FAIR Data and Interpretable AI Framework for Architectured Metamaterials

DOE ASCR PI Meeting

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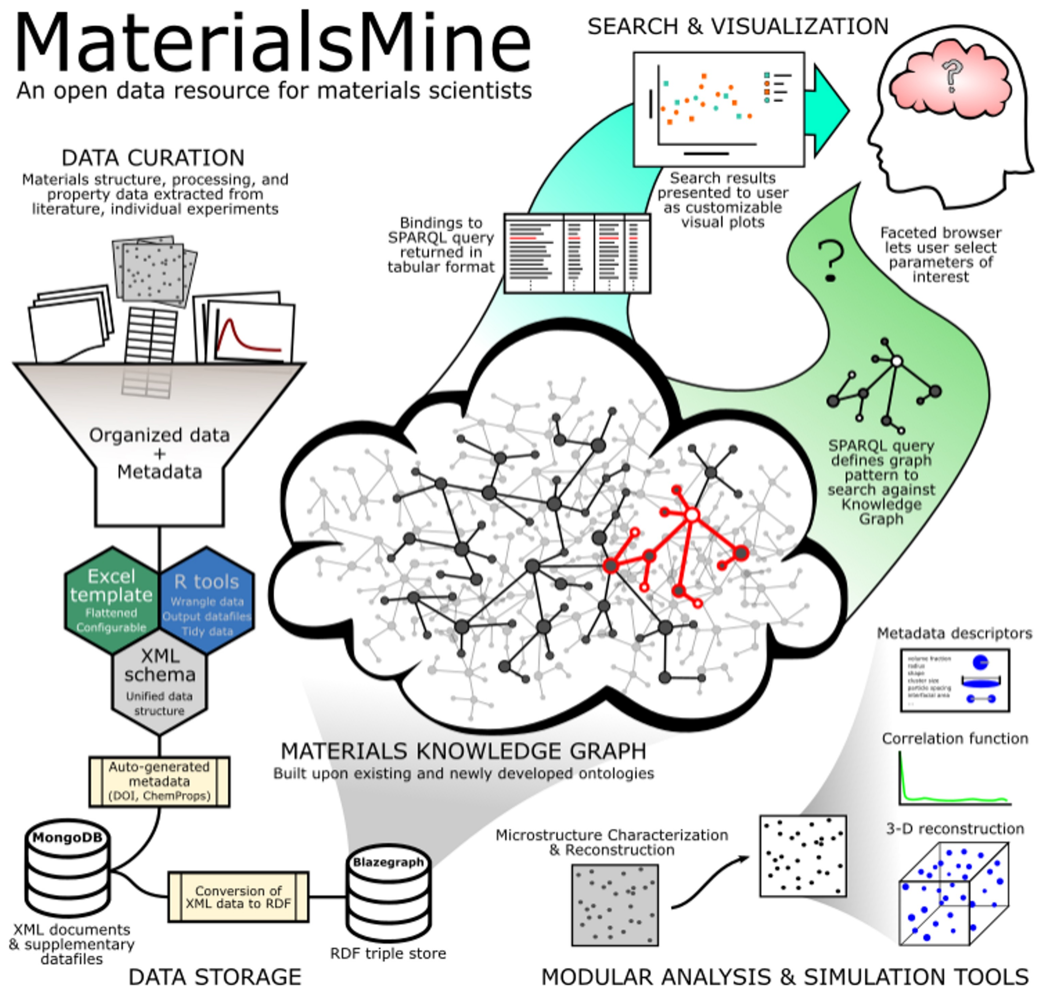
Institution: Northwestern

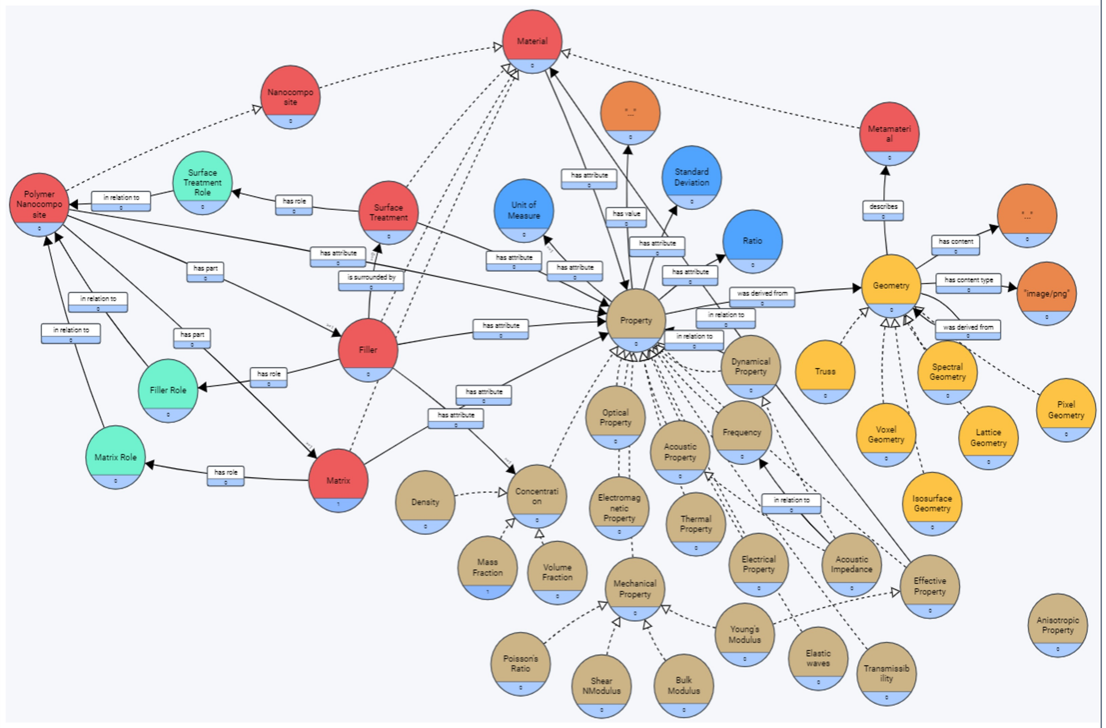
Duke Caltech

Award #
OAC-1835677

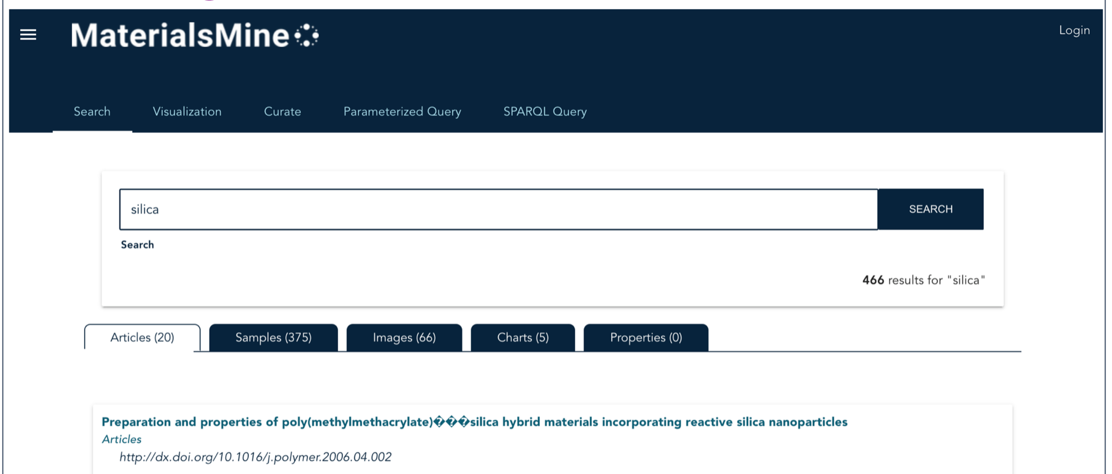
MaterialsMine



Ontology



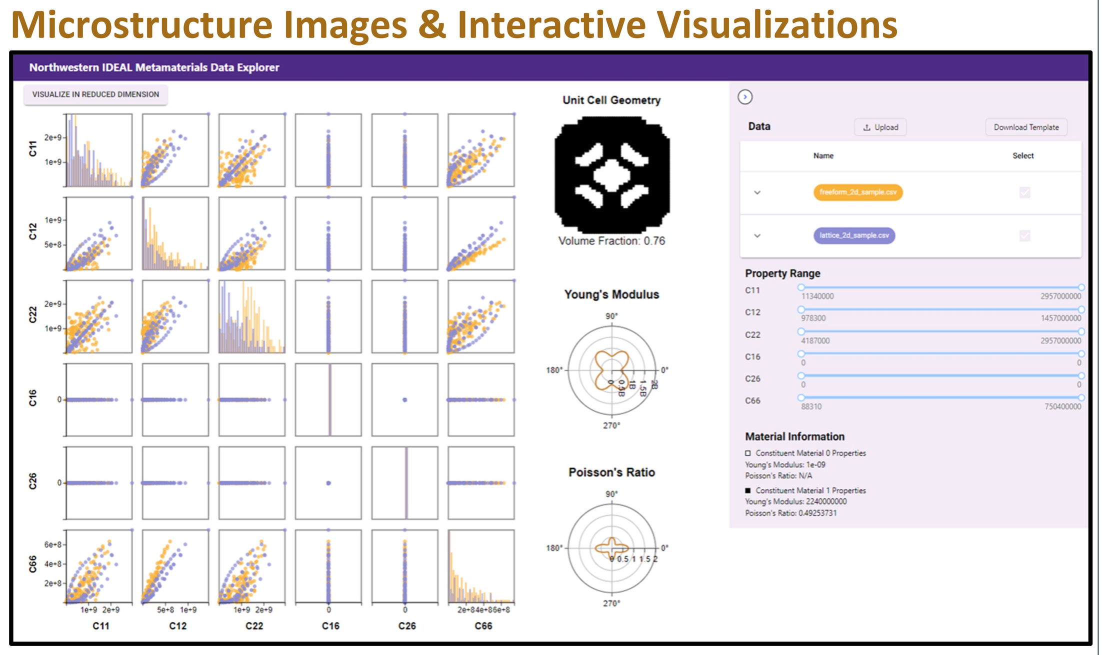
Data Storage & Search

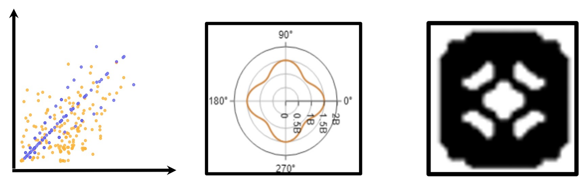


Semantic Data Dictionary (SDD) for curating FAIR (Findable, Accessible, Interoperable, Reusable) data

Column	Label	Attribute
unit_cell_x_pixels		sio:Count
unit_cell_y_pixels		sio:Count
geometry_full	Geometry encoding (full, row-major)	mm:FullMaterialPropertyFieldMatrix
condition	Plane Stress/Plane Strain	mm:Condition
C11	(sxx-exx)	mm:C11
C12	(sxx-eyy)	mm:C12
C22	(syy-eyy)	mm:C22
C16	(sxx-exy)	mm:C16
C26	(syy-exy)	mm:C26
C66	(sxy-exy)	mm:C66

Microstructure Images & Interactive Visualizations





APIs with Documentation

DELETE `/admin/es` Removes resource item from search service. Examples of a resource item are charts, samples or articles

Curation

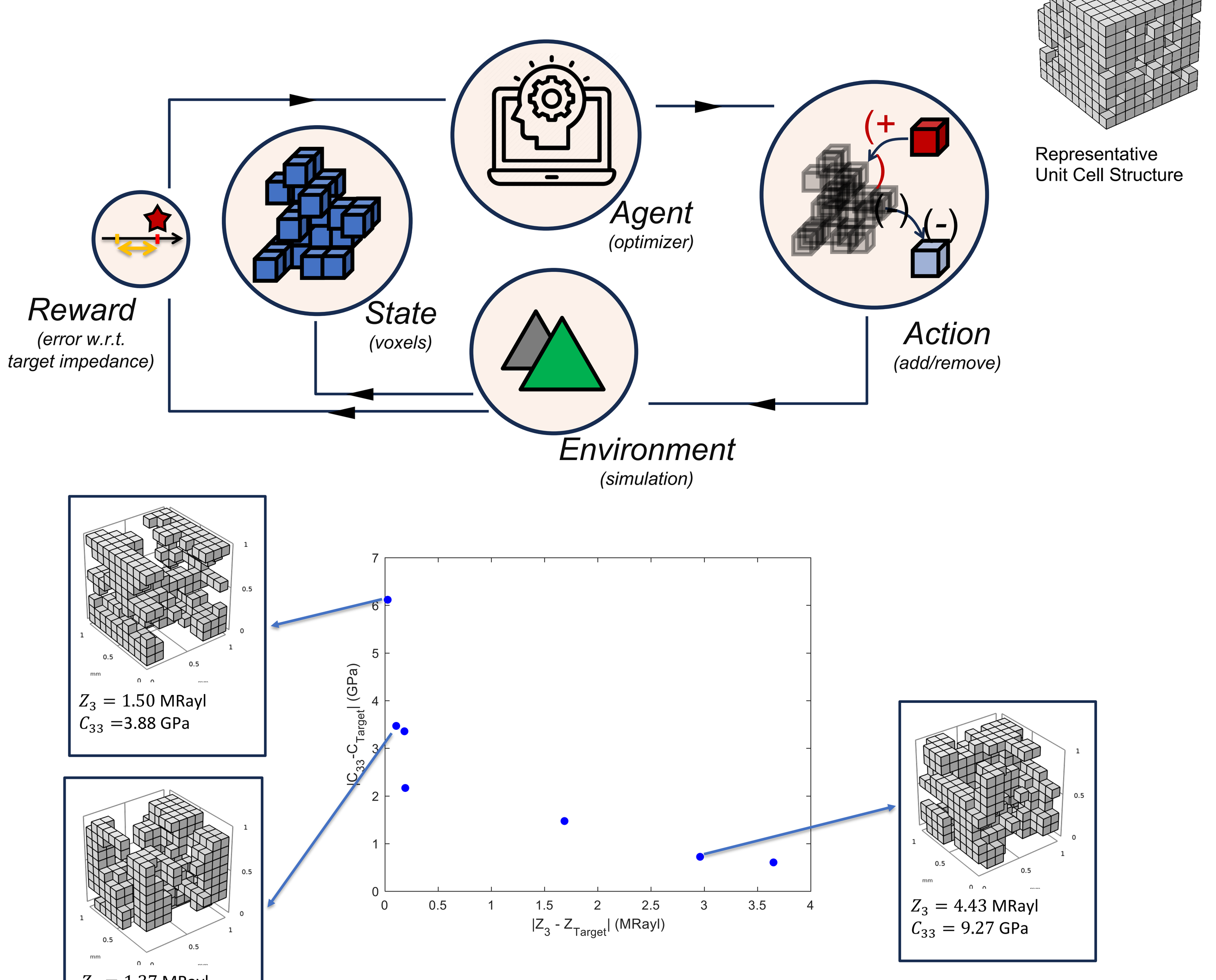
GET `/curate` Gets curation Base Object

POST `/curate` Creates a new curation

MetaMine

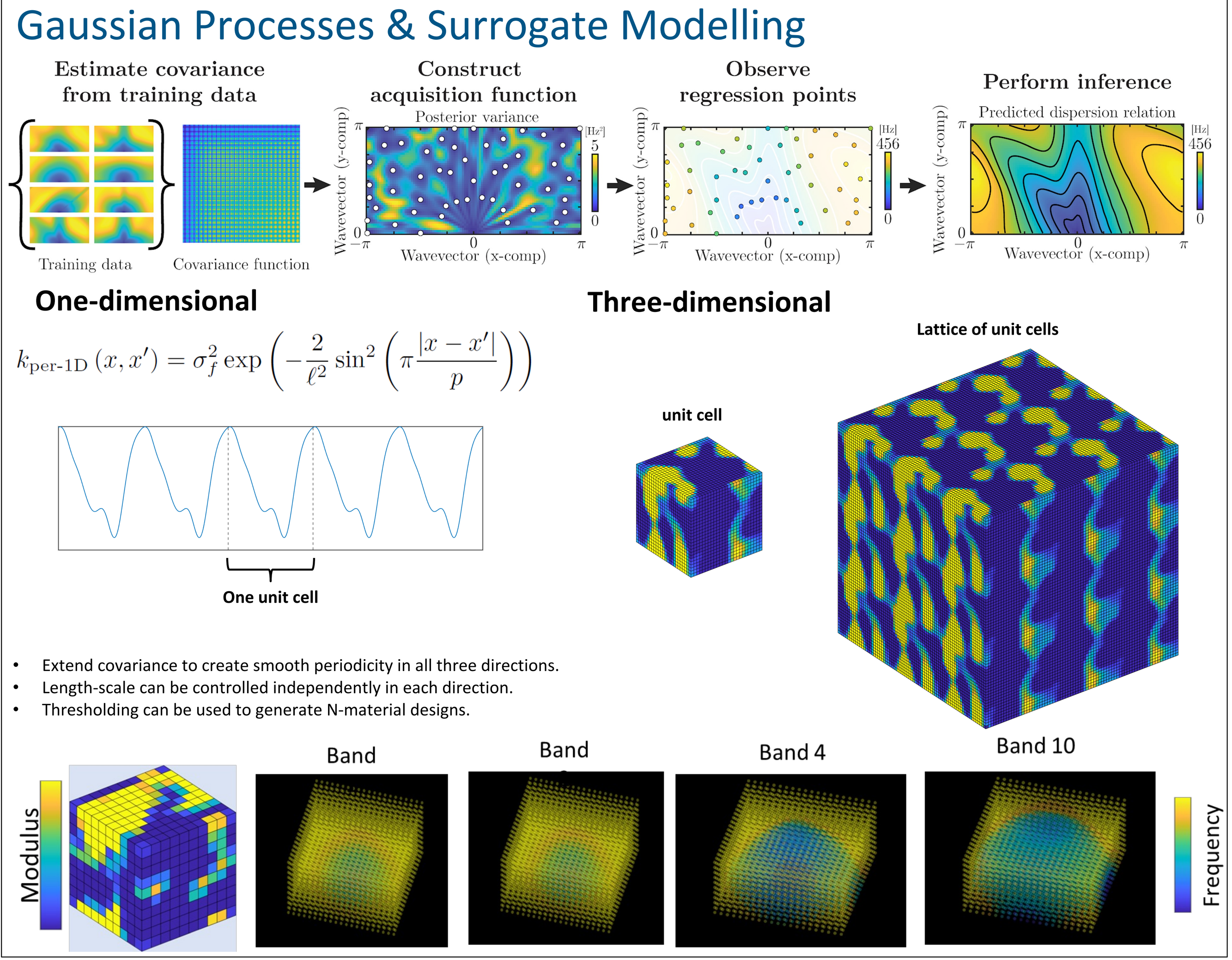
is an open source, data resource for the metamaterial community, involving data from projects like the below

Reinforcement Learning & Evolutionary Algorithms



Objectives:
- Impedance near 1.48 MRayl (at 250kHz))
- Stiffness near 10 GPa

Gaussian Processes & Surrogate Modelling



$$k_{\text{per-1D}}(x, x') = \sigma_f^2 \exp\left(-\frac{2}{\ell^2}\sin^2\left(\pi\frac{|x-x'|}{p}\right)\right)$$

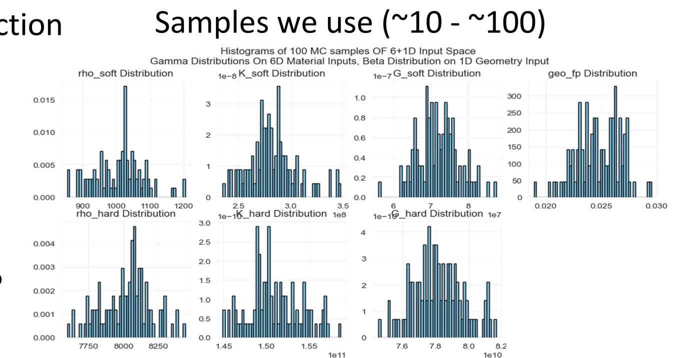
- Extend covariance to create smooth periodicity in all three directions.
- Length-scale can be controlled independently in each direction.
- Thresholding can be used to generate N-material designs.

Uncertainty Quantification for Stochastic Material & Geometries

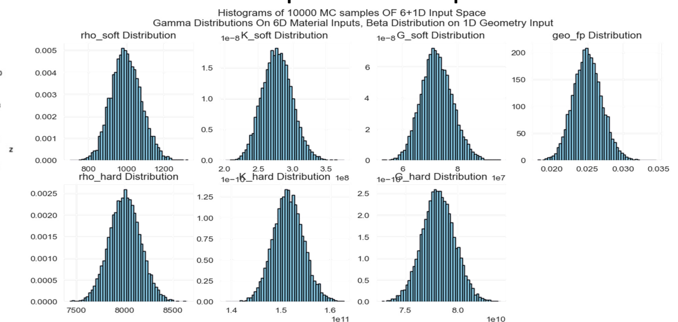
Polynomial Chaos Expansion & Spectral Projection

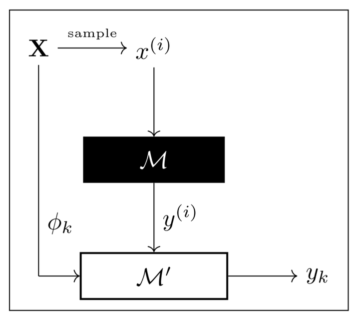
1. Sample Input distributions (X) with Monte Carlo, Quadrature Rule, or Sparse Grid
2. Compute outputs (Y) with true model (M)
3. Form polynomial basis from X (P)
4. Build Surrogate Model (M') from X, Y and P
5. Generate surrogate outputs Y'

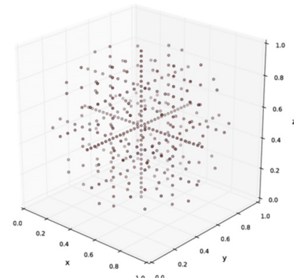
Samples we use (~10 - ~100)



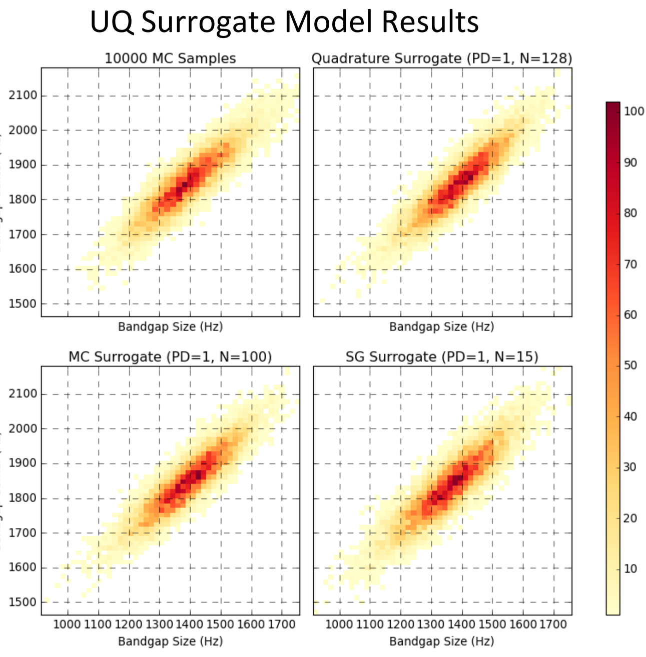
10000 Samples As Comparison



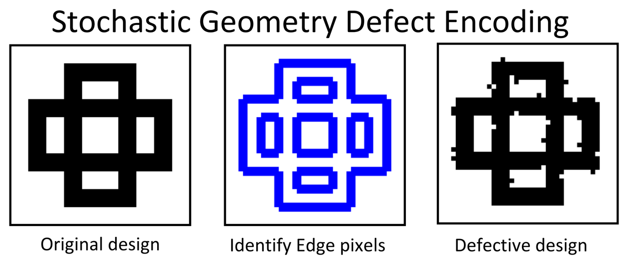




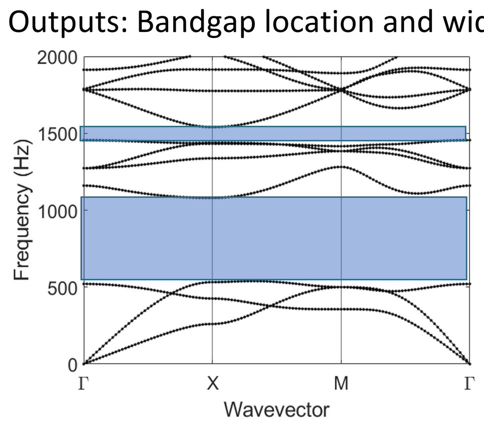
UQ Surrogate Model Results



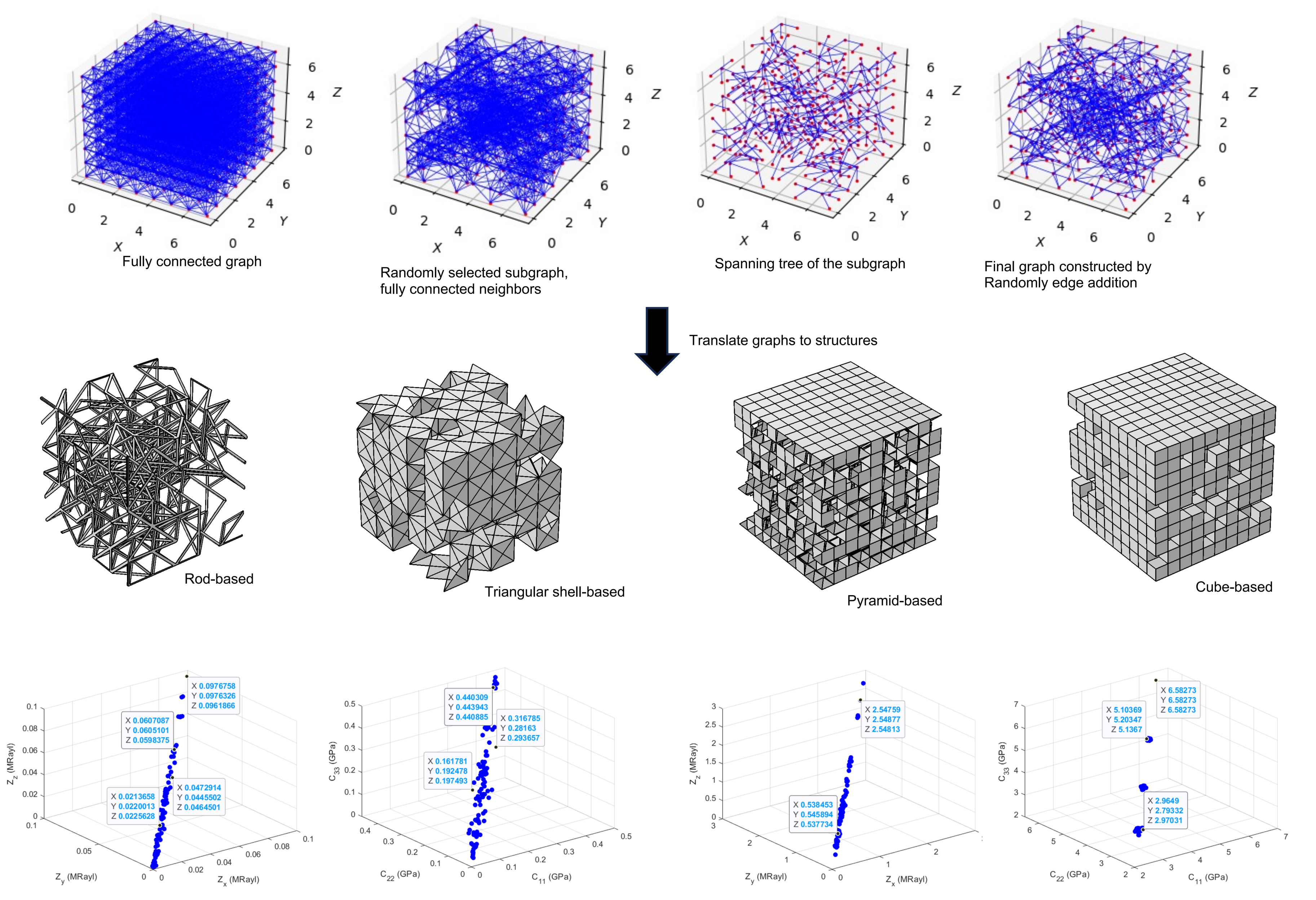
Stochastic Geometry Defect Encoding



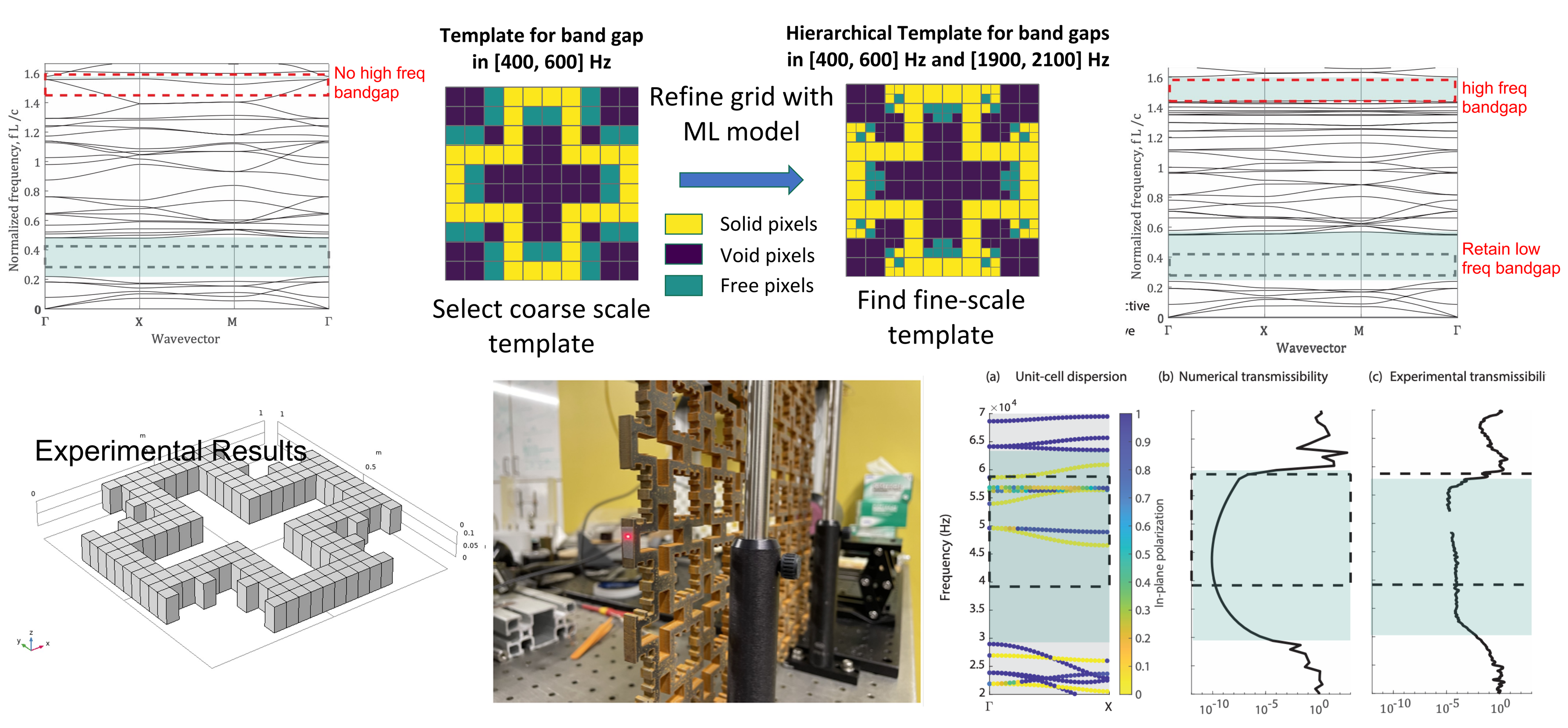
Outputs: Bandgap location and width



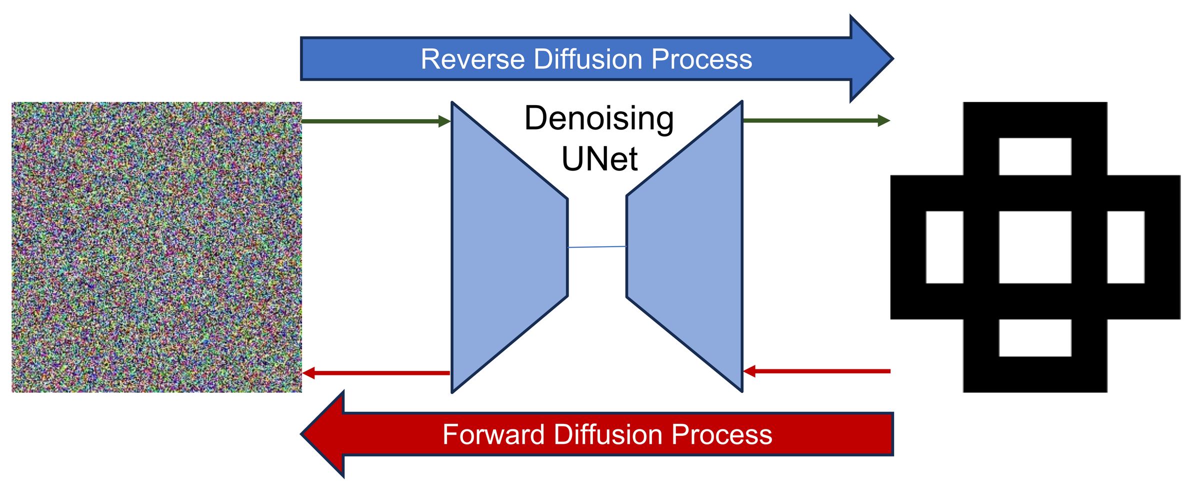
Graph Based Designs



Hierarchical Phononic Metamaterials With Machine Learning



Diffusion Models for Geometry Generation



Training

- Start with sample geometries and context text for relevant material properties, i.e. [BGS:1000; BGC:5000]
- Add noise $\vec{\epsilon_t}$ in incremental amounts t to geometry
- Given t, the noisy image with $\vec{\epsilon_t}$ noise added, and the text prompt, have diffusion model attempt to predict $\vec{\epsilon_t}$.
- With appropriate metric, iterate over many images and text prompts to gain understanding of distribution of geometries conditioned on text prompts

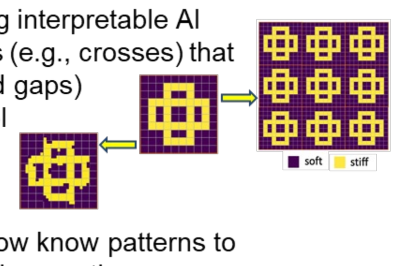
Evaluation

- Start with seed noise and text prompt i.e. [BGS:1000; BGC:5000]
- Model attempts to predict a likely geometry, given seed prompt, by removing a prediction $\vec{\epsilon_t}'$, checking using an appropriate metric if there is still substantial noise remaining. If so, iterate to further remove noise.
- After some iterations, image converges to a geometry, which if model is well trained, exhibits desired properties expressed in text prompt.

Potential Impact

Scientific Achievement

- Custom architectured metamaterials discovered using interpretable AI
- Interpretable AI finds meaningful patterns in unit-cells (e.g., crosses) that give the materials extraordinary properties (e.g., band gaps)
- User-specified, adaptable frequency band gap control
- AI accounts for possible manufacturing defects

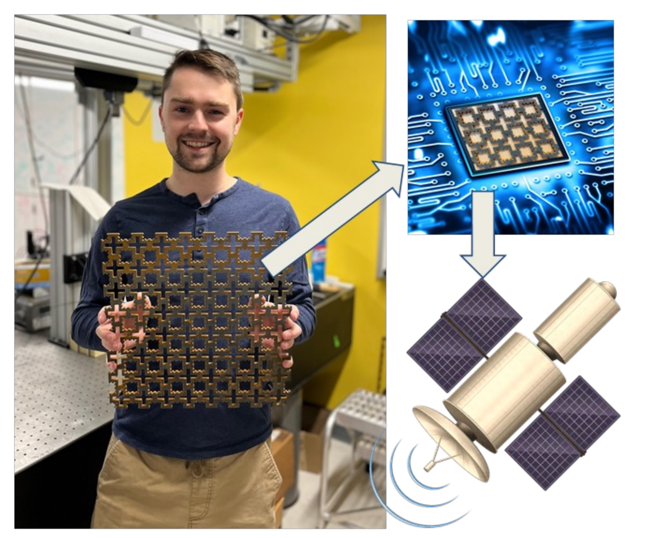


Significance and Impact

- Transformation of metamaterial design with AI. We now know patterns to include in unit cells to achieve specific useful material properties.
- Generalized across design spaces of varying resolutions
- Empowered users with fine-resolution design flexibility
- Designed metamaterials enable custom vibration isolation & ultrasound tech
- Potential for design of next-gen telecommunications devices (SAW/BAW)

Technical Approach

- Our work enables AI exploration of materials in human-understandable way
- Demonstrators prove that real, fabricated designs are successful



The geometry of the metamaterial above was designed by our interpretable AI methods to exhibit specific signal processing behavior. Developed tools enable material designs from large to miniaturized scales. Metamaterials designed for advanced signal processing have potential for impact in medical devices (e.g. ultrasound), structural engineering (e.g. vibration isolation, and non-destructive testing), and telecommunications (e.g. SAW/BAW devices in cellular communications for more compact signal processing, RFID tags, GPS receiver, wireless sensors, remote controls, and satellite communication).