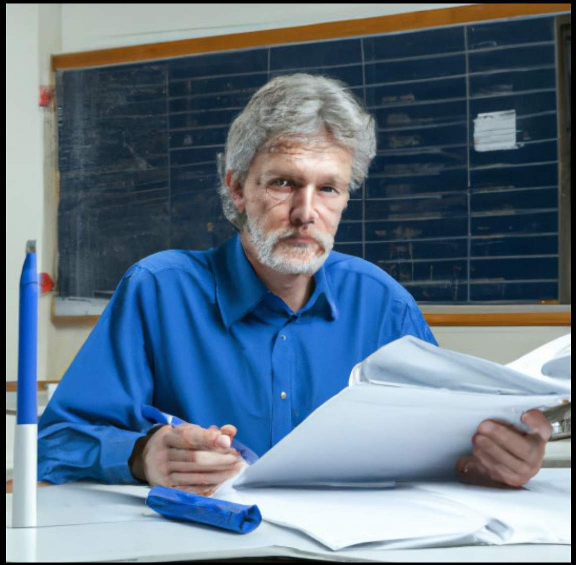


# AI-Generated Images & Videos

How can I help you today?

DK Photo of an engineering professor solving a hard problem

DALL·E *(early 2023)*:

# AI-Generated Images & Videos

*A drone camera circles around a beautiful historic church built on a rocky outcropping along the Amalfi Coast, the view showcases magnificent architectural details and tiered pathways and patios…*

OpenAI
Sora
*(early 2024)*:

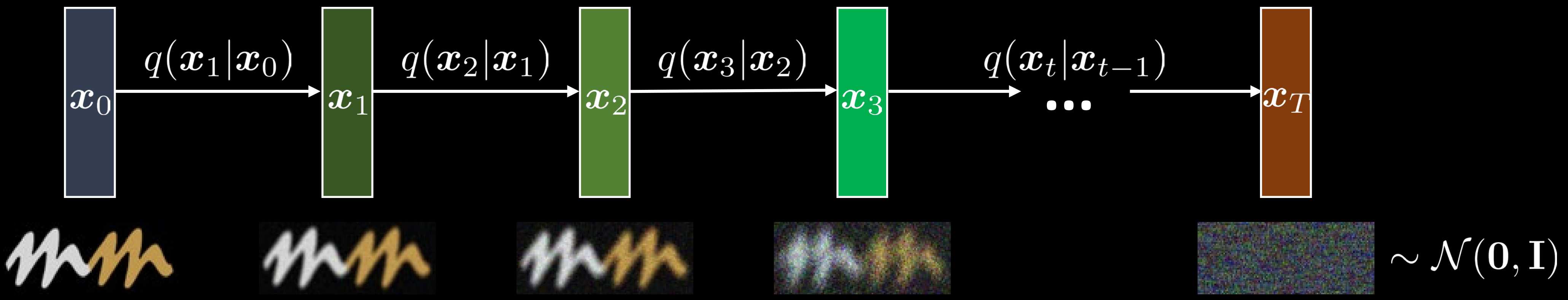
*https://openai.com/sora*

# Diffusion Models in a Nutshell: The Forward Process

Idea: transform an image to an **isotropic Gaussian distribution** by iteratively adding **Gaussian noise**.

Forward diffusion is a fixed Markov chain with some variance schedule $\beta_1, \ldots, \beta_T$:

$$q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0) = \prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) \qquad \text{with} \qquad q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{1-\beta_t}\boldsymbol{x}_{t-1}, \beta_t \boldsymbol{I}).$$



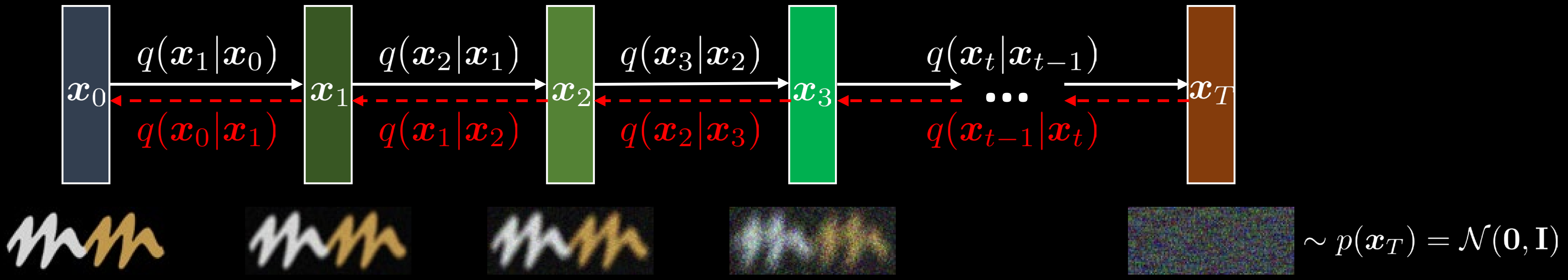

*(Sohl-Dickstein et al., 2015)*

# Diffusion Models in a Nutshell: The Reverse Process

Approximating the reverse diffusion ("*denoising*") process of a Markov chain in *reverse direction,*

$$p_\theta(\boldsymbol{x}_{0:T}) = p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t), \quad p_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t) = \mathcal{N}(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_\theta(\boldsymbol{x}_t, t), \boldsymbol{\Sigma}(\boldsymbol{x}_t, t))$$

while **conditioning** it on a **prompt**:




(realization based on 3D U-Nets)

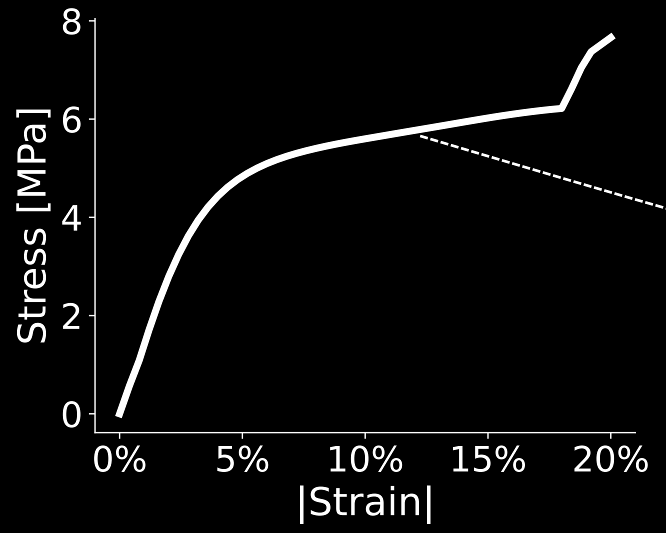
*(Sohl-Dickstein et al., 2015)*

# The Vision

## How can I help you today?

DK

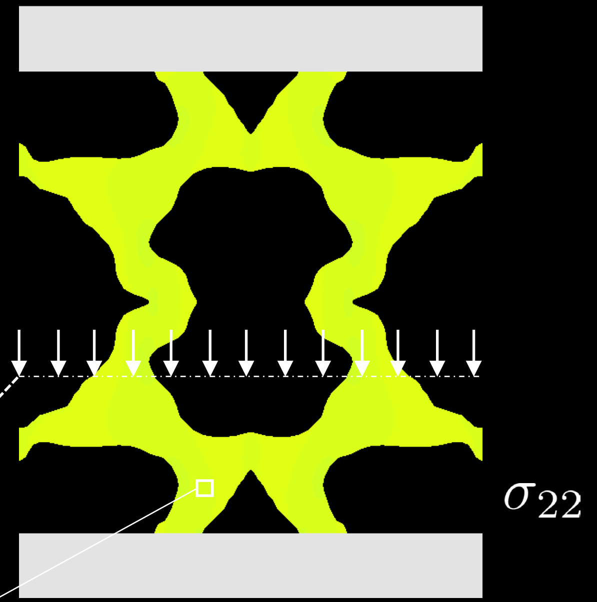
Video showing the finite element simulation of a periodic unit cell having the following overall stress-strain response in compression:




video
diffusion (?)

$(\mathrm{R,G,B}) = (u_1, u_2, \sigma_{22})$
+ physics

Of course, here you go:

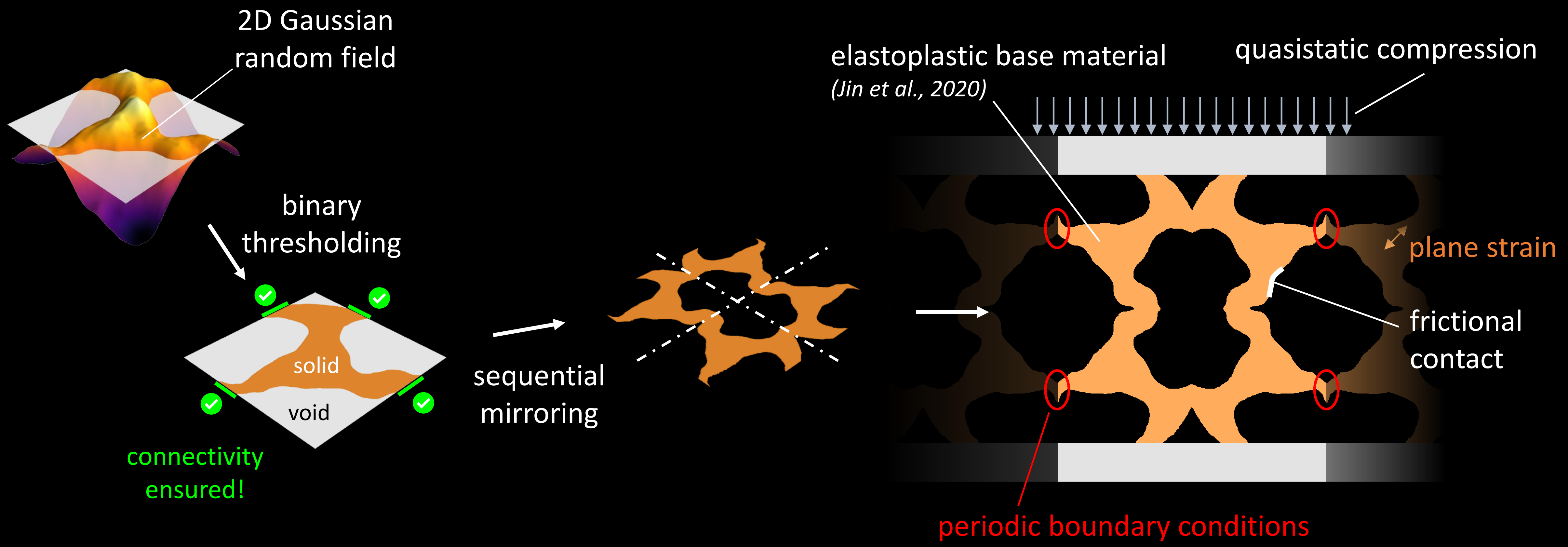



**optimal structure**
**+**
**simulated deformation**

*(Bastek & Kochmann, Nature Mach. Intell. 2023)*

# Parameterization Example #4: Pixel-Based Cellular Solids

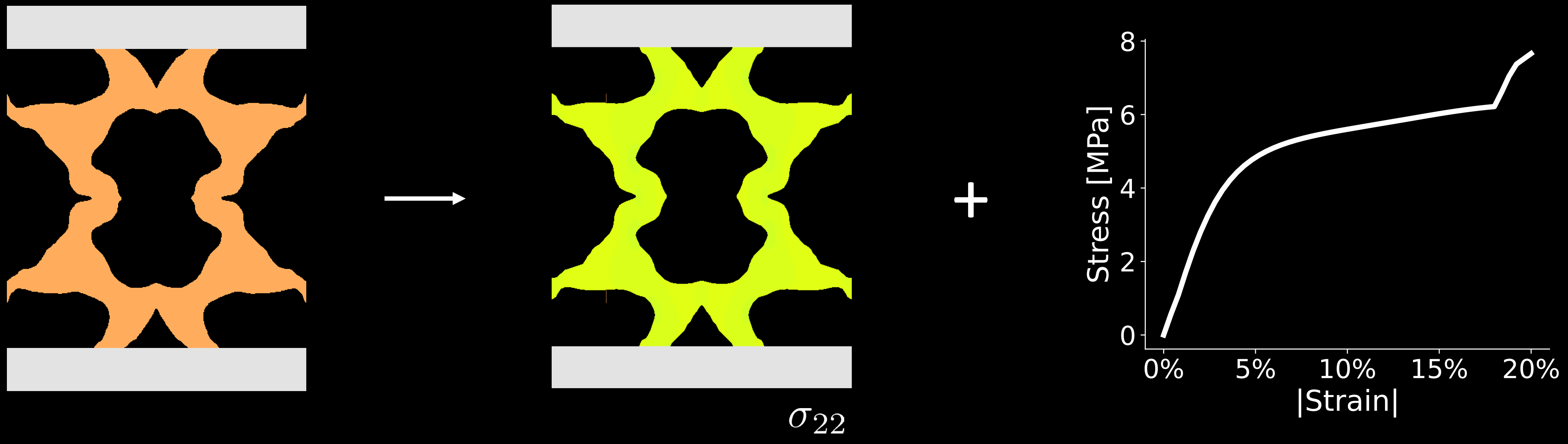
We generate **spatially correlated** pixel distributions by considering **Gaussian Random fields**:




*(Bastek & Kochmann, Nature Mach. Intell. 2023)*

# Data Generation

We generate the corresponding stress-strain response and stress distribution via FE simulations and train a video diffusion model (based on 3D U-Nets, parametrization by 96 $\times$ 96 pixels):

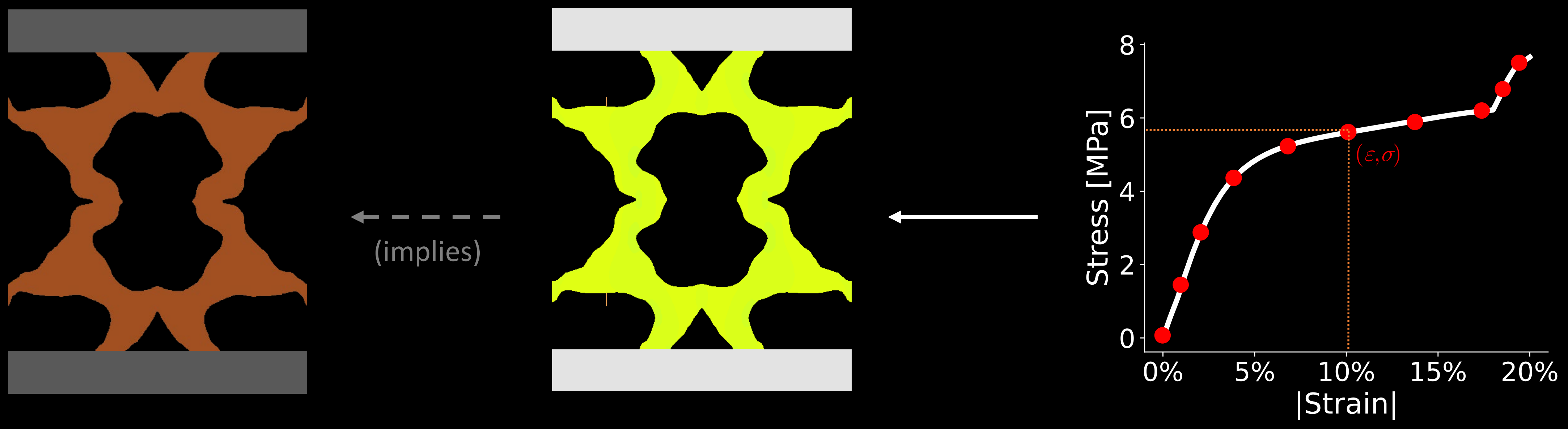



ca. 53,000 finite element simulation videos + average stress-strain curve

*(Bastek & Kochmann, Nature Mach. Intell. 2023)*

# Inverse Design Challenge

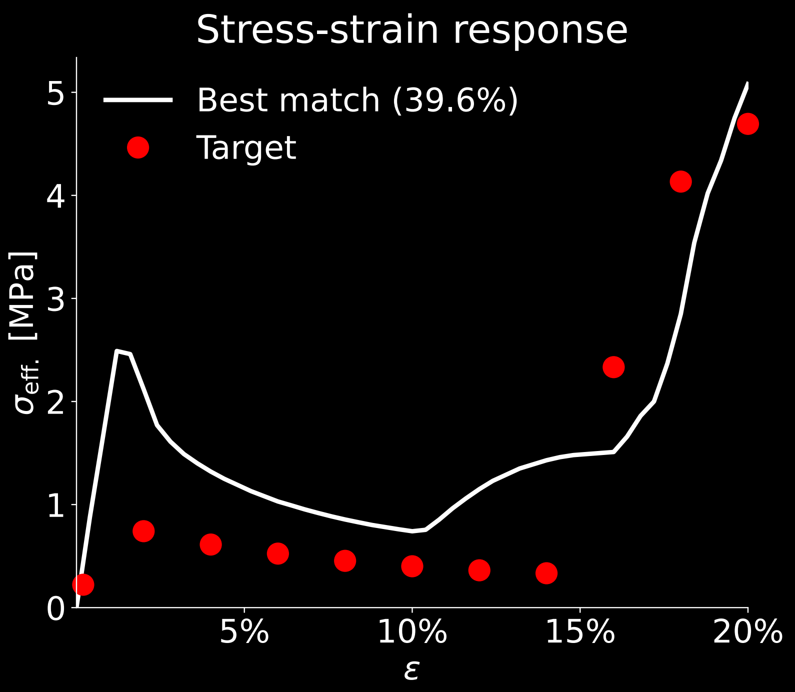
For a given stress-strain response, generate a cellular structure!




(Bastek & Kochmann, Nature Mach. Intell. 2023)

# Results: Video Generation Based on Stress-Strain Data

How well can the model generalize to unseen target responses? Let’s make it challenging!
*Lagrangian frame*




*(Bastek & Kochmann, Nature Mach. Intell. 2023)*

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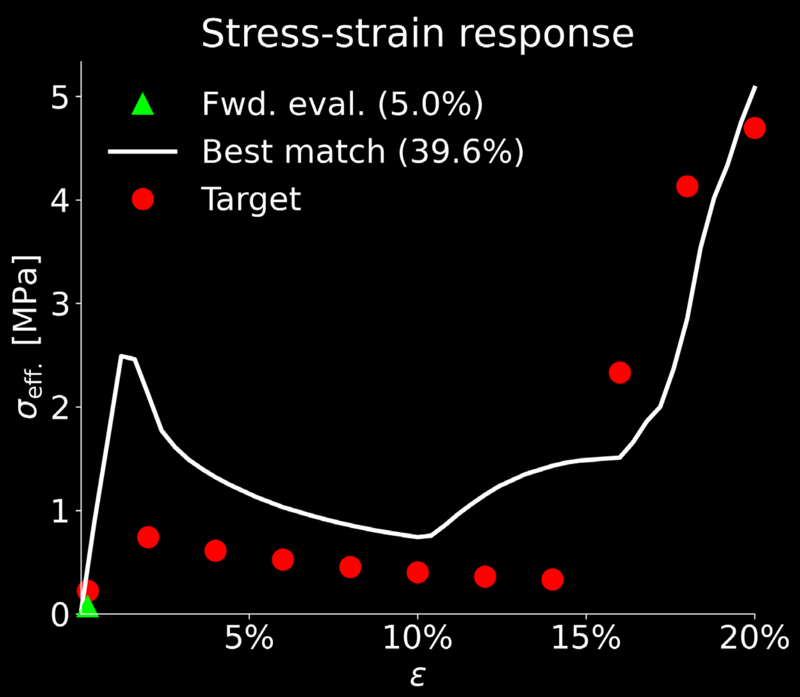


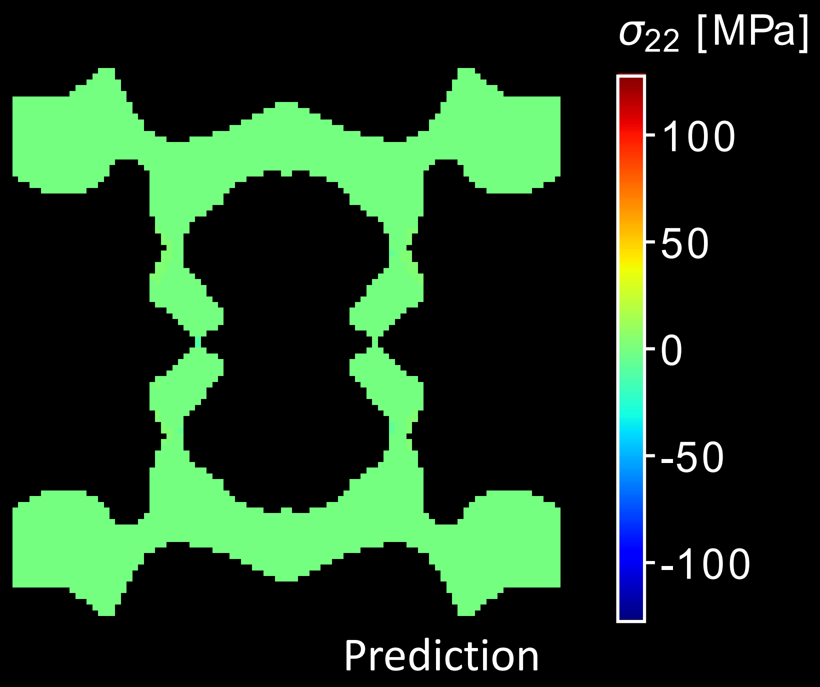


*(Bastek & Kochmann, Nature Mach. Intell. 2023)*

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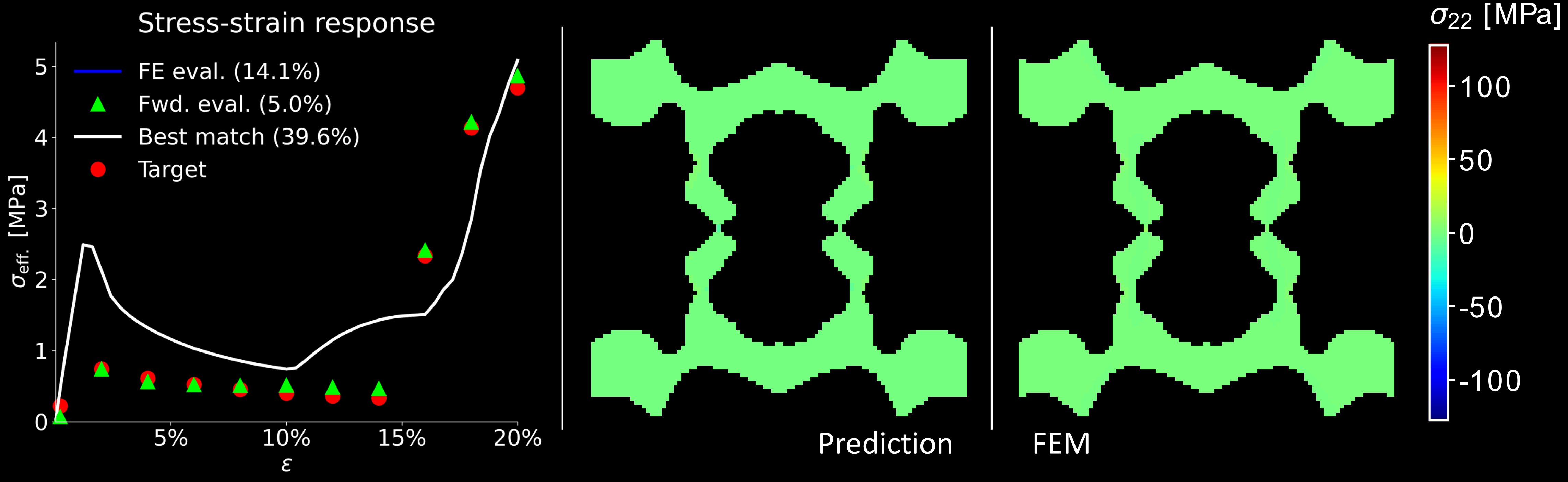
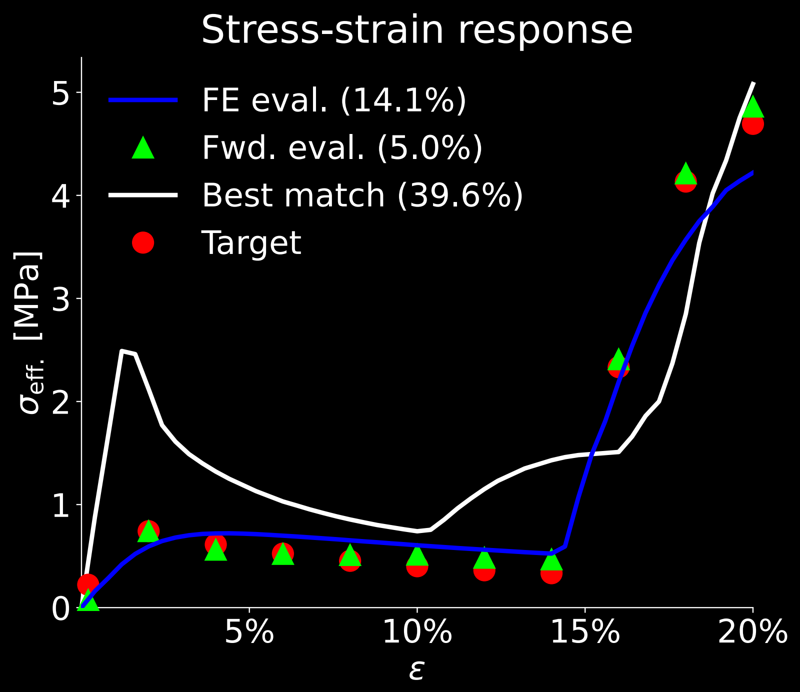
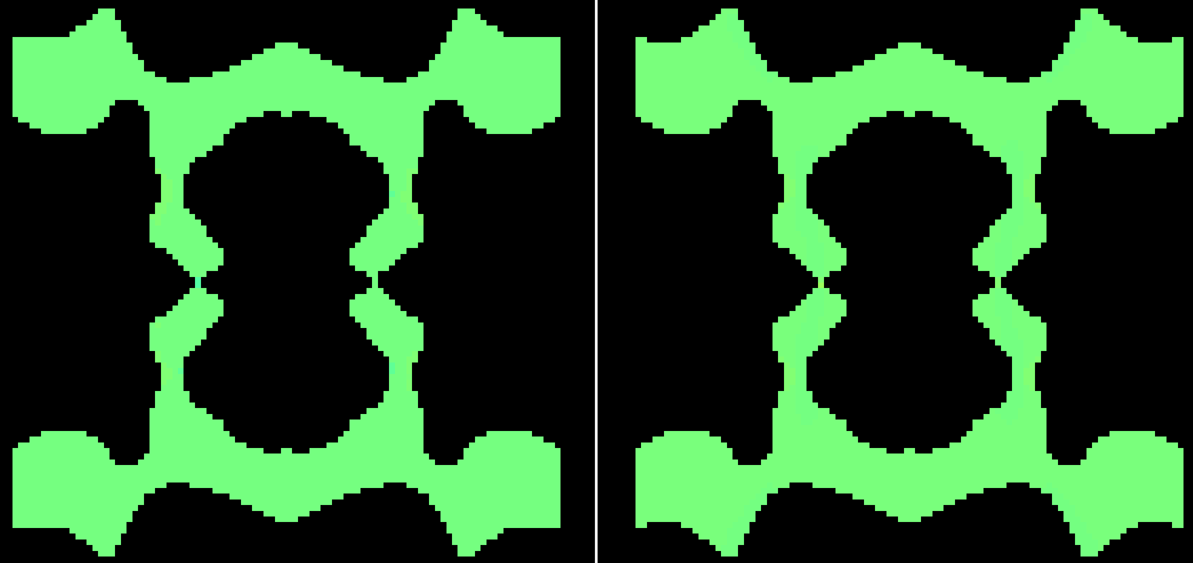



(Bastek & Kochmann, Nature Mach. Intell. 2023)

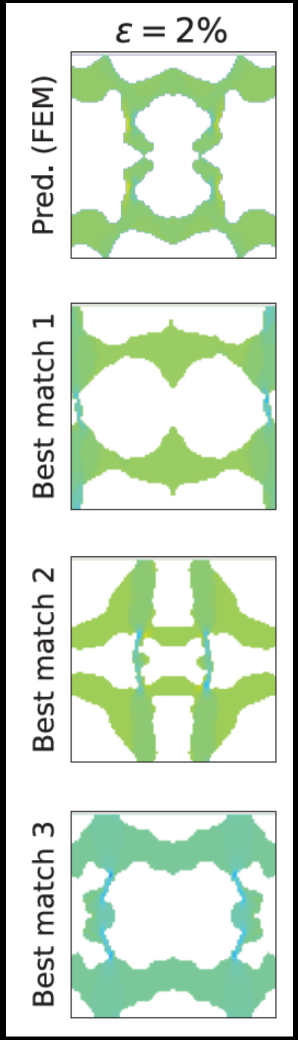
# Results: Video Generation Based on Stress-Strain Data

How well can the model generalize to unseen target responses? Let's make it challenging!
(*Eulerian frame)*



Prediction FEM




(*Bastek & Kochmann, Nature Mach. Intell. 2023)*

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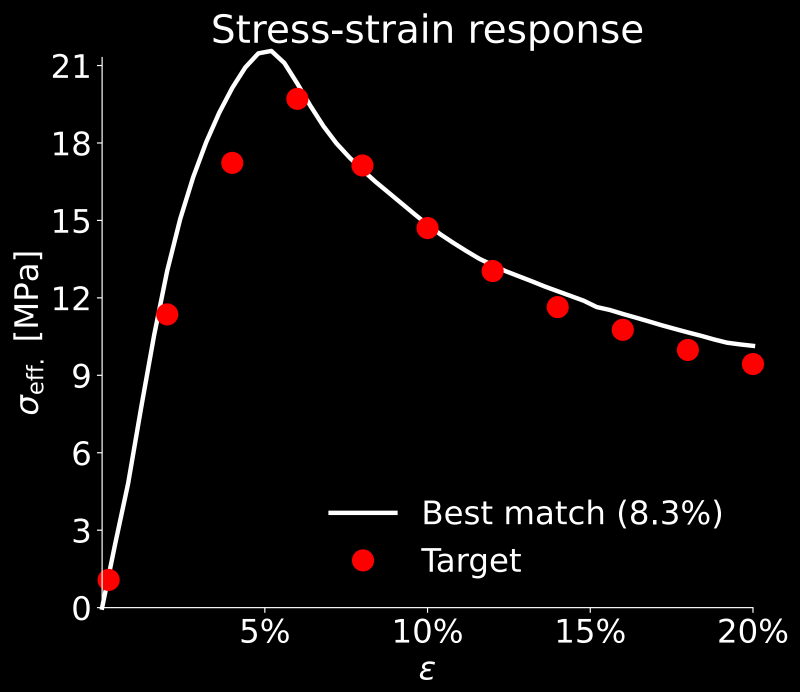


(Bastek & Kochmann, Nature Mach. Intell. 2023)

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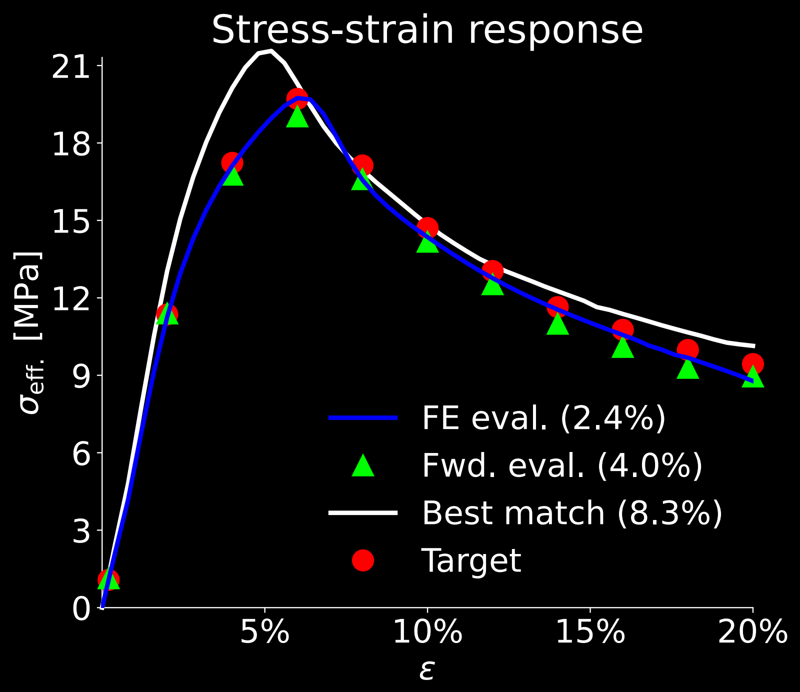


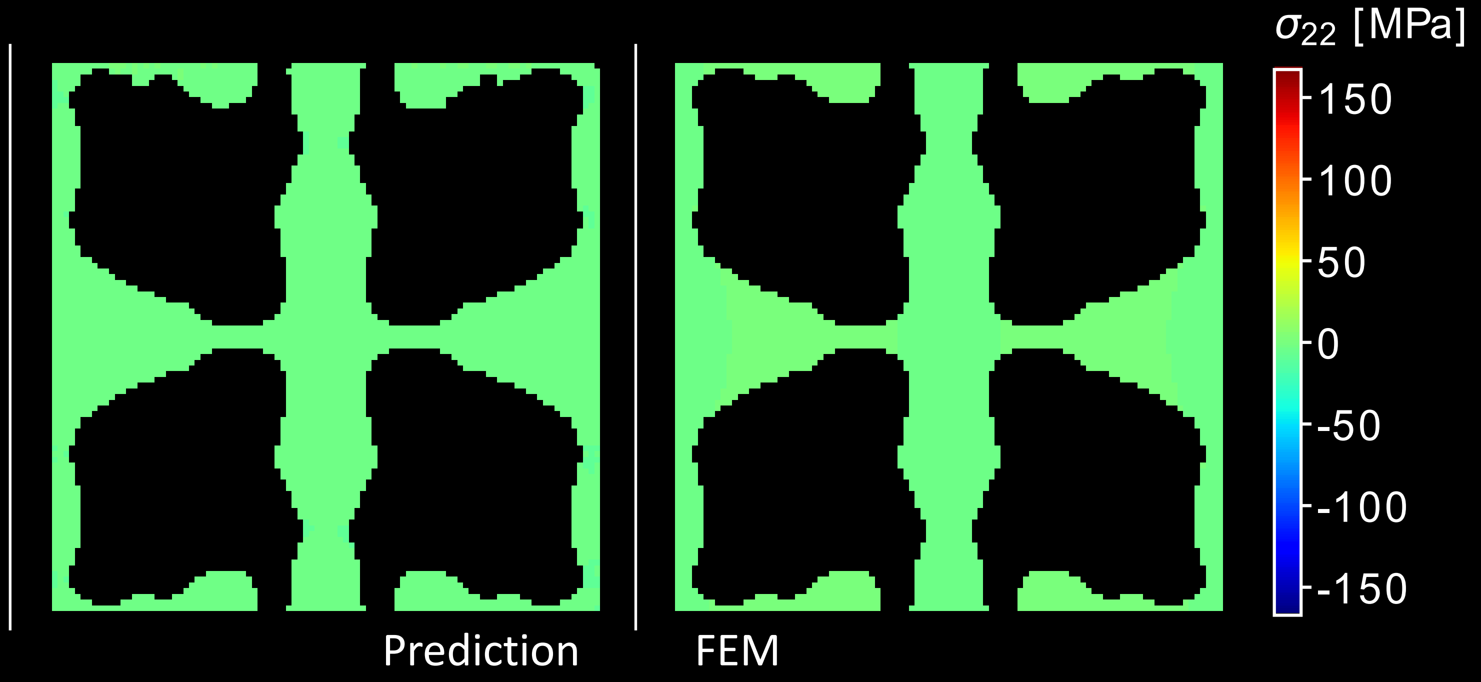


*(Bastek & Kochmann, Nature Mach. Intell. 2023)*

# Take-Away Messages

- Inverse design and multiscale optimization are topical computational challenges.
- There is a tremendous **design space** (beams, plates, shells, …) and **property space** (stiffness, anisotropy, strength, toughness, wave motion, …) to be explored.
- **AI-based approaches offer alternatives** for the inverse design– especially when paired with engineering/scientific insight.
- Many approaches can be and are being **extended to materials** (in the classical sense).

**Spinodoid Inverse Design**
*(Kumar et al., npj Comp. Mater. 2020)*

**Truss Inverse Design**
*(Bastek et al., PNAS 2022)*

**Truss Design by VAEs**
*(Zheng et al., Nature Comm. 2023)*

**Video Diffusion Models**
*(Bastek & Kochmann, Nature Mach. Intell. 2023)*

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mechanics & materials

# Thank you for your invitation, interest & attention!

*Questions & Comments?*

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**Acknowledgements:**

Jan-Hendrik Bastek & Li Zheng (ETH Zurich), Sid Kumar (TU Delft)

Financial support from adidas & ETH Zurich.