



Sandia
National
Laboratories

CENTER
5500

Data-Driven Optimization of Interlocking Metasurface Design



Nathan Brown, Benjamin Young, Brett Clark, Ophelia Bolmin, Brad Boyce, Philip Noell

Sandia National Laboratories

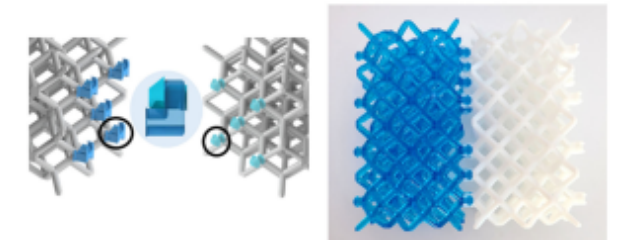
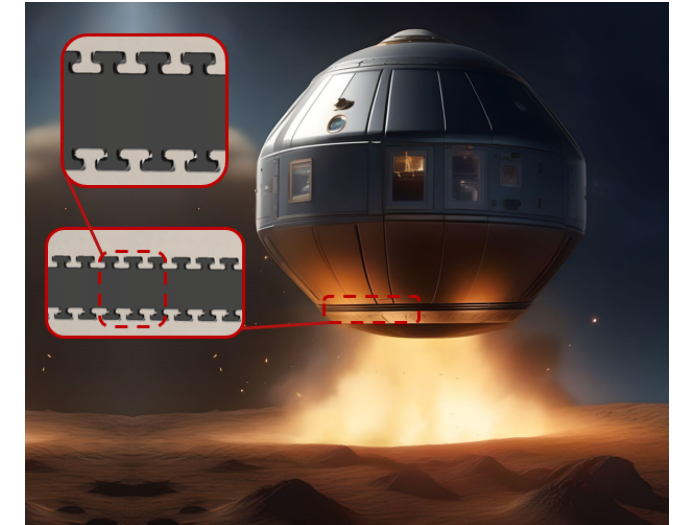
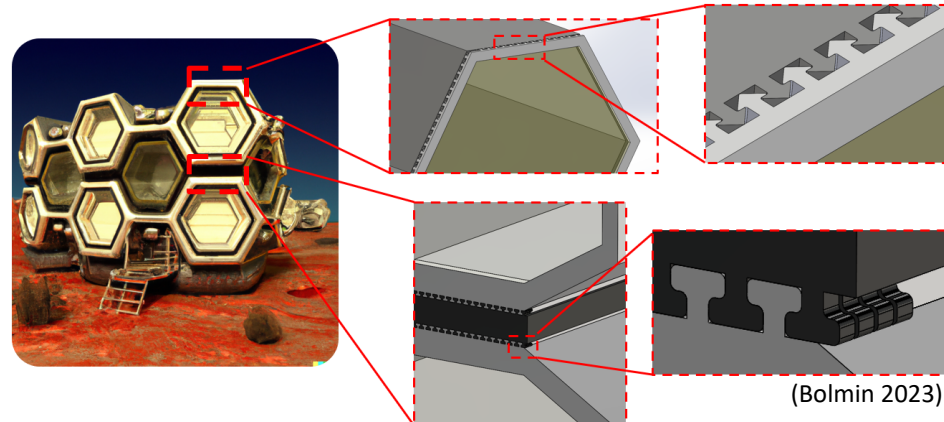
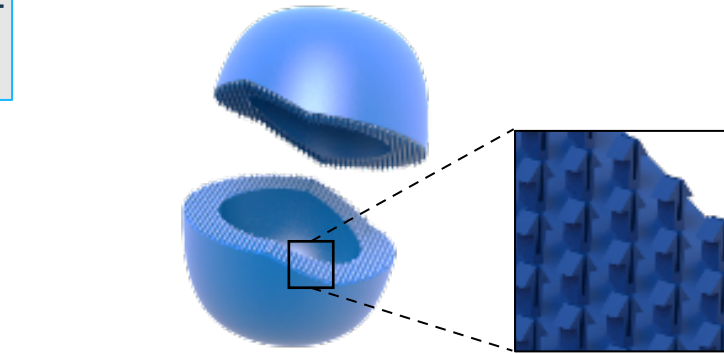
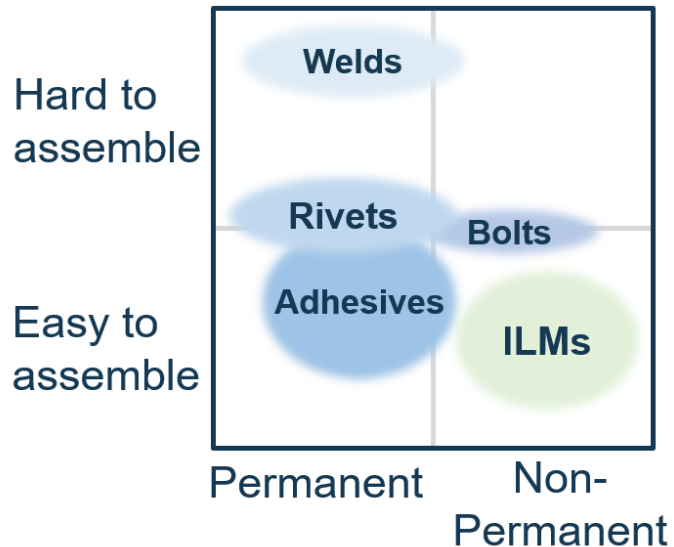
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.



What are interlocking metasurfaces (ILMs)?



ILMs overcome many limitations of existing joining methods

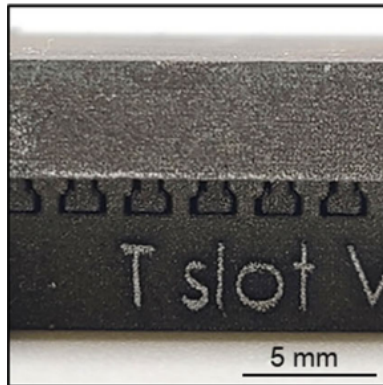


(Bolmin 2023)

Tailoring Mechanical Performance

- Robustness controlled by ILM's **unit cell design**, constitutive material, and unit cell interaction

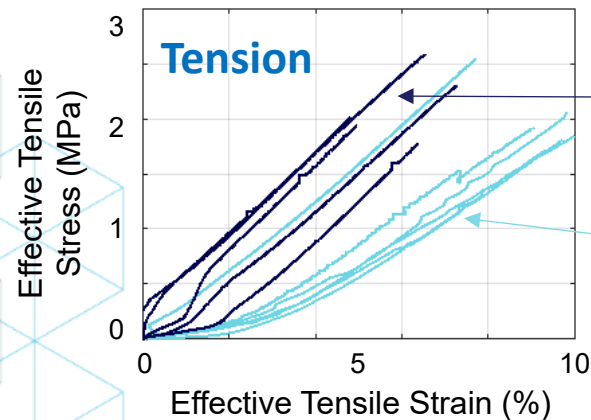
Failure Criteria



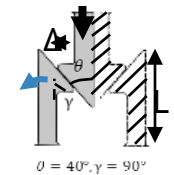
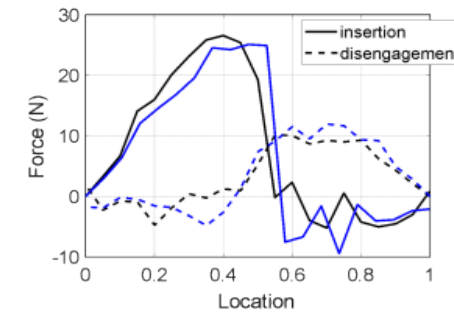
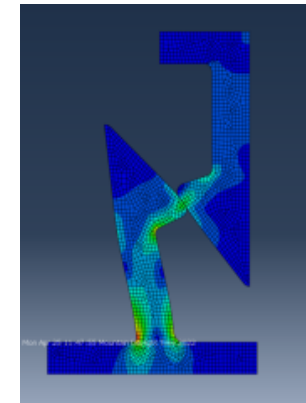
Snapping T-slots



Sliding T-slots



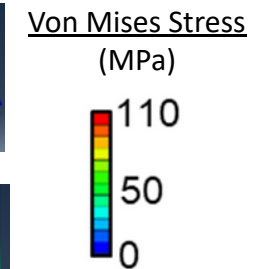
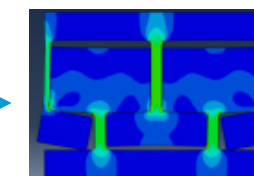
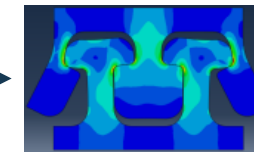
Remateability



$$\begin{aligned} & \text{--- } \theta = 40^\circ, \gamma = 60^\circ \\ & \text{--- } \theta = 40^\circ, \gamma = 70^\circ \end{aligned}$$

$$F > \frac{3EI}{l^3} \Delta \frac{\mu + \tan(\theta)}{1 - \mu \tan(\theta)}$$

Stress Uniformity



Design Methodology Comparison



- Evaluate ILM unit cell performance and capabilities of 4 distinct design methods

Human Intuition

- Expertise
- Experiences
- Nature

Parametric Opt.

- Geometrically parameterize a design
- Optimize parameters according to objectives and constraints

Genetic Algorithm

- Elementally Discrete domain (voxelized design)
- Evolutionary algorithm: Cross-populating and mutations

Conditional Diffusion Model

- Single-shot generation
- Conditions based on objectives/constraints
- Thermo-mechanical properties

Direct design comparison in tension and shear, including experimental validation

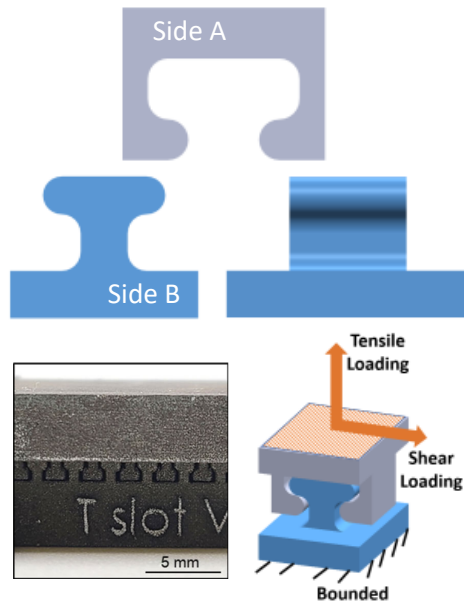
Rapid unit cell generation with emphasis on generalizability

Topology Comparison Methods



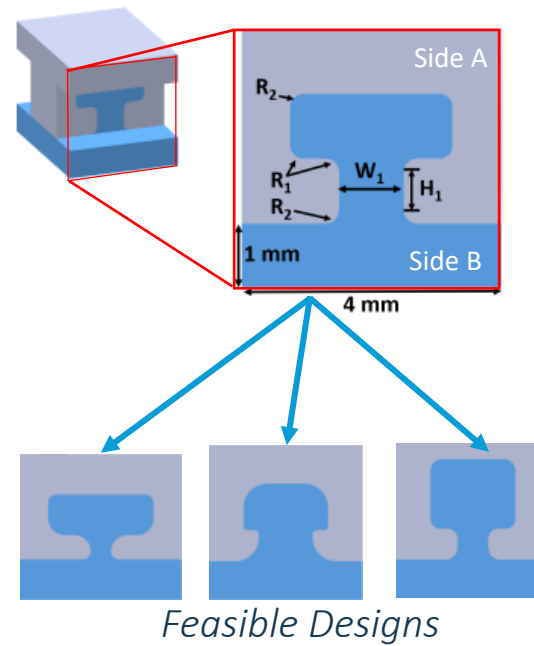
Human Intuition

- “Sliding T-slot”
- Based on designer’s expertise
- No additional optimization



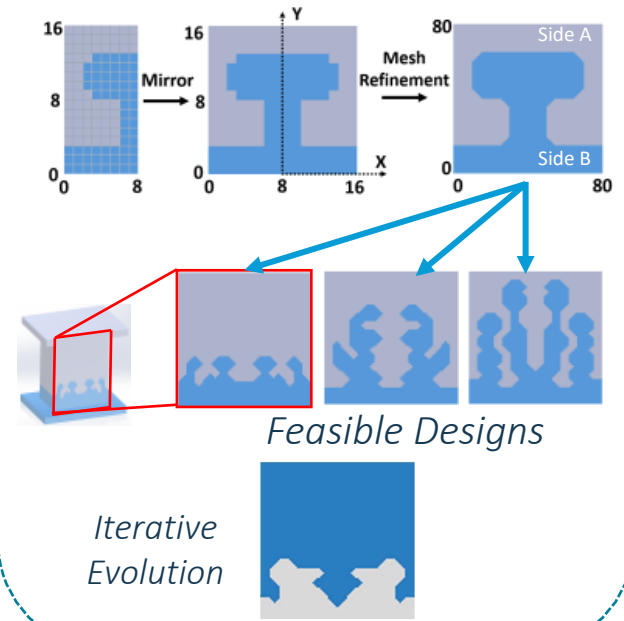
Parametric Optimization

- Parameterized T-slot
- Gradient-based optimization
- Maximize Strength: Tension, Shear, Weighted-sum



Genetic Algorithm

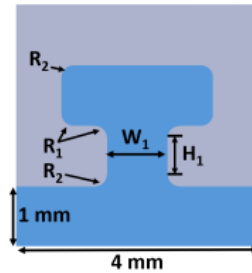
- Evolutionary optimization
- 16x8 mirrored discretized design domain
- Single and Multi-Objective Optimization (Tension/Shear)



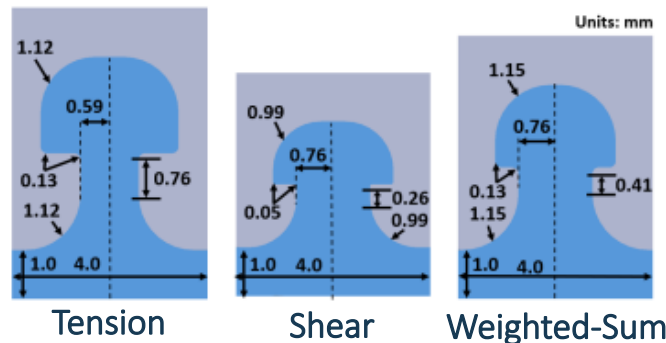
Parametric Optimization

- Parametrization limit uniqueness between topologies
- Differences in height and width

Initial Design

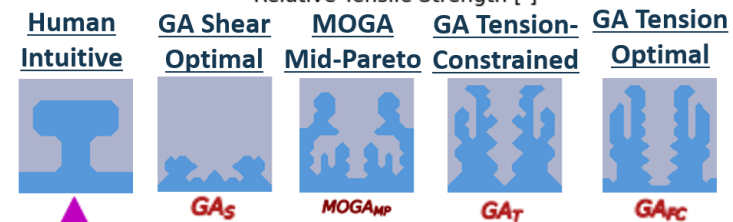
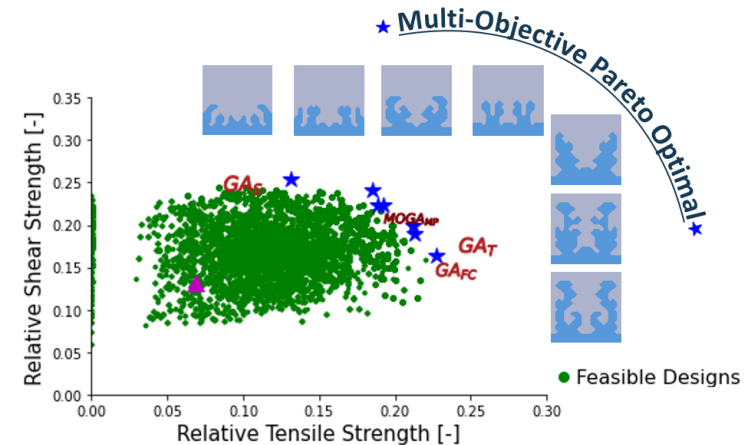


Optimized Designs



Genetic Algorithm

- Considerable change in topology corresponding to objective
- Non-intuitive designs
- **Tension:** Tall, Dendritic **Shear:** Short, sturdy



MOGA: Multi-Objective Genetic Alg.

Constrained: Mimics "infinite" unit cell tessellation

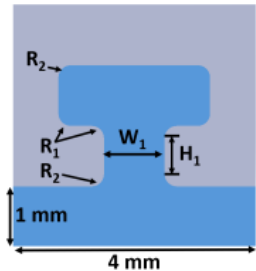
Design Results



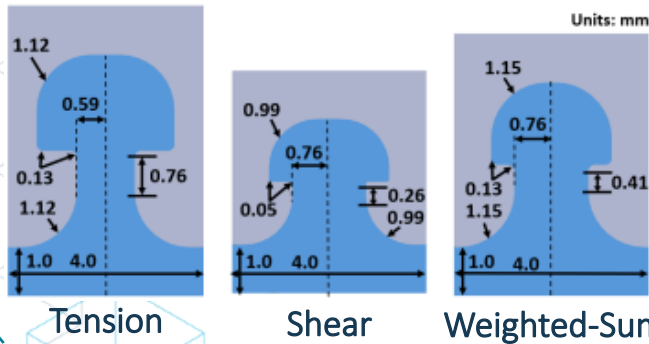
Parametric Optimization

- Parametrization limit uniqueness between topologies
- Differences in height and width

Initial Design

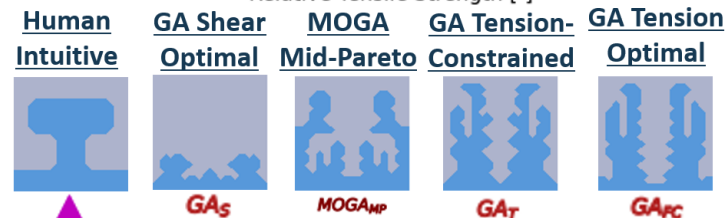
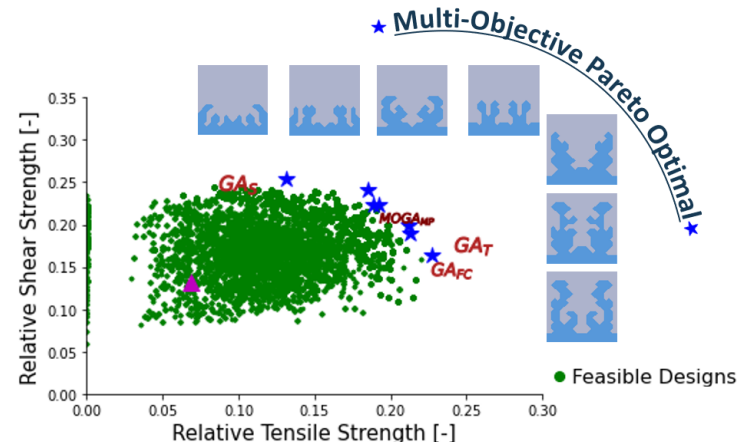


Optimized Designs



Genetic Algorithm

- Considerable changed in topology corresponding to objective
- Non-intuitive designs
- **Tension:** Tall, Dendritic **Shear:** Short, sturdy



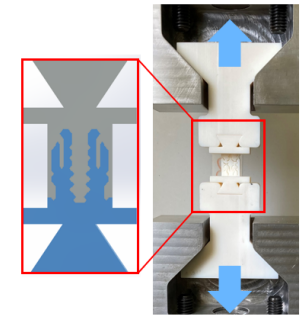
MOGA: Multi-Objective Genetic Alg.

Constrained: Mimics "infinite" unit cell tessellation

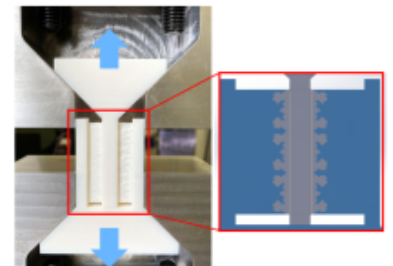
Experimental Testing

- Tested in 1x1, 1x3, and 1x1 Fully Constrained configurations
- Extruded 2D surfaces

Tension Testing



Shear Testing

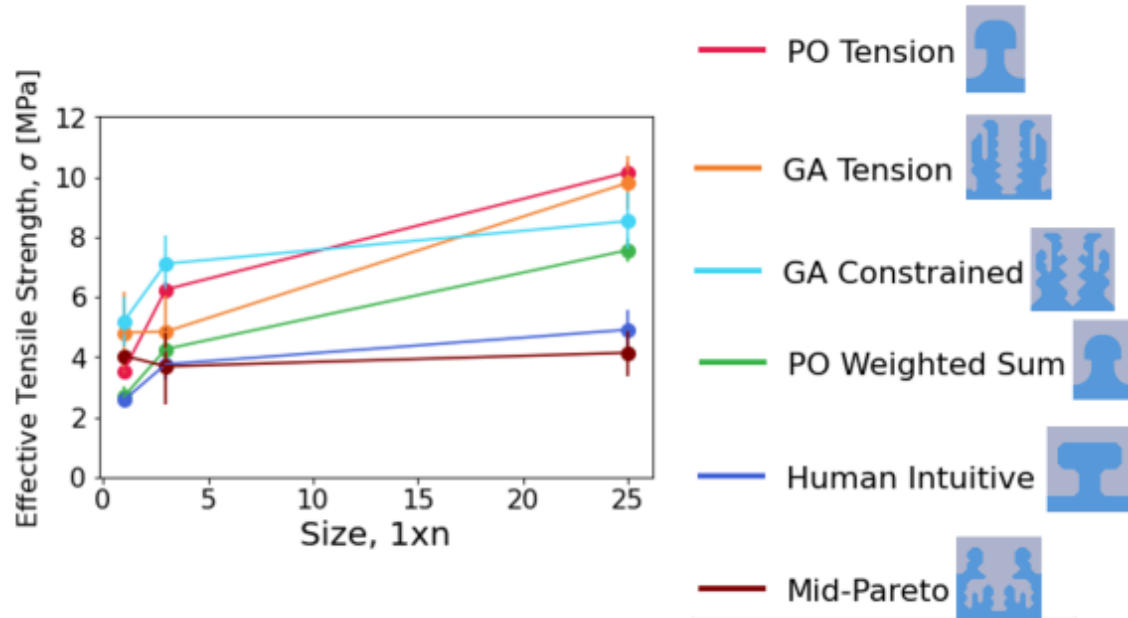


Experimental Results

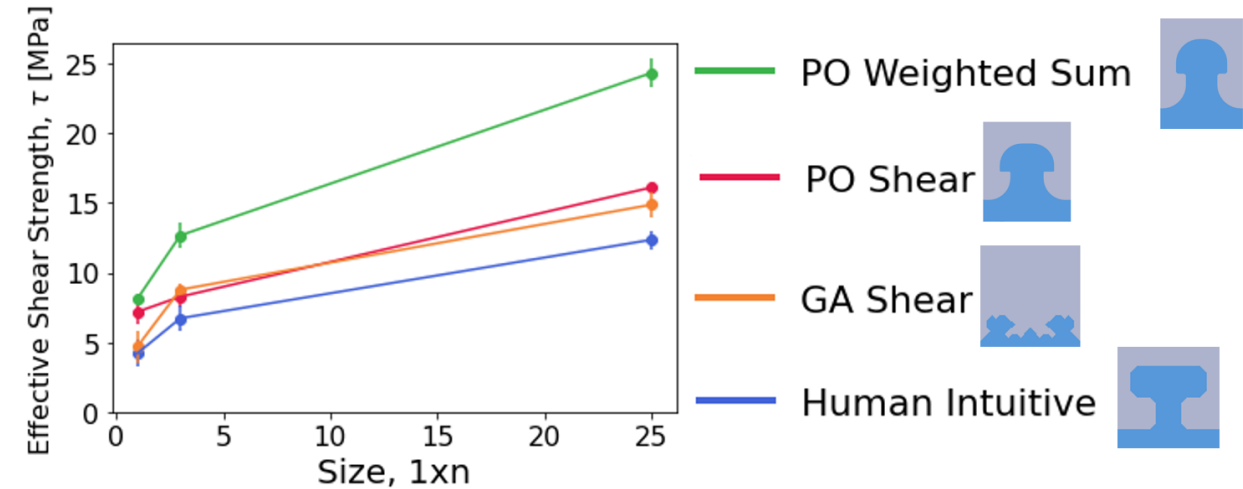


- Both optimization method result in considerable strength increase
- Effective strength increases with tessellation size \rightarrow Unit Cell Interactions

Tension



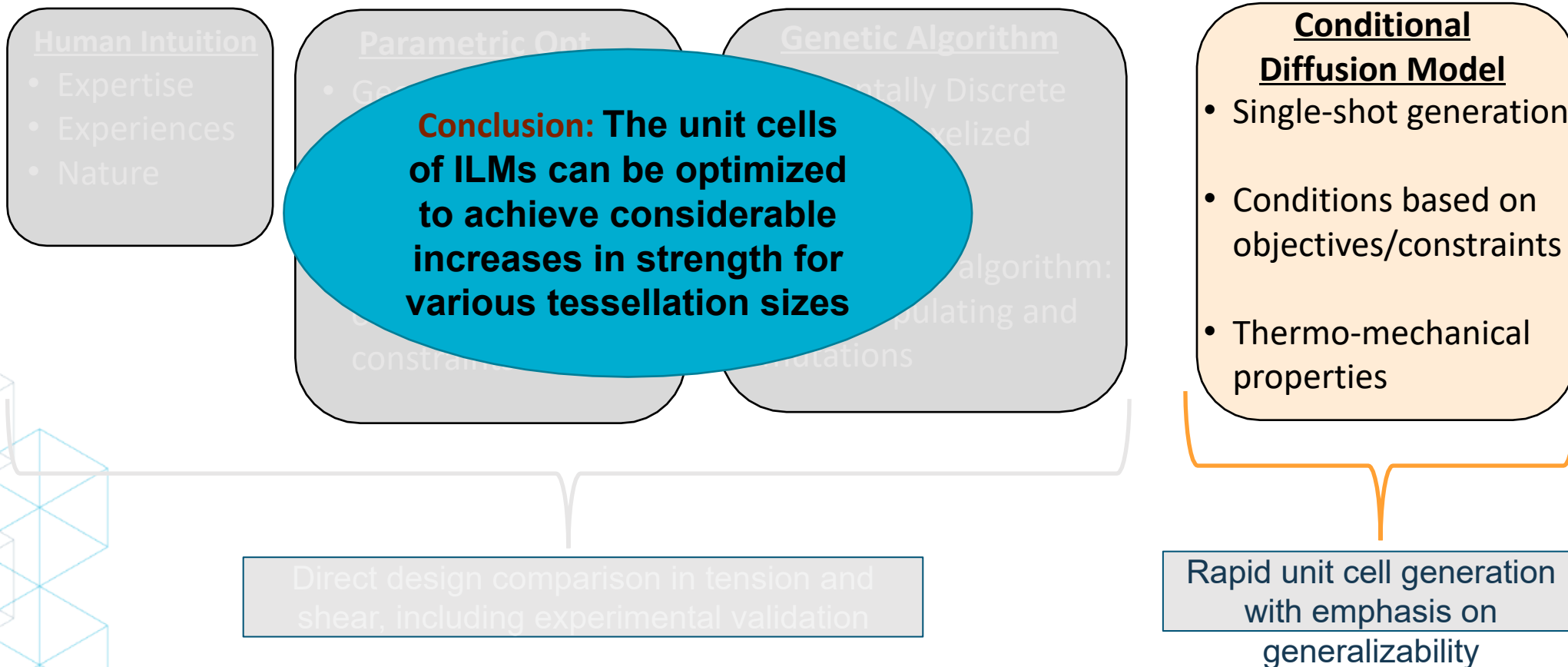
Shear



Design Methodology Comparison



- Evaluate ILM unit cell performance and capabilities of 5 distinct methods



Condition Diffusion Models (CDMs)

- **CDM**: Generative AI method to generate data by iteratively refining random noise, guided by specific conditions or inputs, to produce highly realistic/practical outputs
- Commonly used for “text-to-art” generation →



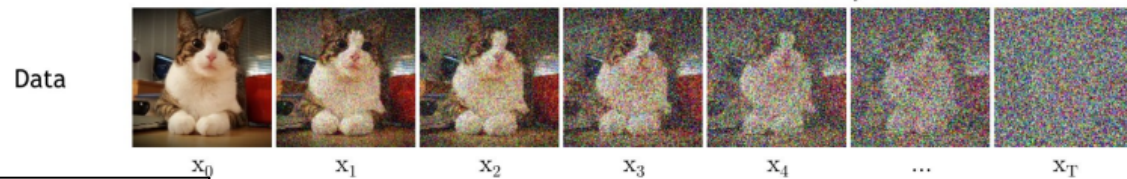
(MidJourney)



(Gemini)

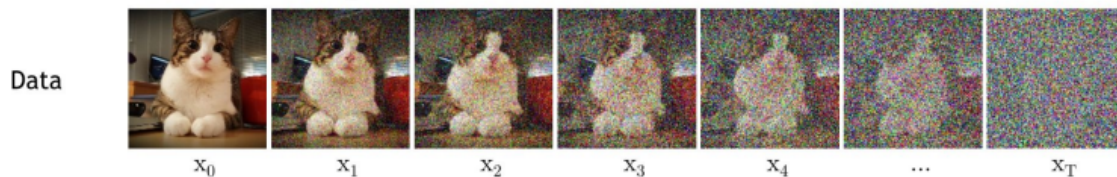
Training

Forward diffusion process (fixed)



$$q(x_t | x_{t-1}, Y)$$

Reverse denoising process (generative)



$$p_\theta(x_{t-1} | x_t, Y)$$

Noise

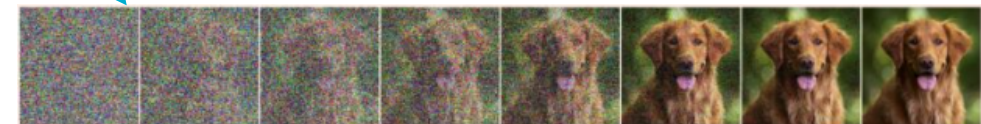
Noise

Testing

Y

“Front facing
photo of large
breed dog”

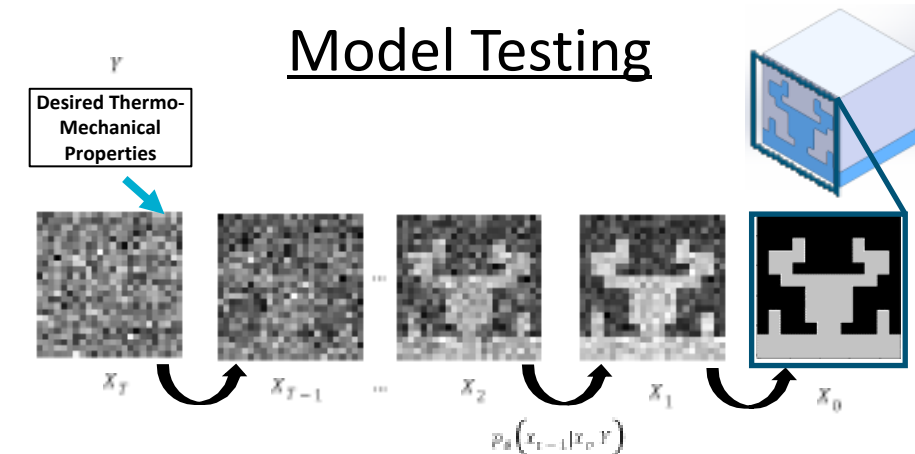
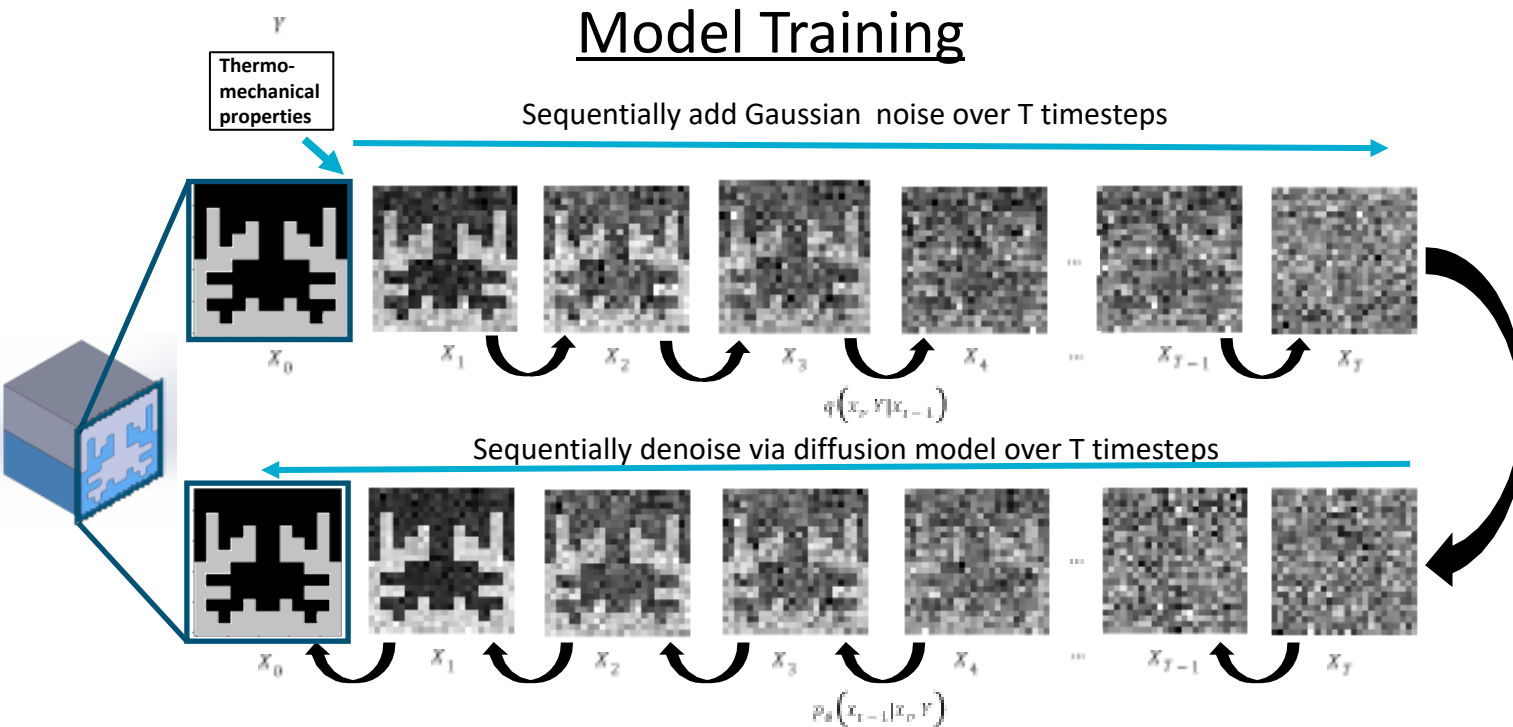
$$p_\theta(x_{t-1} | x_t, Y)$$



CDMs as an Engineering Design Tool



- Use the denoising process to go from complete noise to a viable design candidate
- Replace “text-description” with performance criteria → Desired Thermo-mechanical properties



Generating Training Data

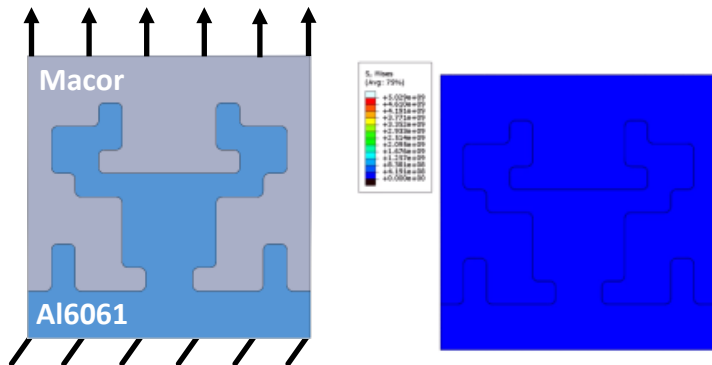


- Training data comprised of **ILM unit cell design** and **corresponding thermo-mechanical properties**
 - Randomly generated ~28k designs and determine properties using finite element analysis (FEA)
 - Voxelized 12x12 (mirrored) design domain, each element either *Macor*, *Al6061*, or void

Thermo-Mechanical Properties

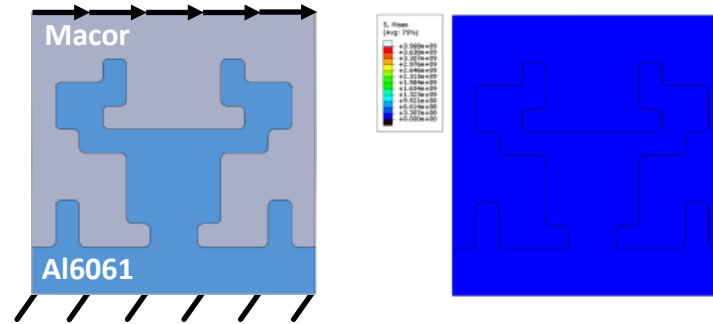
1. Tensile Resultant Force

- Top surface resultant force at material yielding



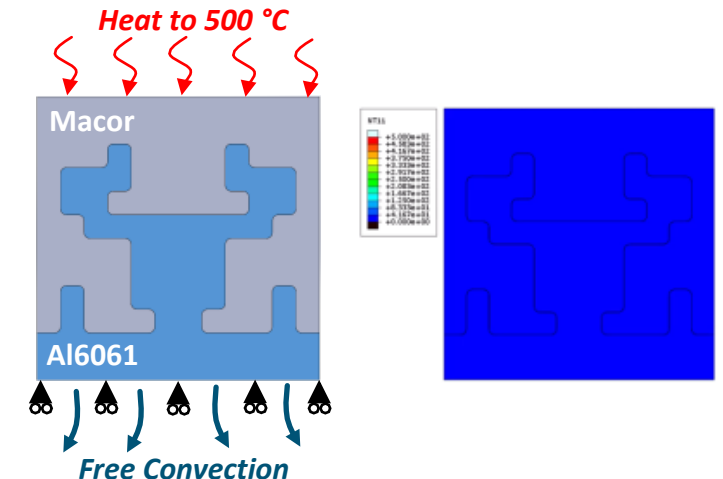
2. Shear Resultant Force

- Top surface resultant force at material yielding



3. Heat Mitigation

- Average bottom surface nodal temperature



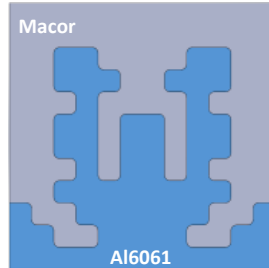
Putting the “Conditional” in CDM



- **40 individual conditions numbers** determined based on thermo-mechanical responses of 28k training samples
- Based on magnitude and ratio of tensile and shear resultant force and average bottom surface nodal temperature

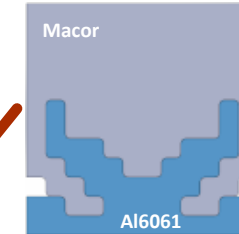
Design 2 (Cond. No. 39)

TRF: 1745 N SRF:566N Temp: 401



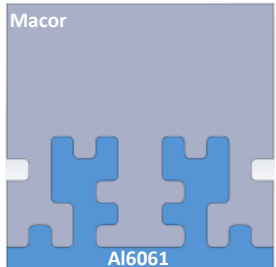
Design 3 (Cond. No. 14)

TRF: 1050 N SRF:965N Temp: 315



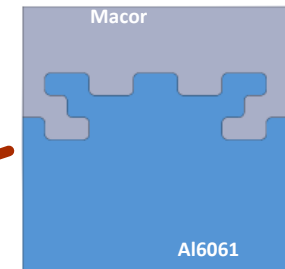
Design 1 (Cond. No. 18)

TRF: 1487 N SRF:515N Temp: 294



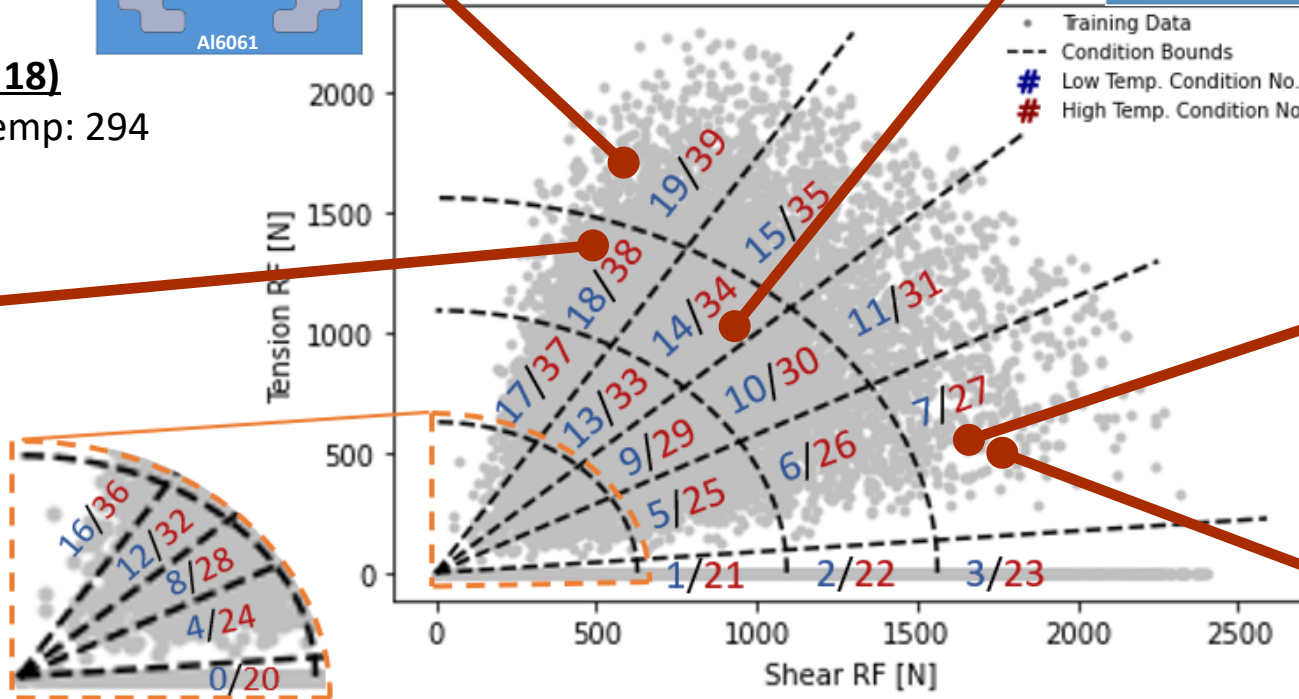
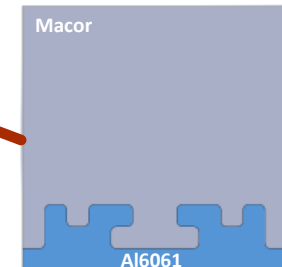
Design 4 (Cond. No. 27)

TRF: 491 N SRF:1659N Temp: 365



Design 5 (Cond. No. 7)

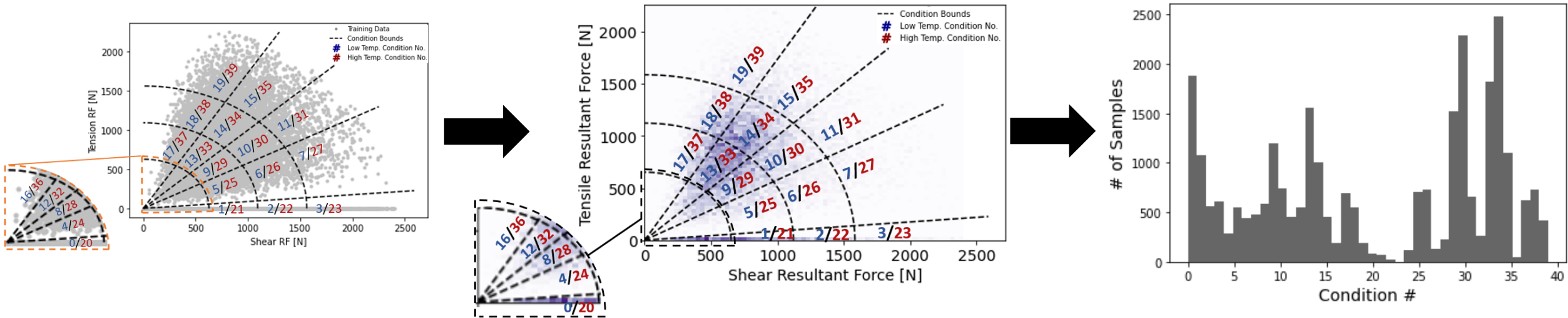
TRF: 384 N SRF:1789N Temp: 281



Putting the “Conditional” in CDM



- **40 individual conditions numbers** determined based on thermo-mechanical responses of 28k training samples
- Based on magnitude and ratio of tensile and shear resultant force and average bottom surface nodal temperature

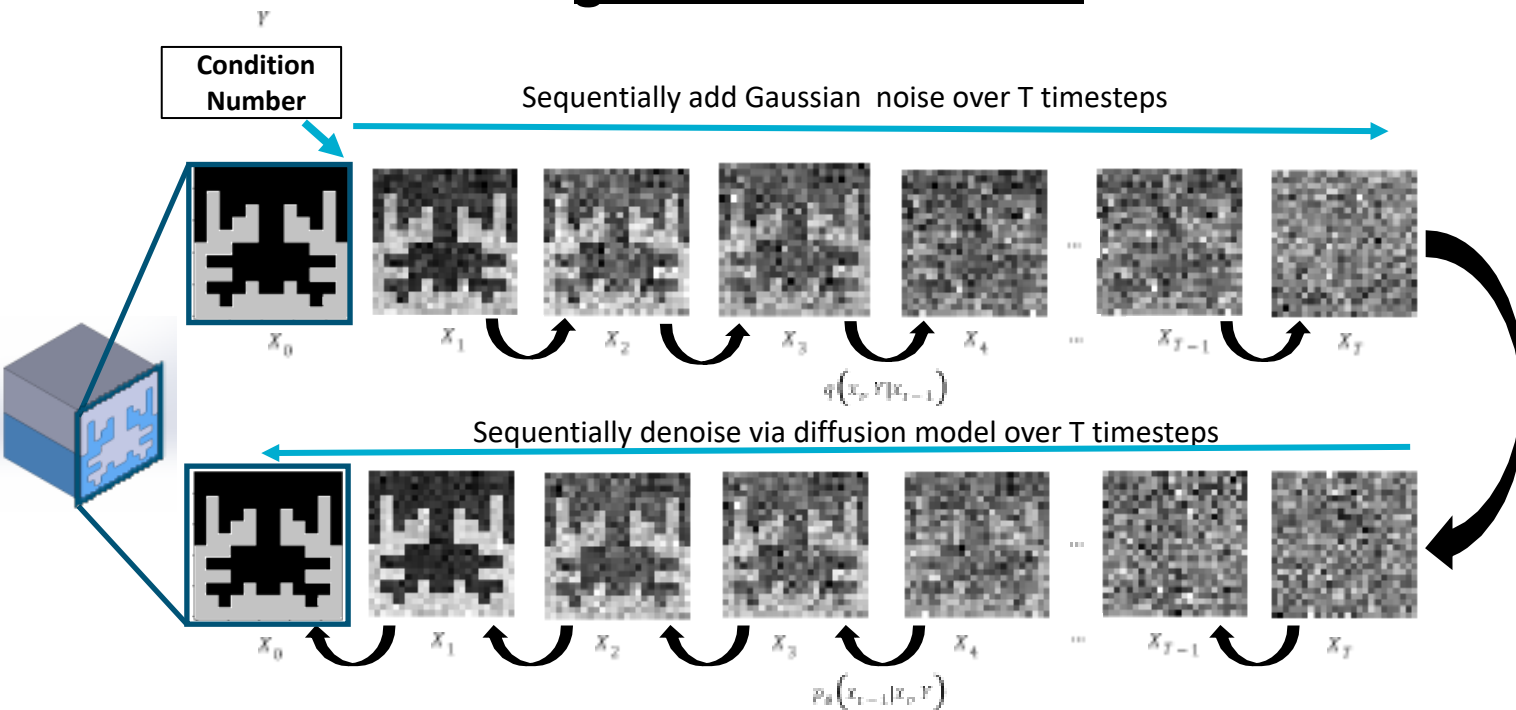


CDMs as an Engineering Design Tool



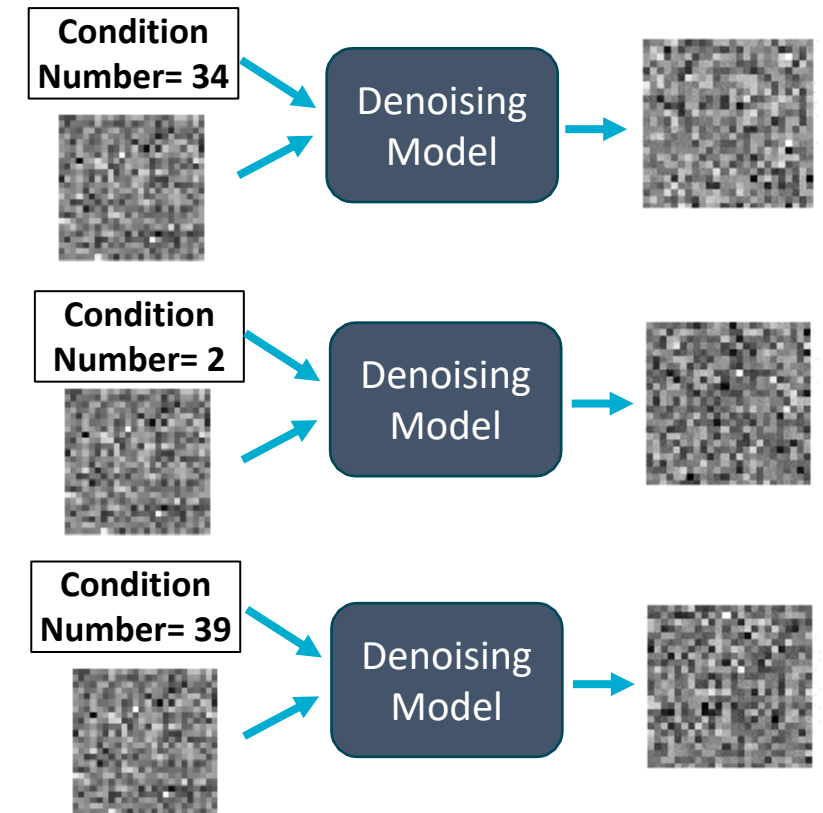
- Feed the 28k unit cell designs and accompanying condition number through the noising and denoising process

Model Training w/ 28k randomly generated unit cells



Model Testing

- Pick condition # based on desired thermo-mechanical properties



Generalized Design Generation

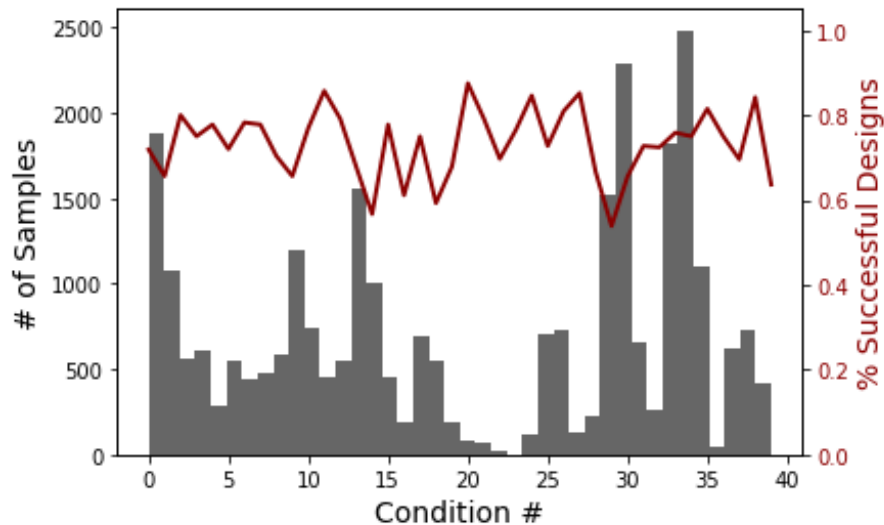


- The model was prompted to generate designs based on 1000 random condition numbers
 - Generate design via CDM → Tested Design via FEA → Compare FEA result to condition bounds

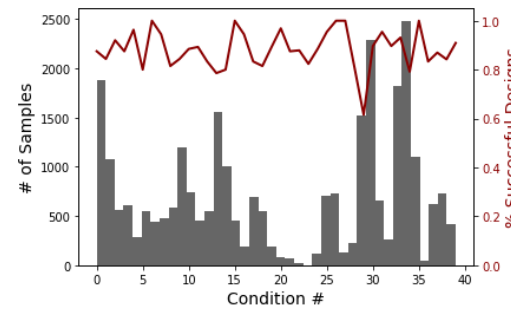
Conditions	Avg. Success Rate
All Conditions	73.3%
Angle	86.0%
Magnitude	88.2%
Thermal	95.6%

- The ability to achieve desired properties does not appear to be condition number dependent!

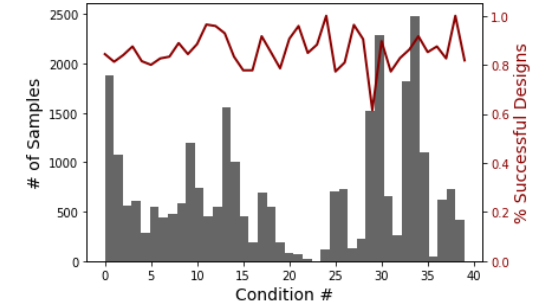
All Conditions



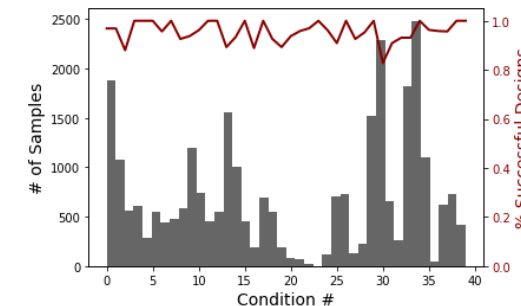
Magnitude



Angle



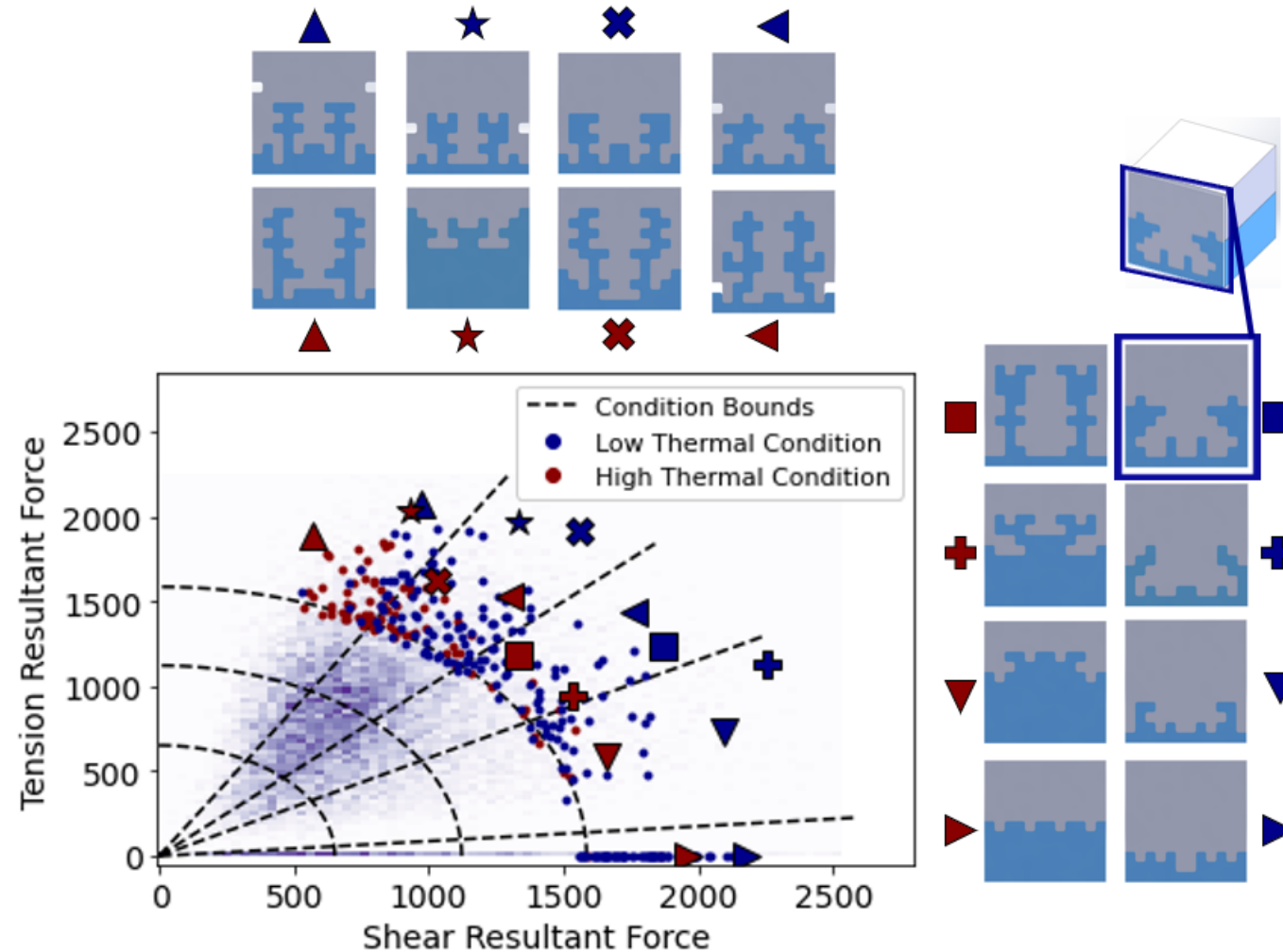
Heat Transfer



“Pareto Front” Approach – 40 conditions



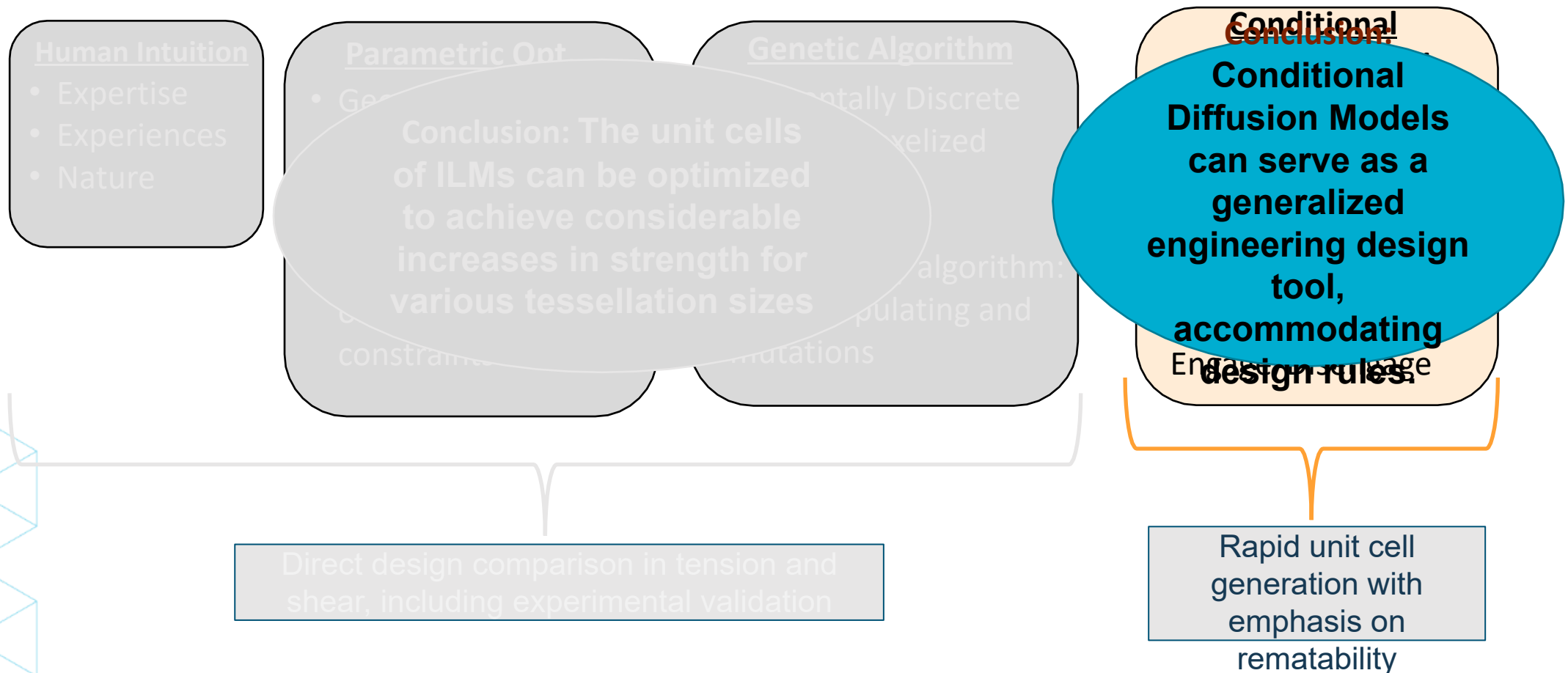
- Testing the model to produce extremes results in plethora of high performing design solutions
- Able to produce designs with high mechanical strength while achieving varying thermal responses



Design Methodology Comparison

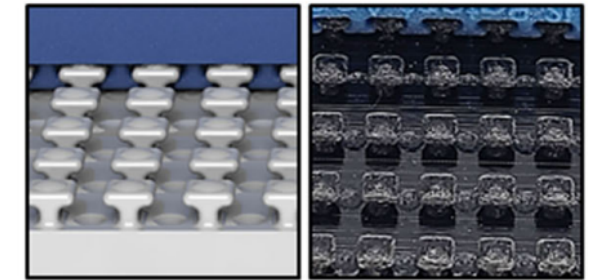
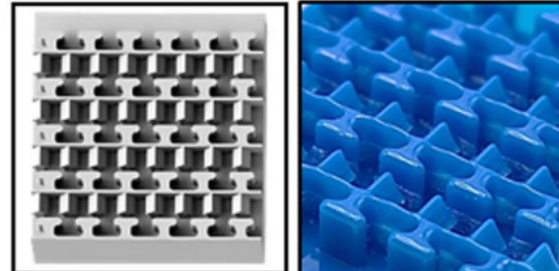
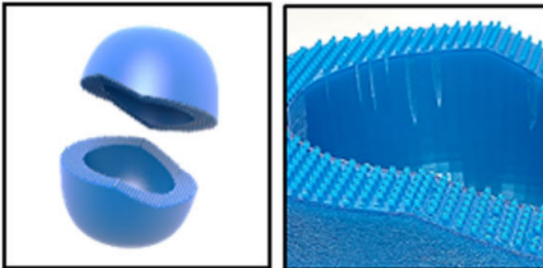
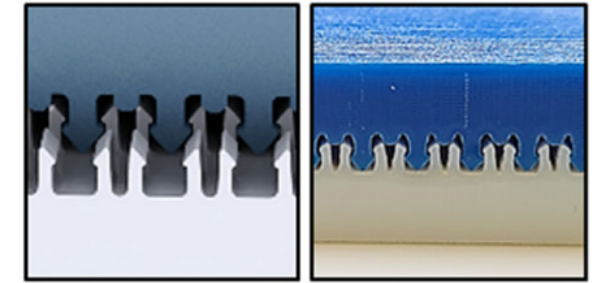
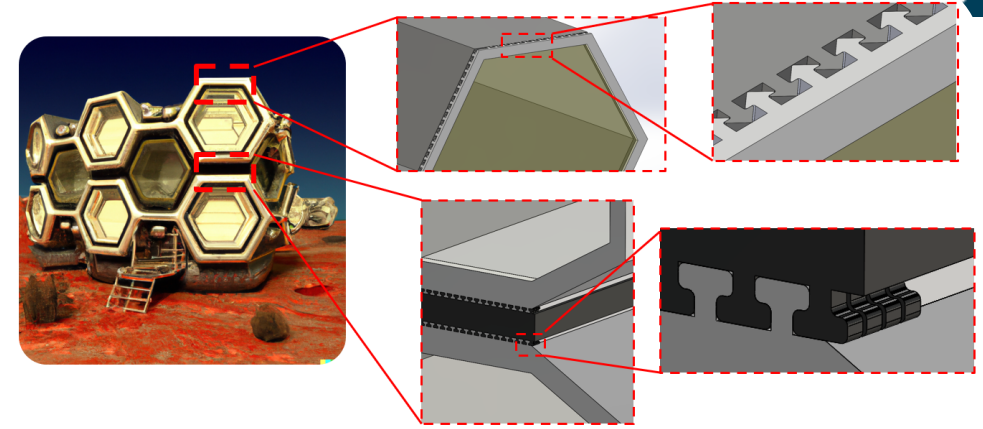


- Evaluate ILM unit cell performance and capabilities of 5 distinct methods



Conclusions

- Interlocking metasurfaces (ILMs) are a mechanically robust, non-permanent, environmentally durable alternative to traditional joining technologies
- ILMs' mechanical (and thermal) properties are dependent on feature topology
- ILMs can be optimized using a host of design methodologies
 - **Human intuition:** Fastest
 - **GA and PO:** Well established methods to achieve high performing solutions
 - **CDM:** Serve as generalizable tools for complex design



Thank you!

Questions?

Nathan Brown – nkbrown@sandia.gov