Deep generative modeling for mechanistic-based learning and design of metamaterial systems

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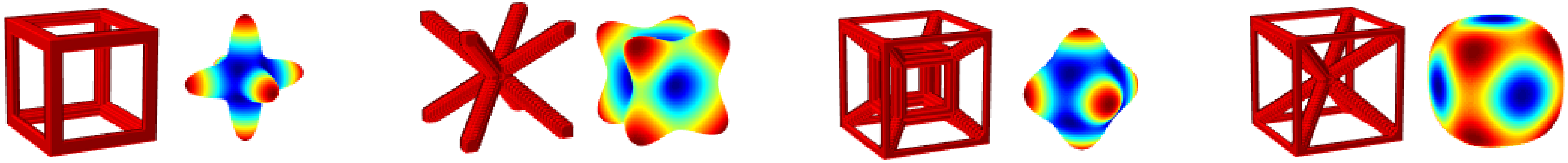
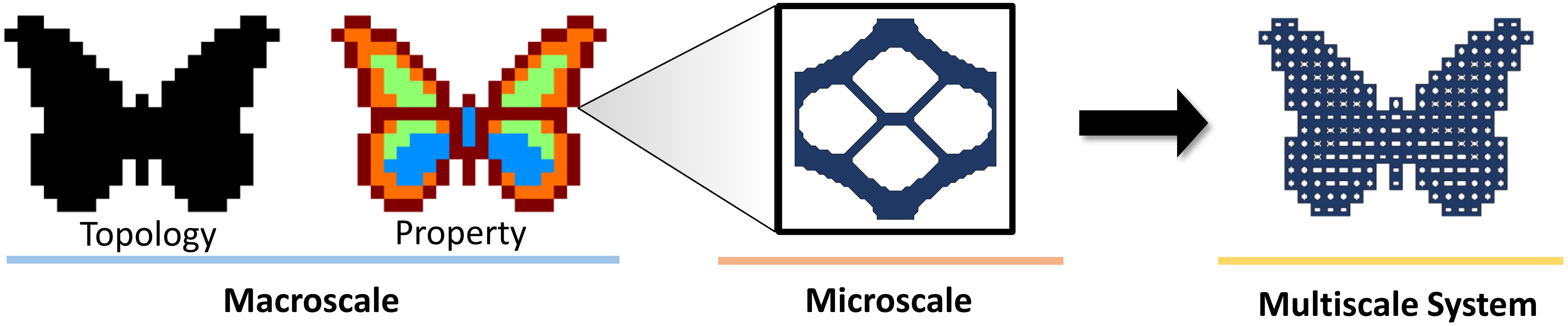
Metamaterial and Multiscale Metamaterial System Design

- Metamaterial: Derive properties from the microstructures rather than the constituents
- Achieve heterogeneous property distribution by assembling different microstructures



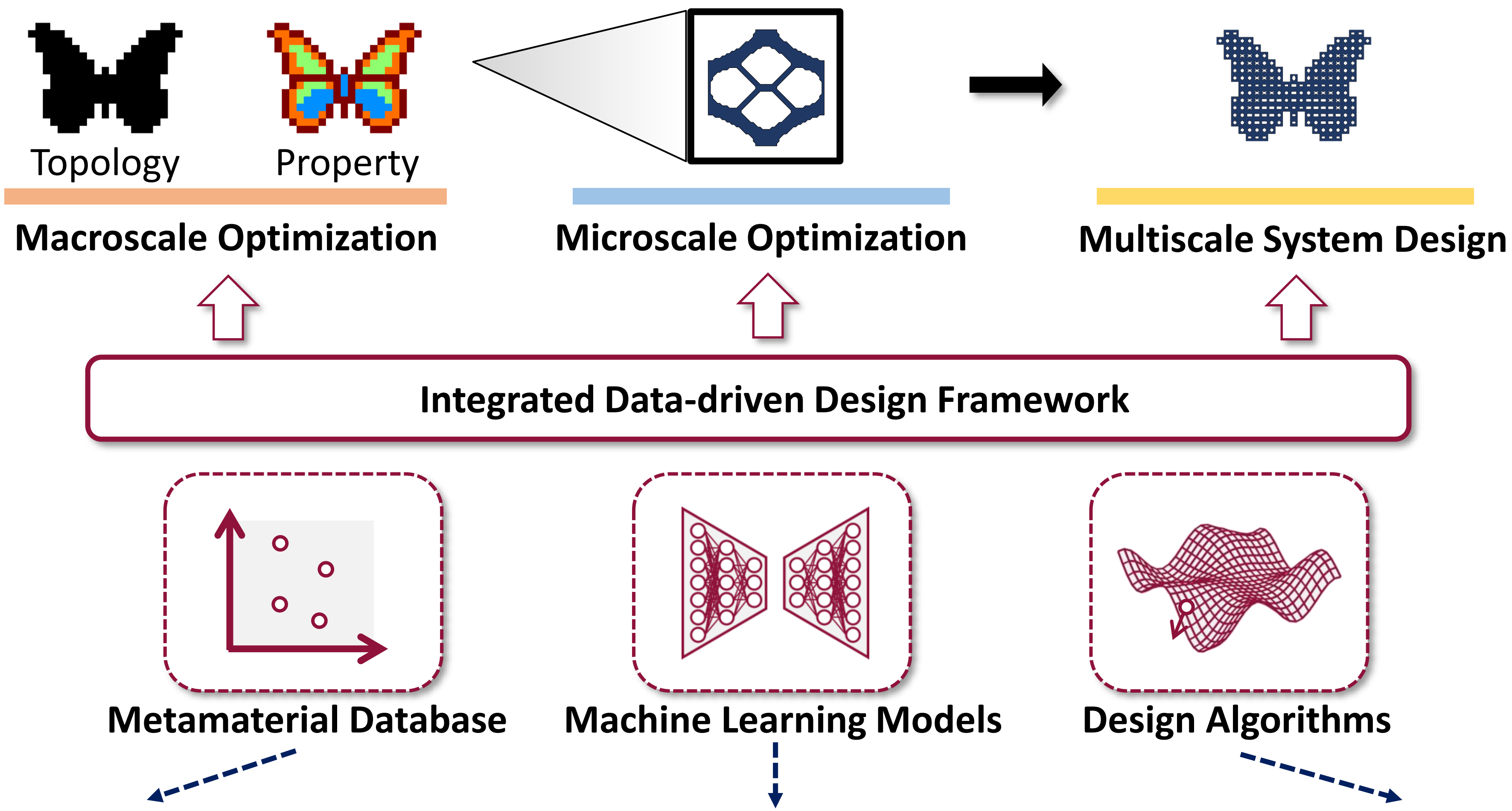
Wang, L. et al., 2020. *J. Mech. Design, 143.*

■ **Different Microstructures and Their Elasticity Surfaces**



■ **Multiscale System Design**

Research Questions and Proposed Data-Driven Design Framework



Database Construction

- How to construct a large database with diverse shapes and properties?

Mechanistic-based Learning

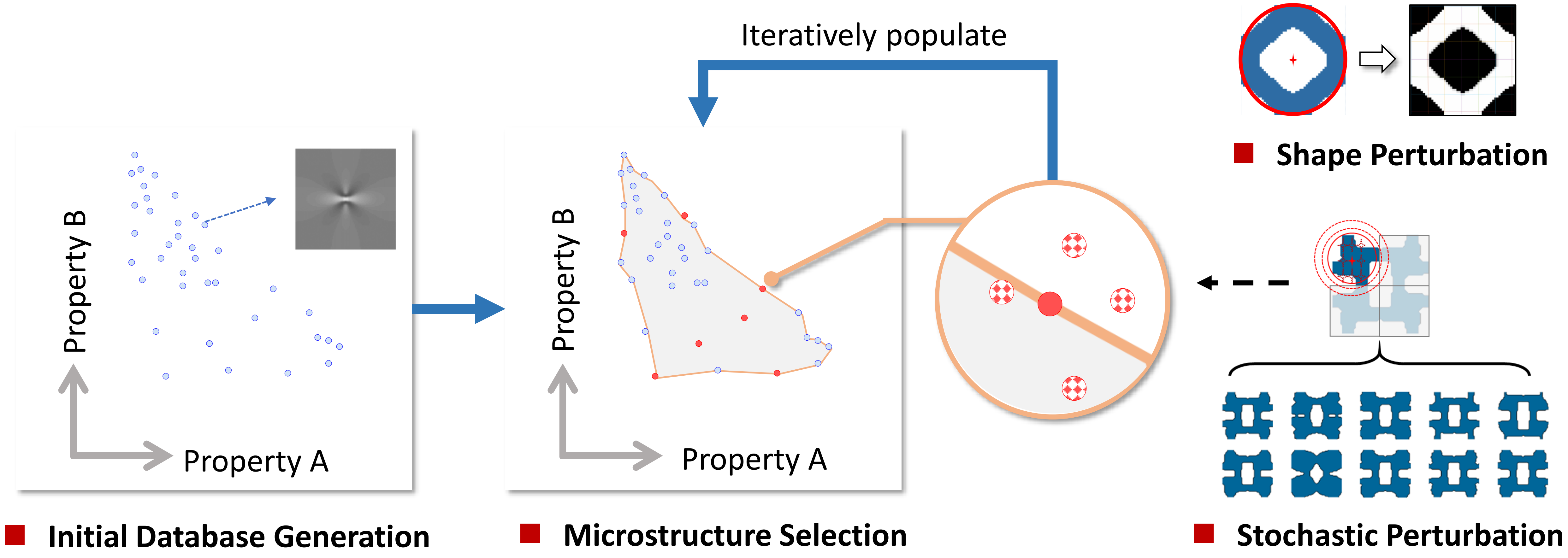
- What mechanics knowledge can be extracted from the database?

Data-driven Metamaterial Design

- How to do scalable multiscale design with well-connected unit cells?

Sequential Generation of Metamaterial Database

- Perform SIMP for uniformly sampled stiffness targets to generate initial database
- Populate the database by sequentially select and perturbate critical structures

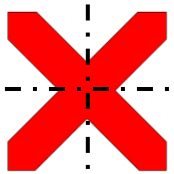


Wang, L. et al., 2020. *Struct. Multidisc. O.*

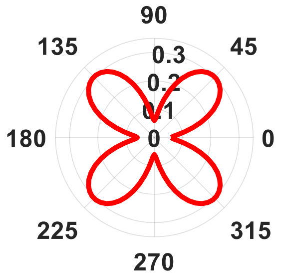
Chan, Y.C. et al., 2020. *J. Mech. Design, 143.*

Large and Diverse Metamaterial Database

- Orthotropic microstructures with four independent entries of stiffness matrix
- A diverse metamaterial database with ~250,000 precomputed microstructures



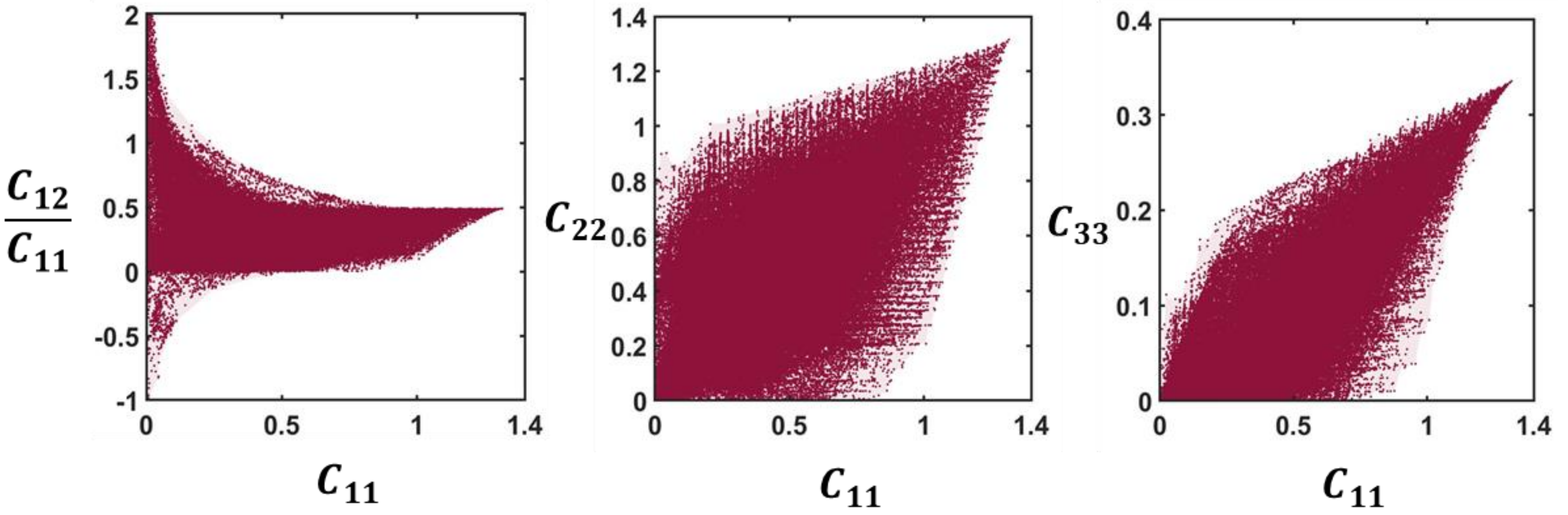
Orthotropic Symmetry



Elasticity Surface

$$\begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{21} & C_{22} & 0 \\ 0 & 0 & C_{33} \end{bmatrix}$$

Stiffness Matrix

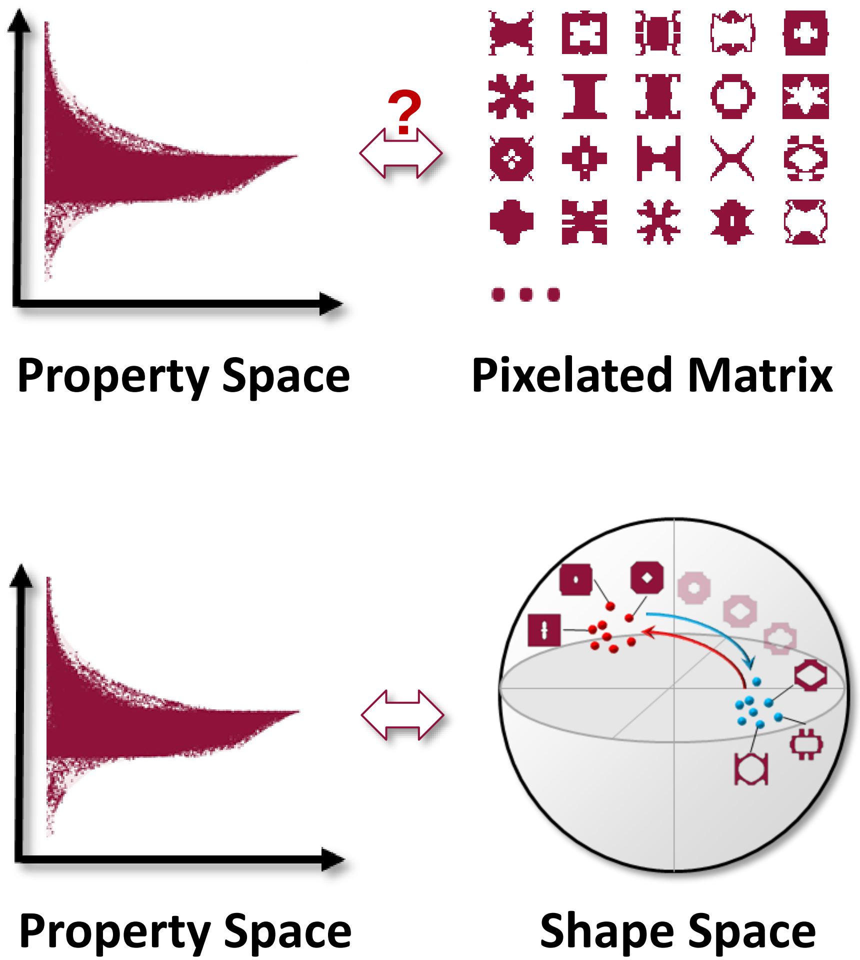


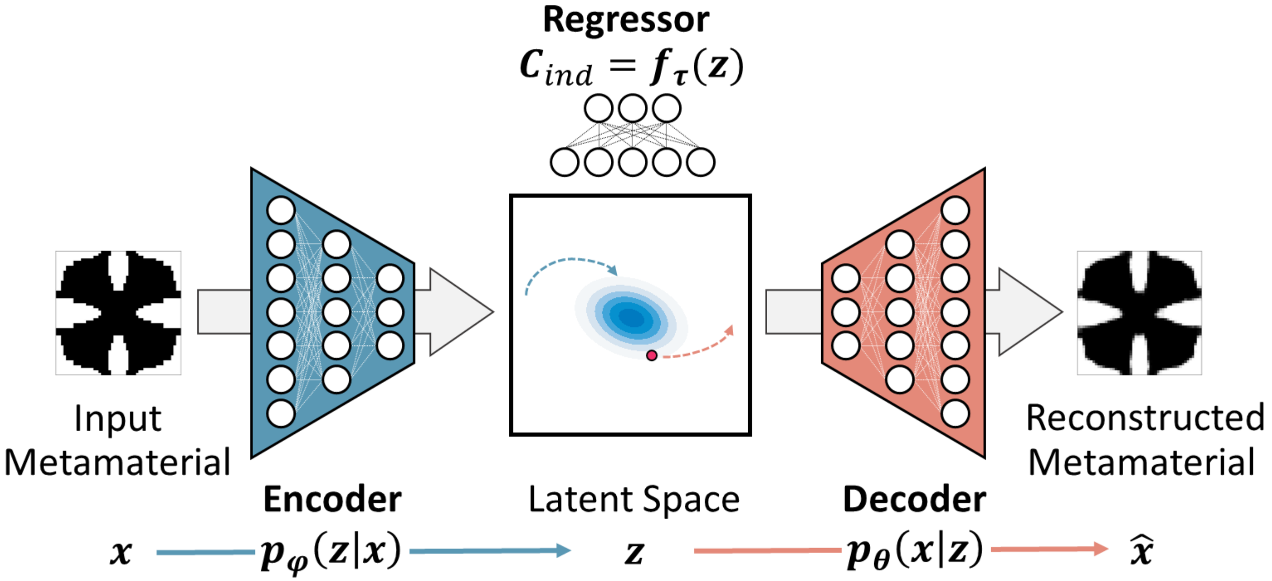
Property Space of the Metamaterial Database

Data available at : https://ideal.mech.northwestern.edu/research/software/

Variational Autoencoder (VAE) for Mechanistic Learning

- A two-way mapping between microstructures and low-dimensional latent vectors
- Unravel the interplay between property and shape spaces

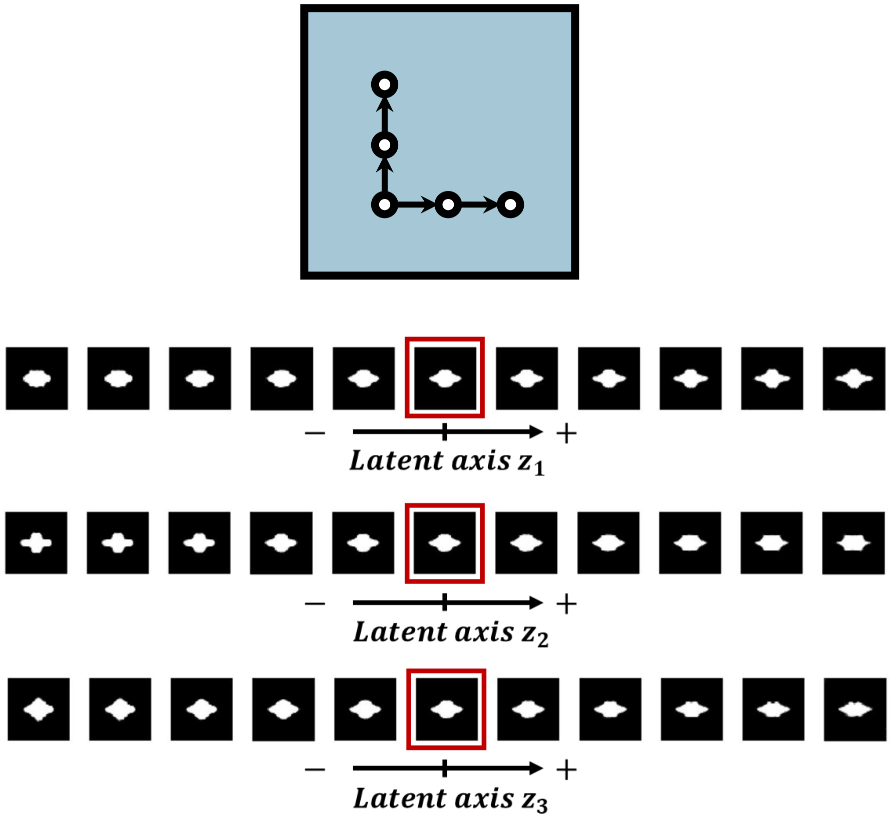




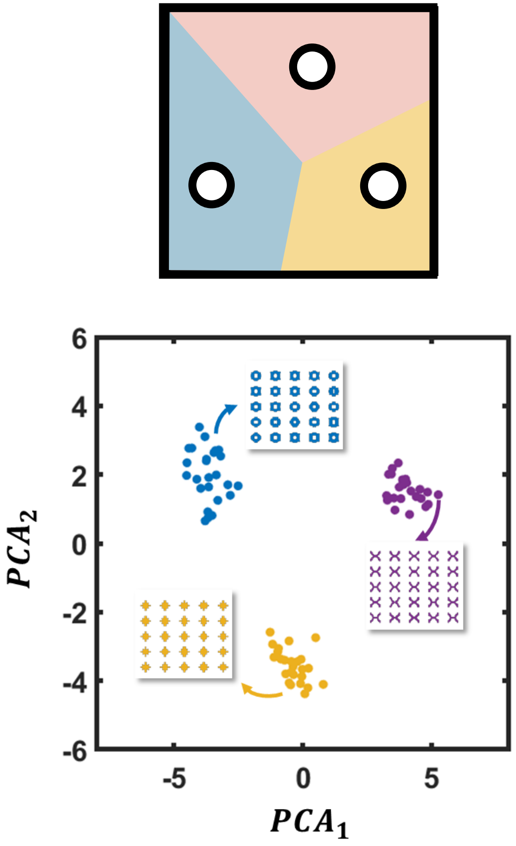
■ **Variational Autoencoder (VAE) Architecture**

Mechanistic-based Learning in Latent Space

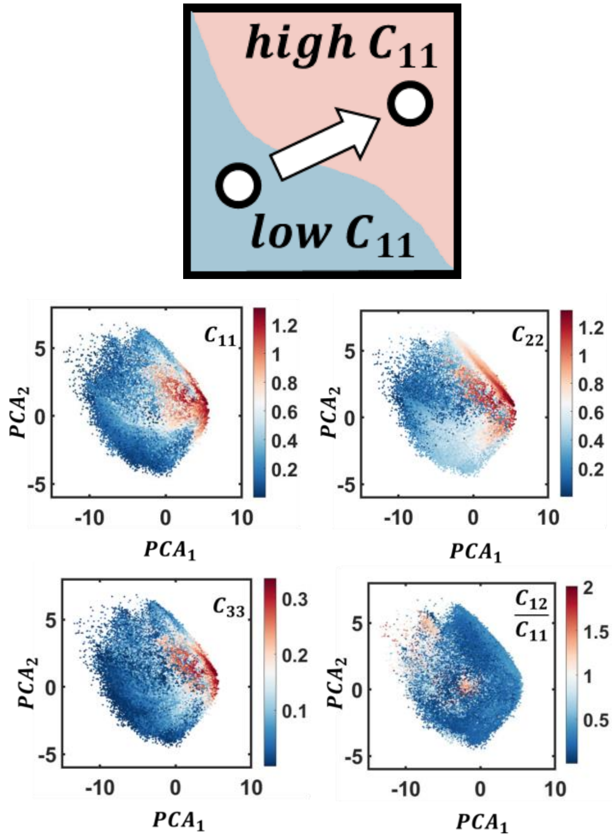
- Meaningful mathematical structure and rich physical information in the latent space
- Latent space as a “control panel” for metamaterial



■ **Meaningful Latent Axis**



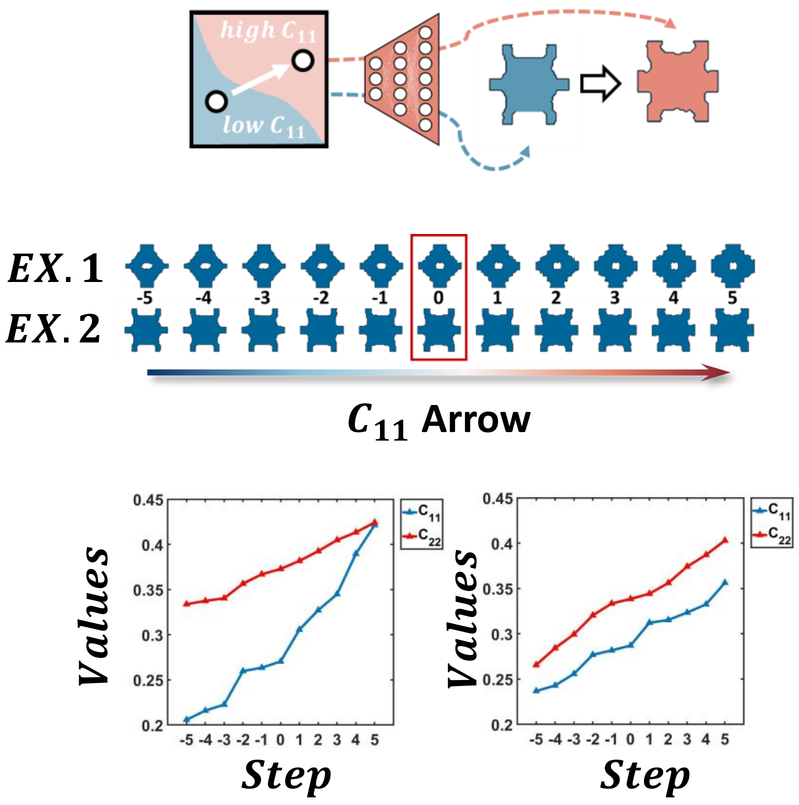
■ **Distance Metric**



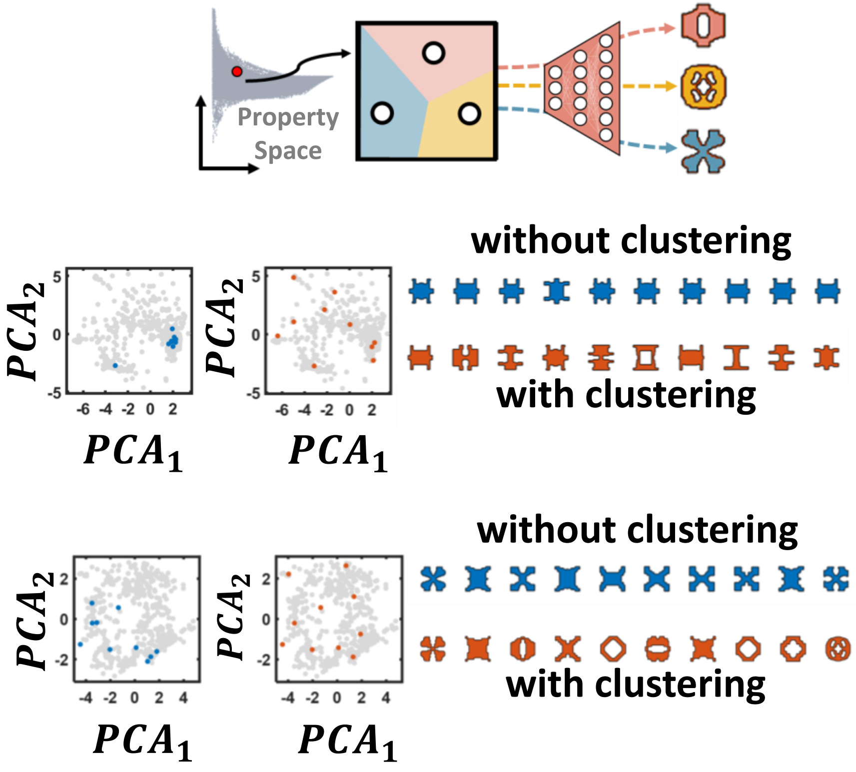
■ **Conceptual Map**

VAE-assisted Inverse Design

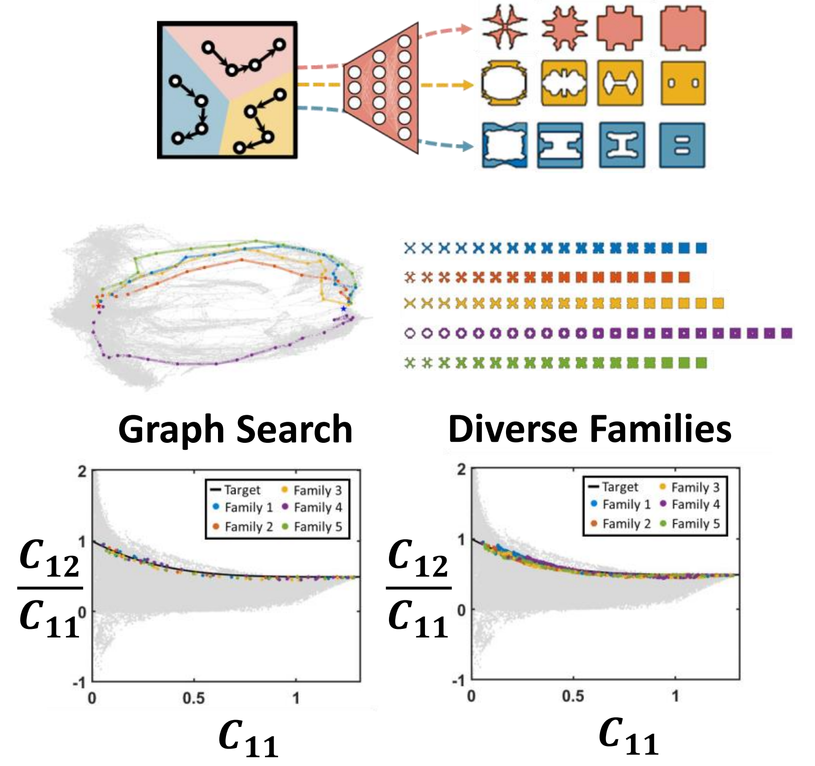
- Easy tuning of properties and geometries by simple vector arithmetic in latent space
- Diverse candidate set selection & generation for target properties
- Efficient generation of metamaterial families with target gradations of properties



■ Semantic Arrow



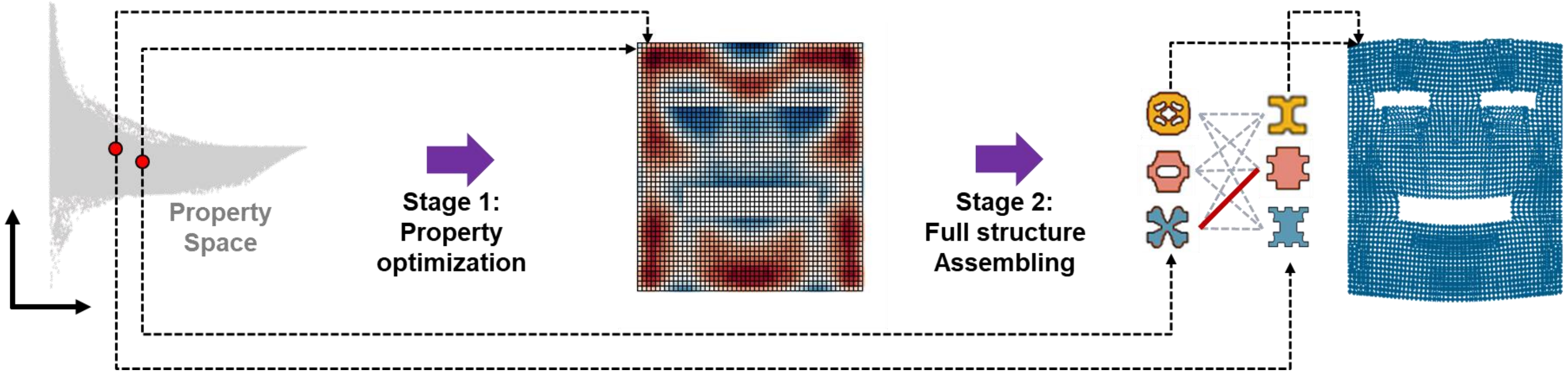
■ Diverse Candidate Set



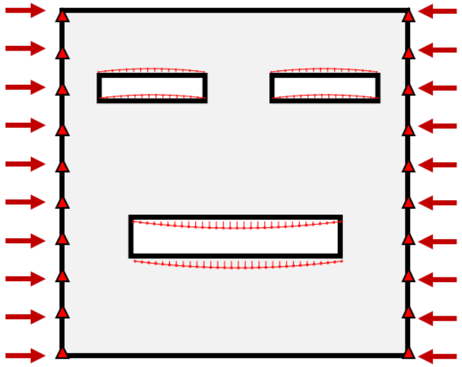
■ Metamaterial Family Generation

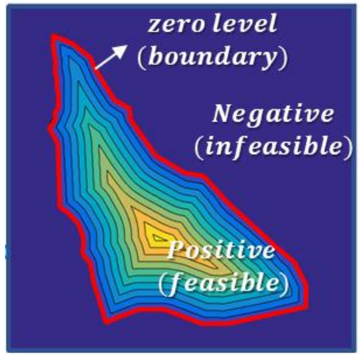
VAE-assisted Multiscale Metamaterial Systems Design

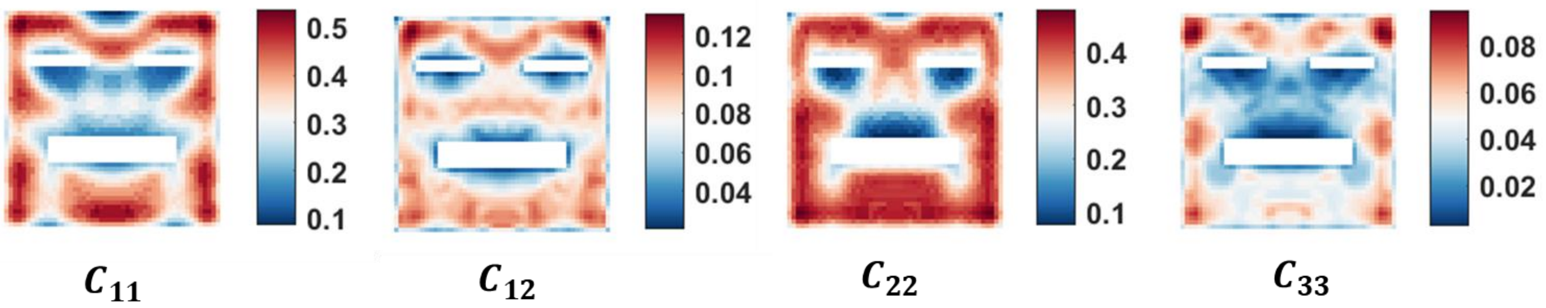
- A two-stage framework for multiscale system design to achieve the prescribed distortion, ensuring the compatibility between adjacent unit cells



■ **Design Framework**



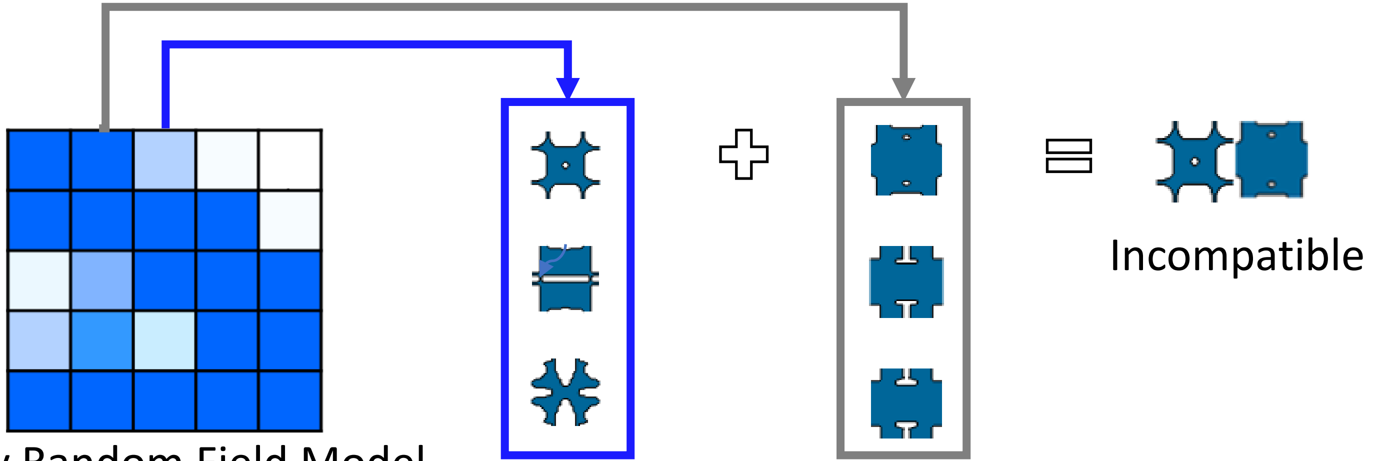




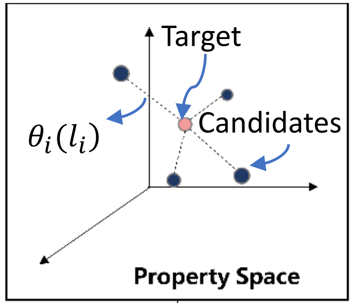
■ **Problem Setting** ■ **Property Constraint** ■ **Optimized Spatially-varying Property Distribution**

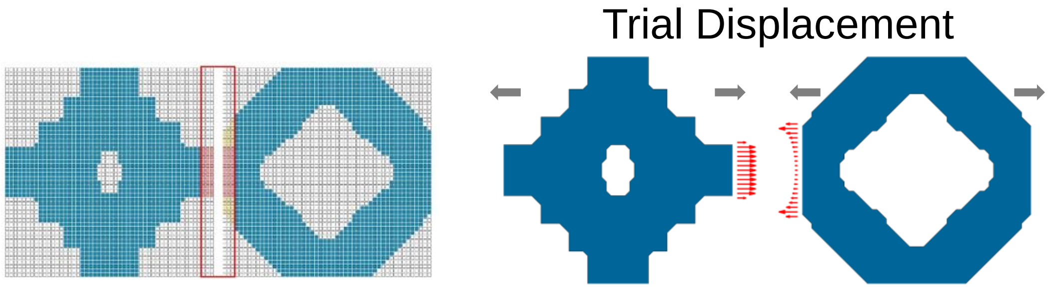
Full Structure Assembling

- Change the full structure assembling into a graph energy minimization problem
- Efficiently solved by dual-decomposition method



Markov Random Field Model





Nodal Energy $\theta_i(l_i)$

Edge Energy $\theta_{ij}(l_i, l_j)$

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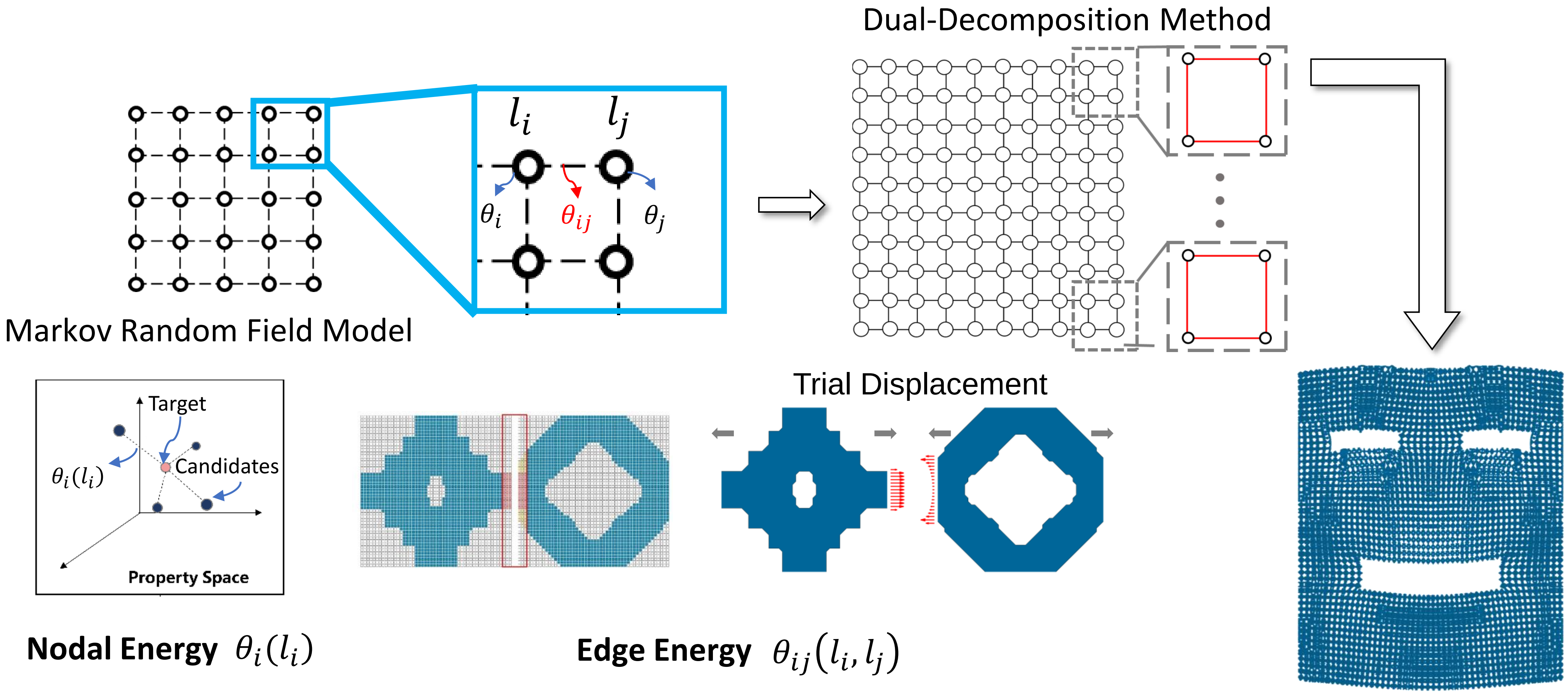

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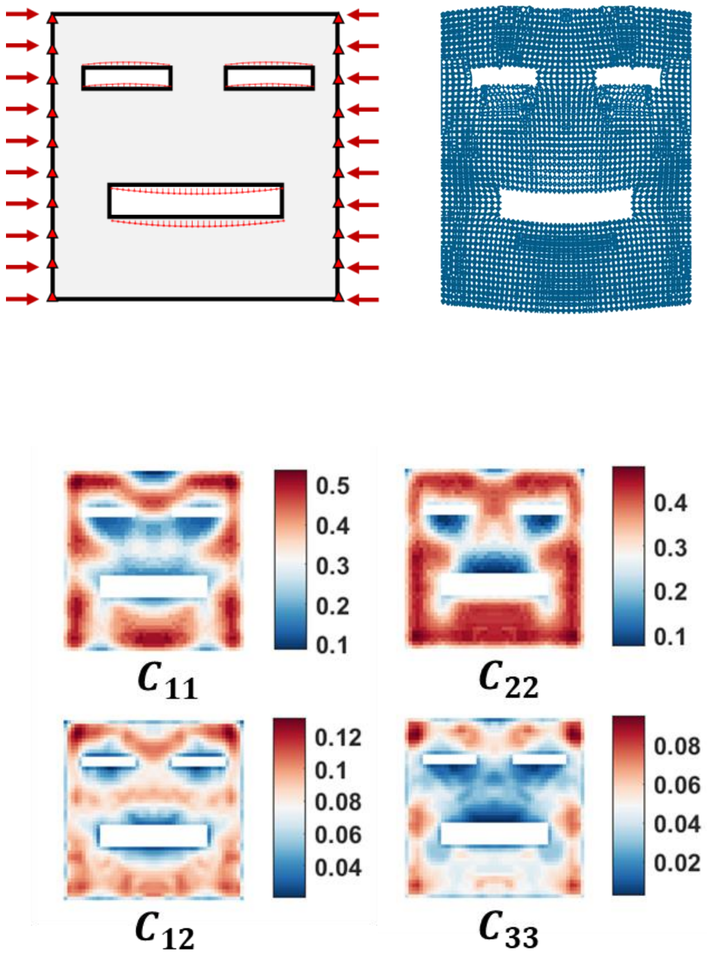
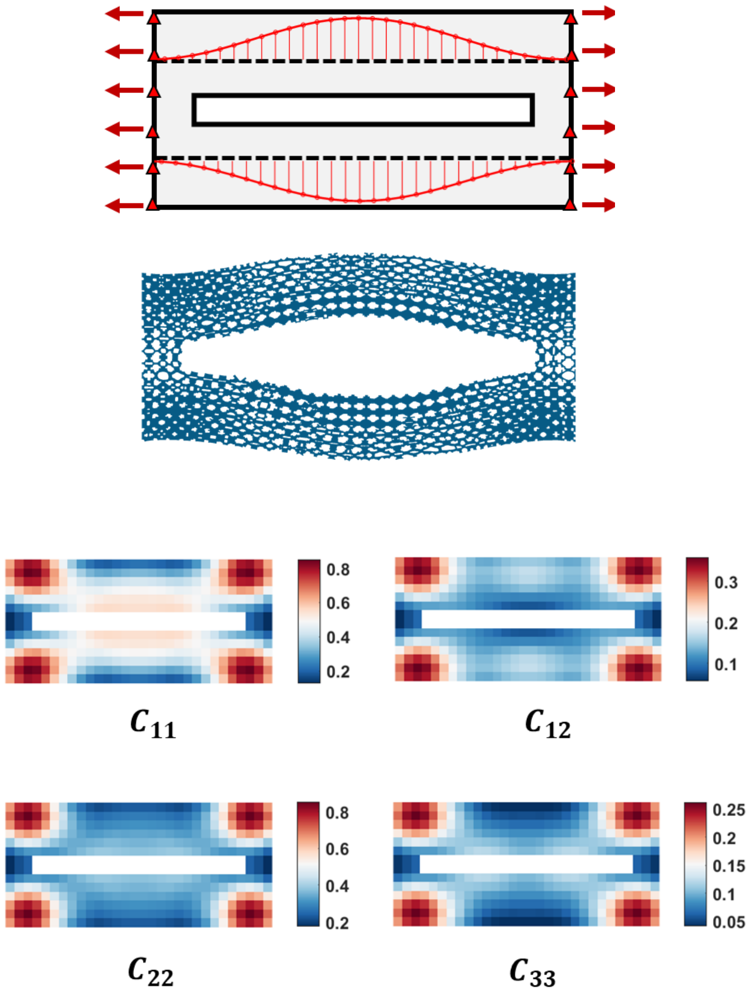
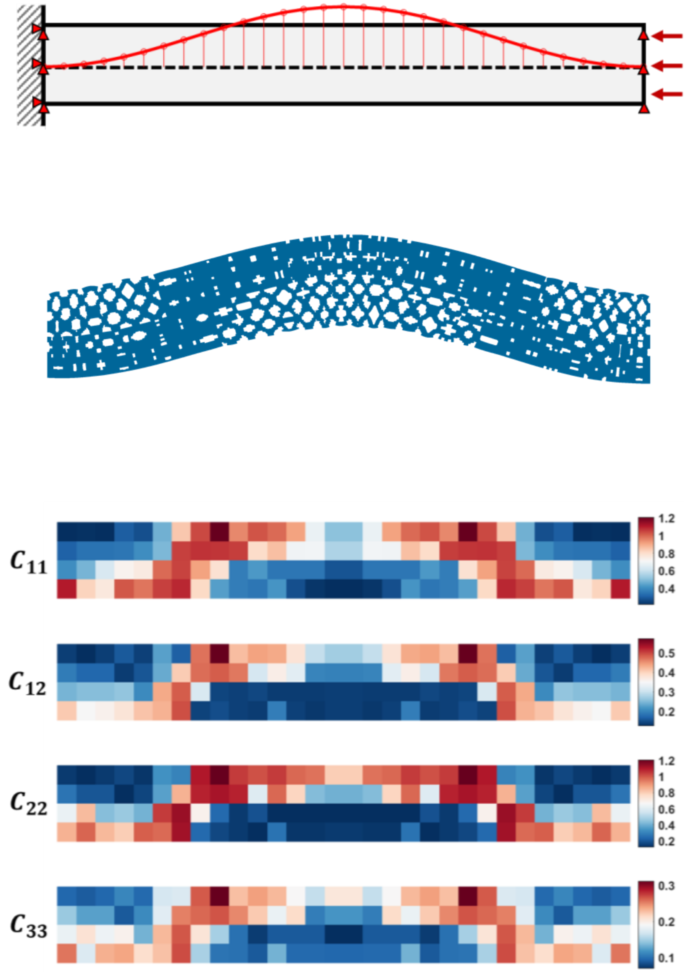
Aperiodic Design with Prescribed Distortion

- Spatially-varying property distribution to achieve prescribed distortion behavior







Summary of Contributions

- Efficient construction of a large database with diverse microstructures and properties
- Insights on the mathematical structure and mechanistic information of latent space
- Easy tuning of properties and geometries by simple vector arithmetic in latent space
- Multiscale design with heterogeneous properties and well-connected aperiodic microstructures

Challenges and Future Opportunities of DATO

- **Design with complicated mechanism or material law**

  - Pattern-switching design, acoustic/ phononic/ photonic design, induced buckling…

  - Structure with manufacturing-induced heterogeneity, e.g. AM

- **Design with multiple scales/components**

  - Nonlinearity, aperiodicity, interaction between components

- **Physics-guided/ “white-box” machine learning method**

  - Bring physics into ML

  - Better generalizability, reduce data requirement, higher interpretability

- **Standard dataset & benchmark problem**

Related papers

[1] **Wang, L.**, Chan, Y.C., Ahmed, F., Liu, Z., Zhu, P. and Chen, W.*, 2020. Deep generative modeling for mechanistic-based learning and design of metamaterial systems. Computer Methods in Applied Mechanics and Engineering, 372, p.113377.

[2] **Wang, L.,** Chan, Y.C., Liu, Z., Zhu, P.* and Chen, W.*, 2020. Data-driven metamaterial design with Laplace-Beltrami spectrum as "shape-DNA". Structural and Multidisciplinary Optimization, pp.1-16.

[3] **Chan, Y.,** Ahmed, F., Wang, L., and Chen, W.* 2020. METASET: Exploring Shape and Property Spaces for Data-Driven Metamaterials Design. Journal of Mechanical Design, 143(3).

[4] **Wang, L**., Tao, S., Zhu, P. and Chen, W*., 2021. Data-Driven Topology Optimization With Multiclass Microstructures Using Latent Variable Gaussian Process. Journal of Mechanical Design, 143(3).

[5] **Bostanabad, R.,** Chan, Y.C., Wang, L., Zhu, P. and Chen, W.*, 2019. Globally Approximate Gaussian Processes for Big Data With Application to Data-Driven Metamaterials Design. Journal of Mechanical Design, 141(11).

Thanks!

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