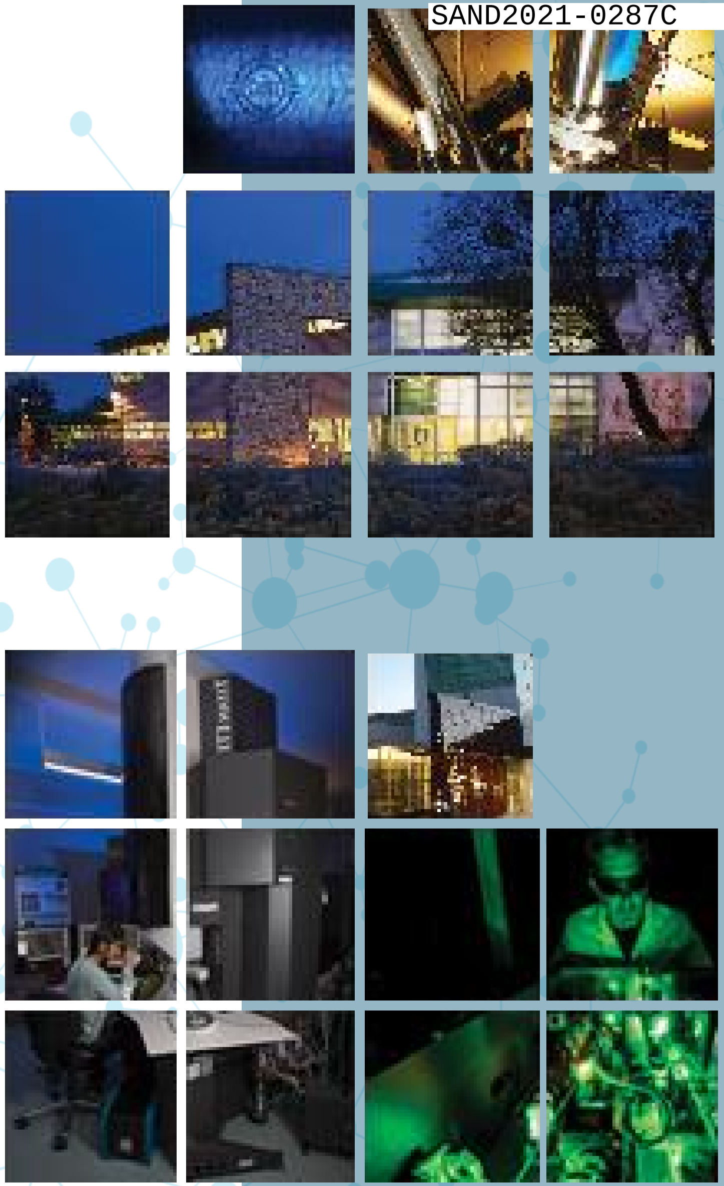
This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

SAND2021-0287C

Pragmatic Generative Optimization of Novel Structural Lattice Metamaterials with Machine Learning



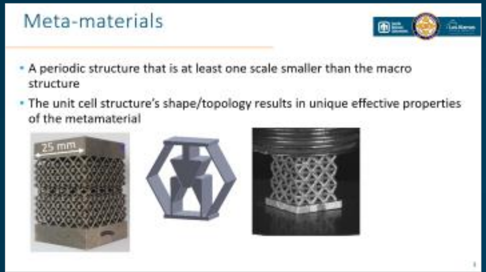
PRESENTED BY

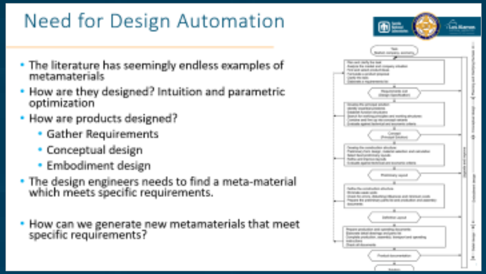
Anthony Garland (agarlan@sandia.gov)

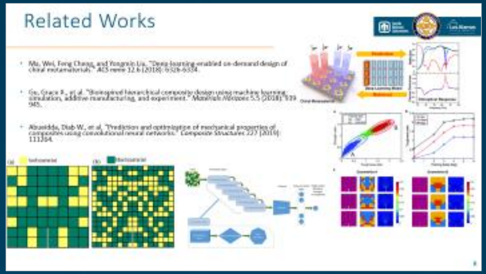
Collaborators: Ben White; Scott Jensen; Brad Boyce

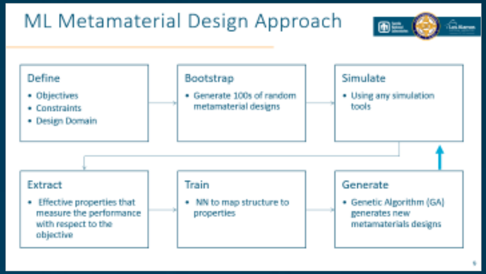
This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.

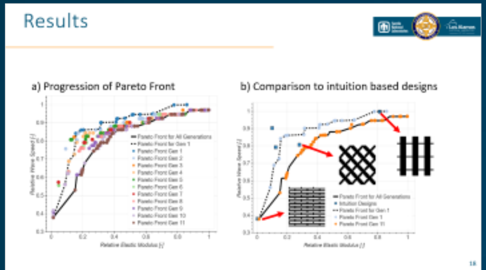
Overview

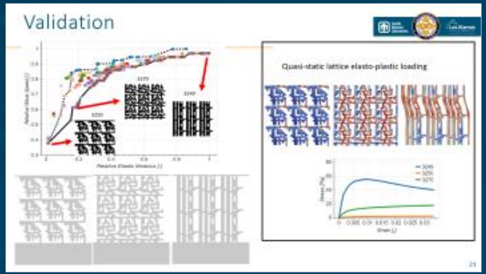

Meta-materials
A periodic structure that is at least one scale smaller than the macro structure
The unit cell structure's shape/topology results in unique effective properties of the metamaterial
25 mm

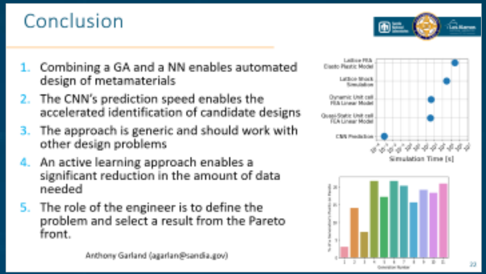

Need for Design Automation
The literature has seemingly endless examples of metamaterials
How are they designed? Intuition and parametric optimization
How are products designed?
Gather Requirements
Conceptual design
Embodiment design
The design engineers needs to find a meta-material which meets specific requirements.
How can we generate new metamaterials that meet specific requirements?


Related Works


ML Metamaterial Design Approach
Define
Objectives
Constraints
Design Domain
Bootstrap
Generate 100s of random metamaterial designs
Simulate
Using any simulation tools
Extract
Effective properties that measure the performance with respect to the objective
Train
NN to map structure to properties
Generate
Genetic Algorithm (GA) generates new metamaterials designs


Results
a) Progression of Pareto Front
b) Comparison to intuition based designs


Validation
Quasi-static lattice elasto-plastic loading


Conclusion
1. Combining a GA and a NN enables automated design of metamaterials
2. The CNN's prediction speed enables the accelerated identification of candidate designs
3. The approach is generic and should work with other design problems
4. An active learning approach enables a significant reduction in the amount of data needed
5. The role of the engineer is to define the problem and select a result from the Pareto front.
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Simulation Time [s]

Meta-materials

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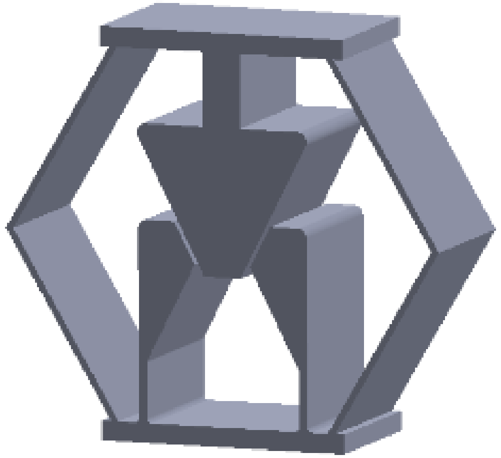

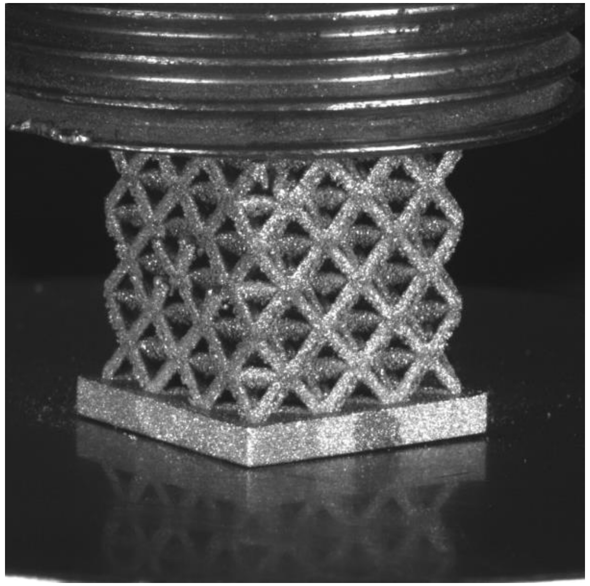

Meta-materials II

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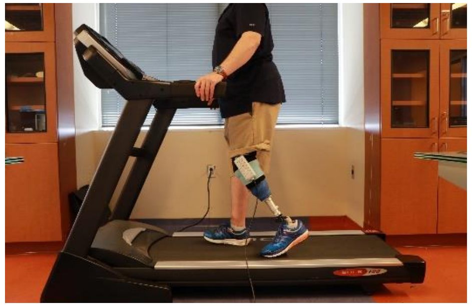

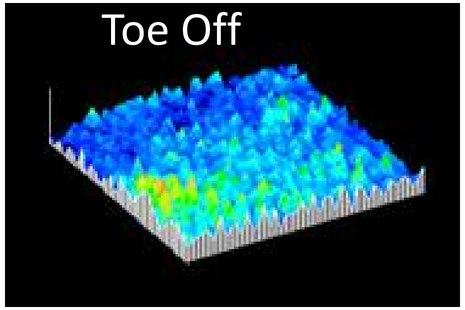

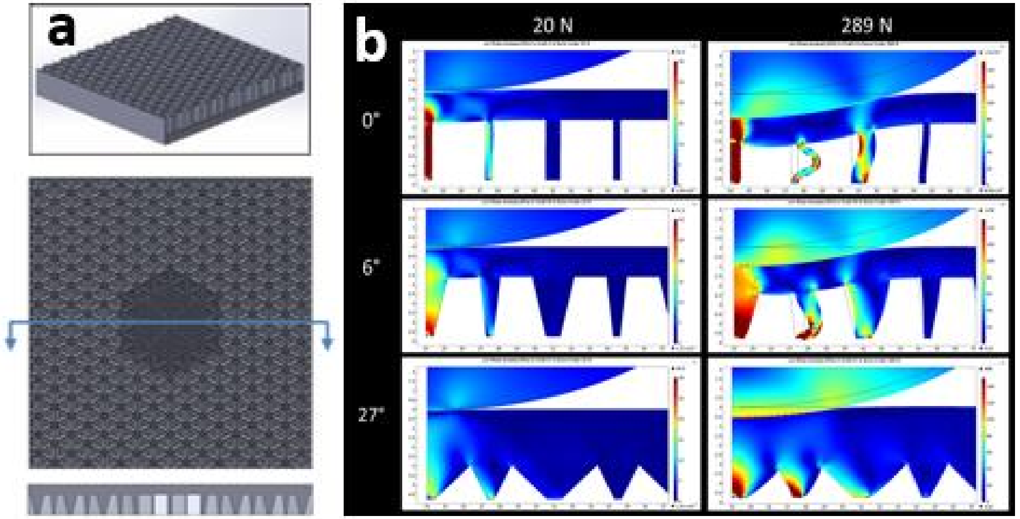

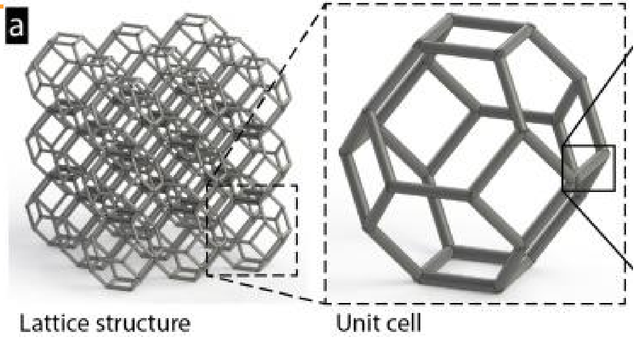

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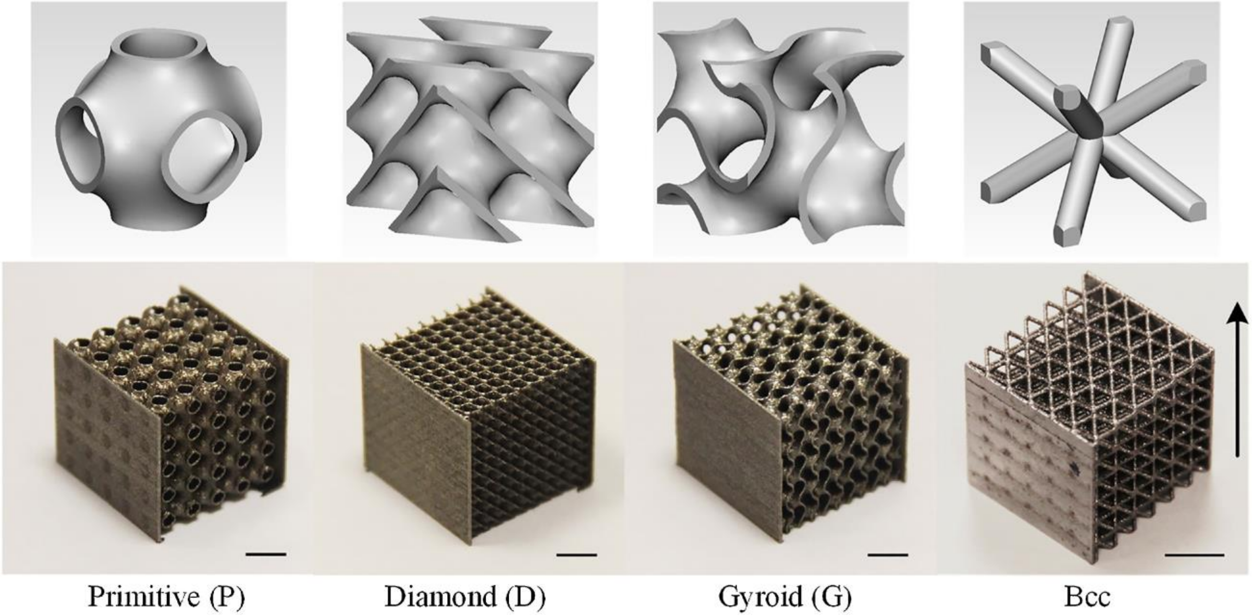
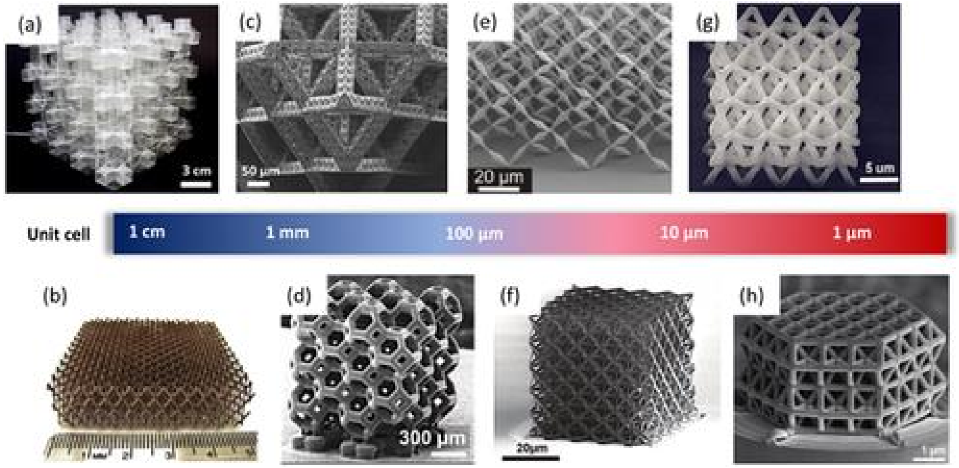
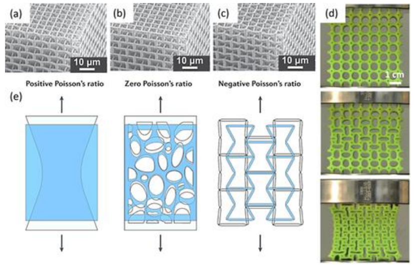
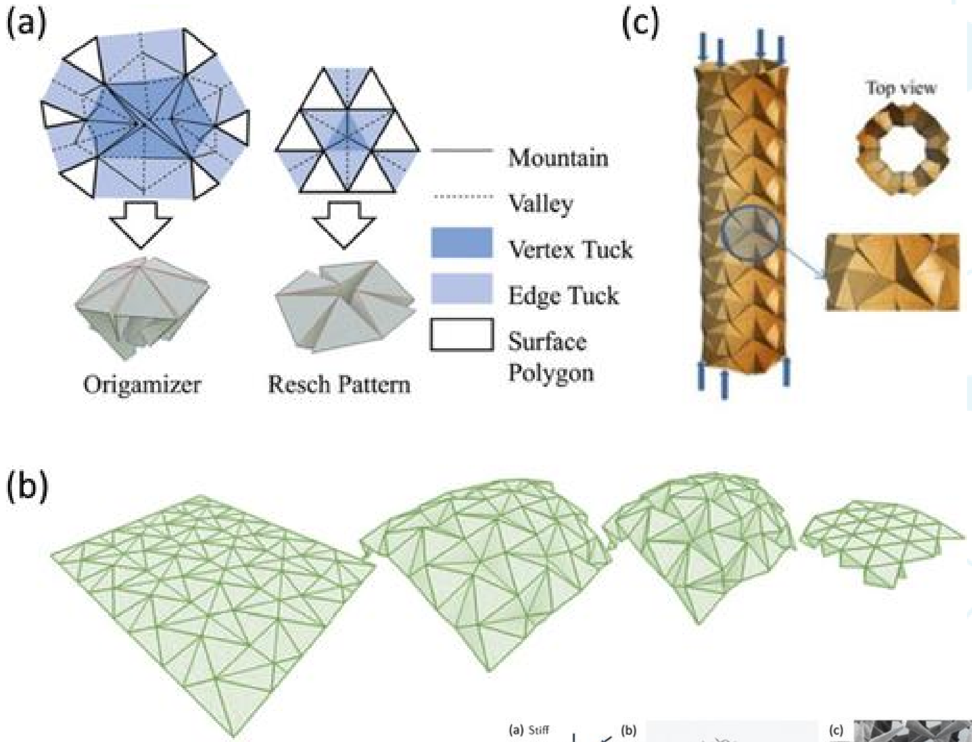
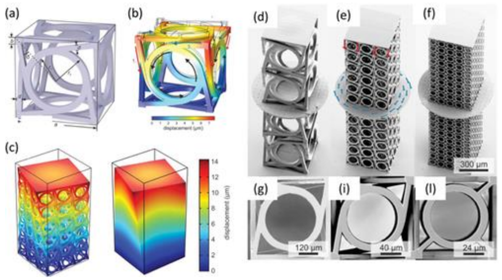


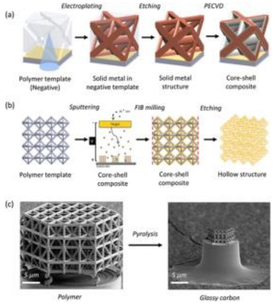
Metamaterials III

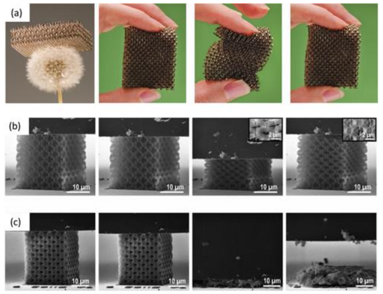












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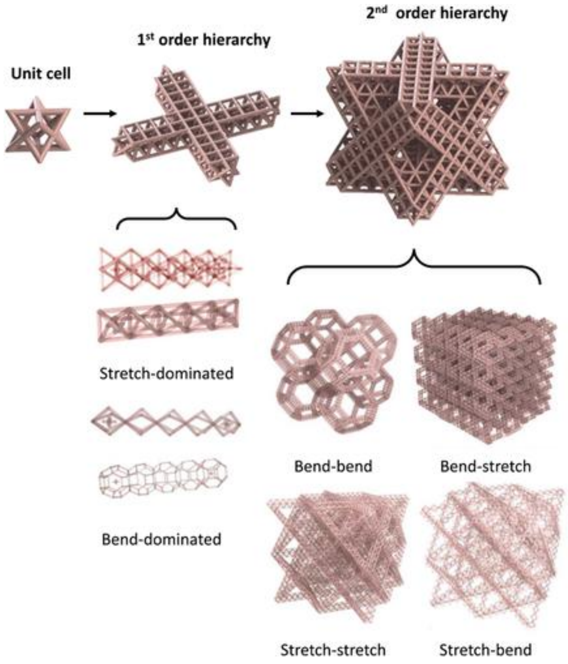

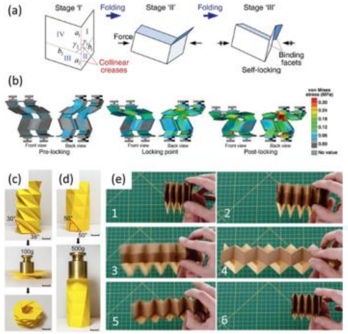

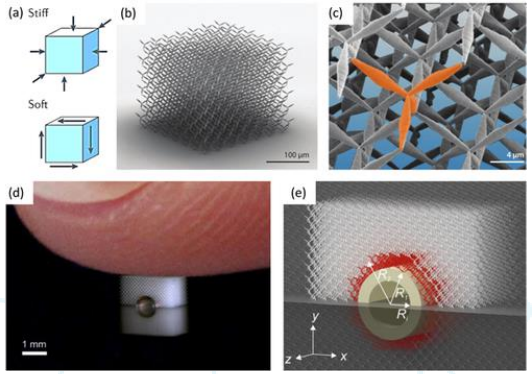

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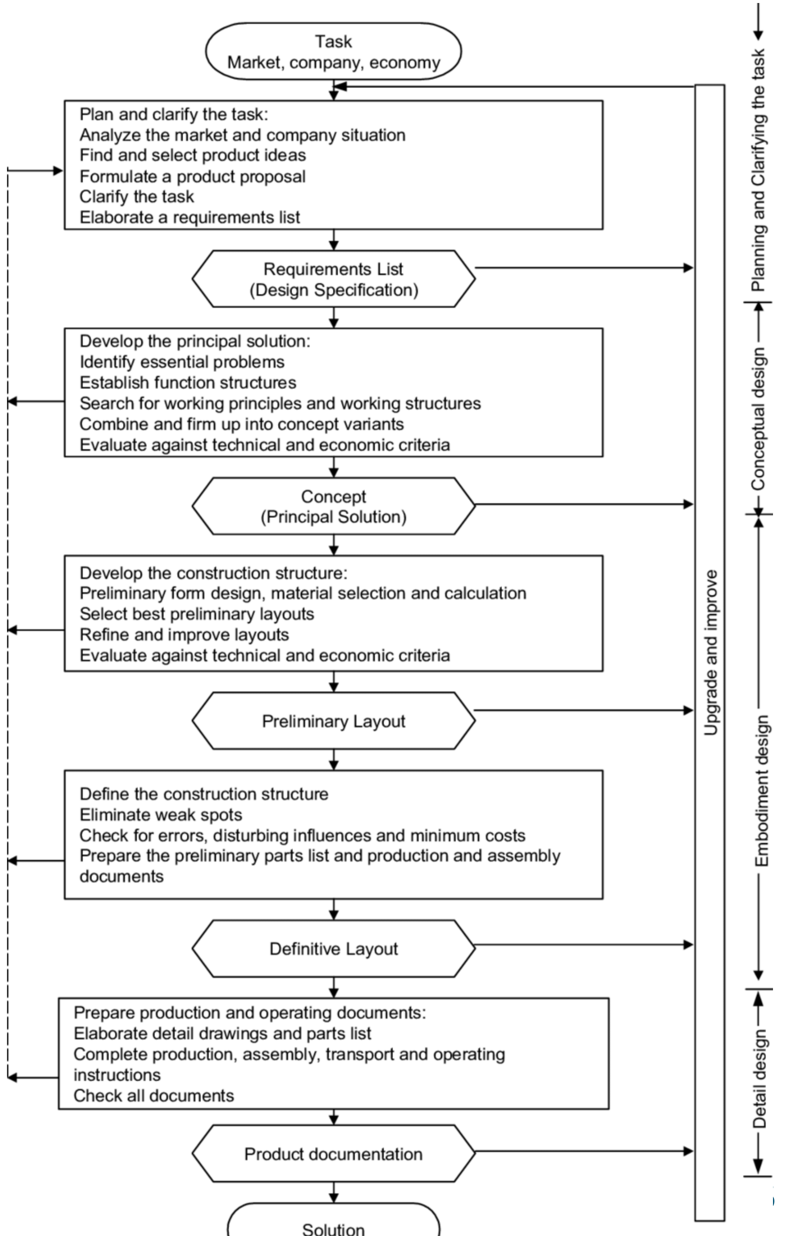
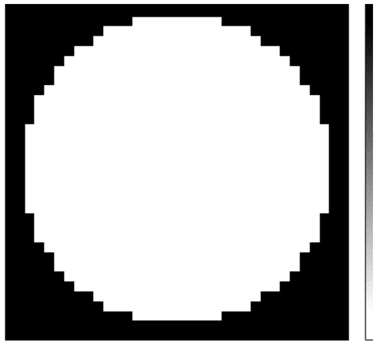
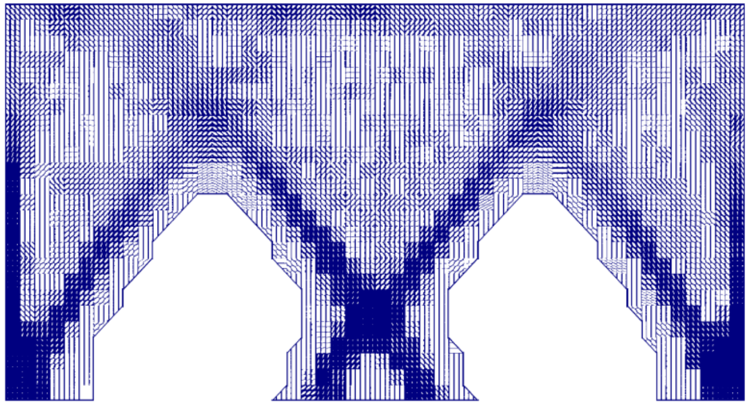


Design automation Methods

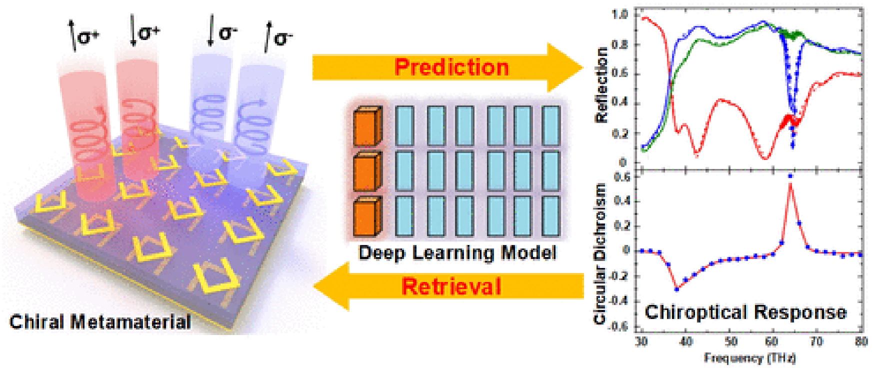
- Topology optimization
  - Requires a formal mathematical description of the problem
    - Difficult/Impossible for many processes
  - The objective function must be continuous and smooth
    - Excludes non-continuous phenomenon like contact and failure
- A generic method of mapping structure to property is needed
  - NN can provide this mapping

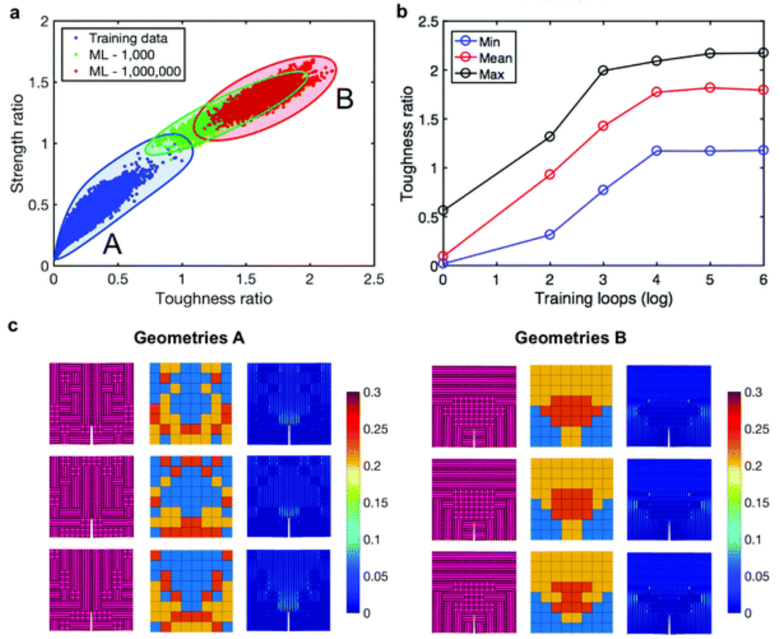


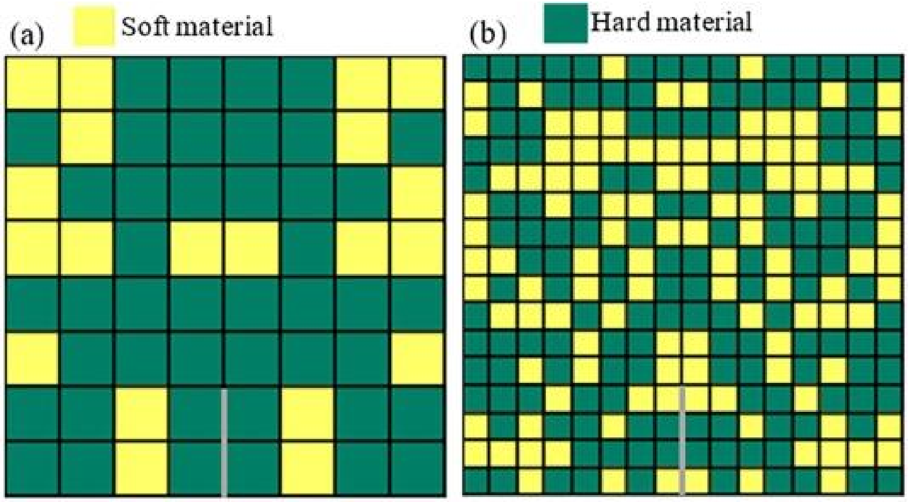


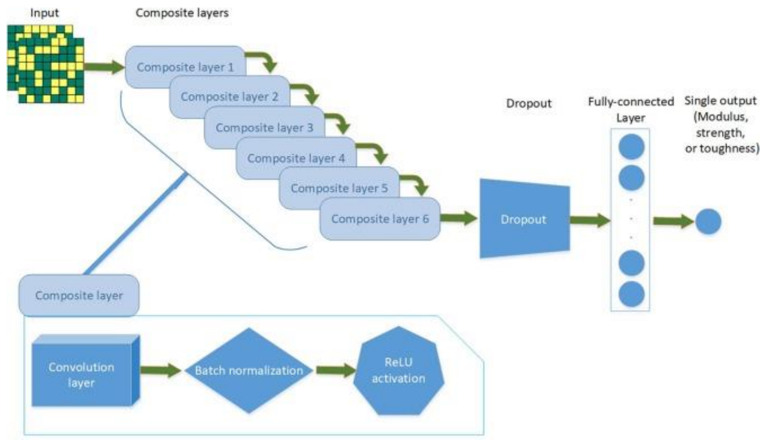
Related Works

- Ma, Wei, Feng Cheng, and Yongmin Liu. "Deep-learning-enabled on-demand design of chiral metamaterials." *ACS nano* 12.6 (2018): 6326-6334.
- Gu, Grace X., et al. "Bioinspired hierarchical composite design using machine learning: simulation, additive manufacturing, and experiment." *Materials Horizons* 5.5 (2018): 939-945.
- Abueidda, Diab W., et al. "Prediction and optimization of mechanical properties of composites using convolutional neural networks." *Composite Structures* 227 (2019): 111264.









ML Metamaterial Design Approach

Define
- Objectives
- Constraints
- Design Domain

Bootstrap
- Generate 100s of random metamaterial designs

Simulate
- Using any simulation tools

Extract
- Effective properties that measure the performance with respect to the objective

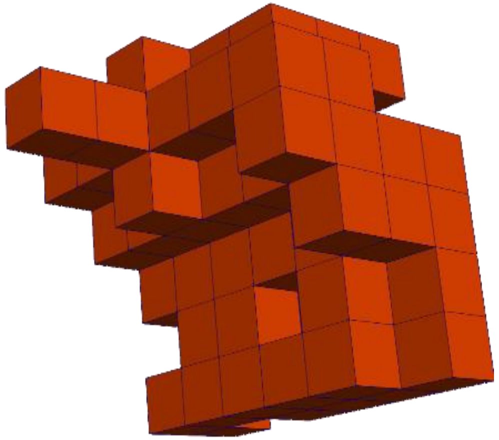
Train
- NN to map structure to properties

Generate
- Genetic Algorithm (GA) generates new metamaterials designs

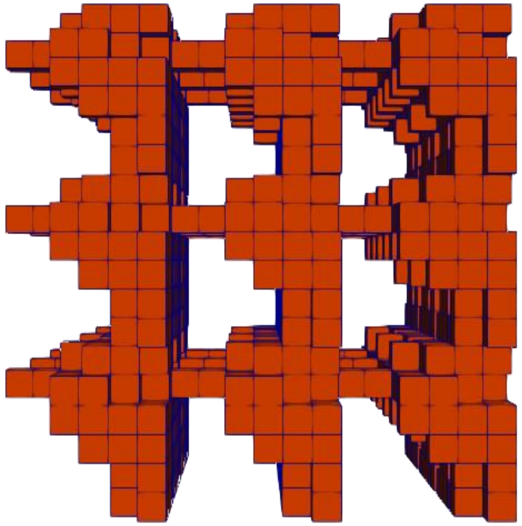
Define

- Objectives
  - Maximize stiffness of the metamaterial
  - Minimize wave-speed through the metamaterial
- Constraints
  - Basic Constraints
    1. A single connected body
    2. Hinge points are not allowed
    3. Design must connect to adjacent cells in all dimensions
    4. Density, $\rho \in [0.4, 0.6]$
  - Additive Manufacturing Constraints
    1. Unsupported overhangs (diving boards) are not allowed. 45 degree angles are ok.
    2. Bridges have a maximum length
- Design Domain (Simplified)
  - Unit cell is 12x12 “pixel” locations can have material or void

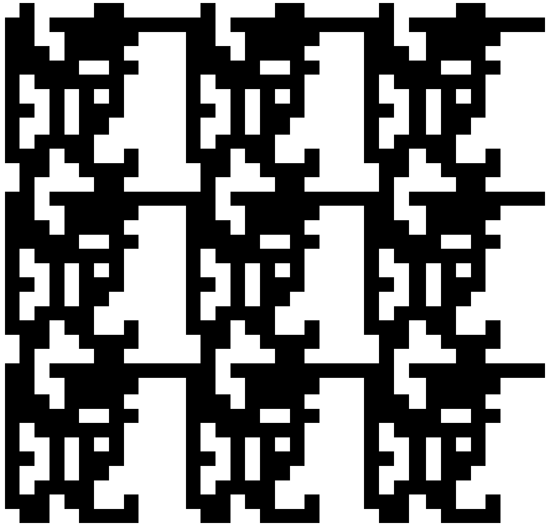
a)



b)

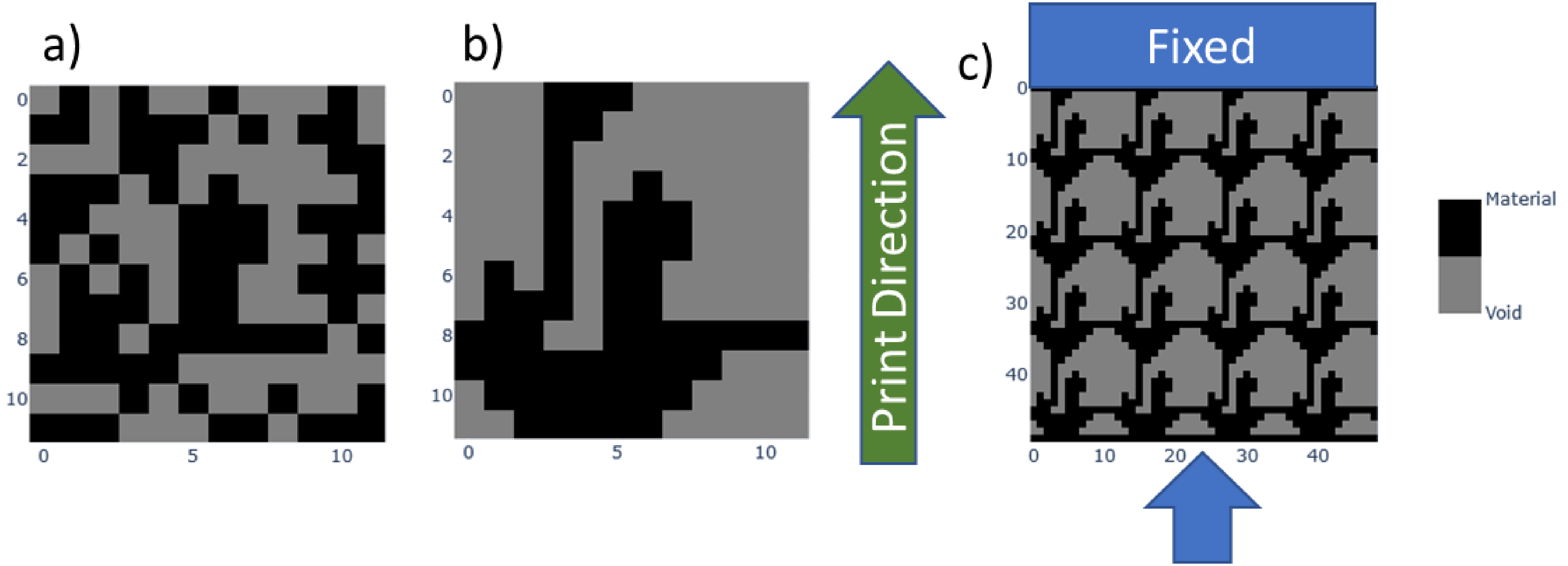


c)

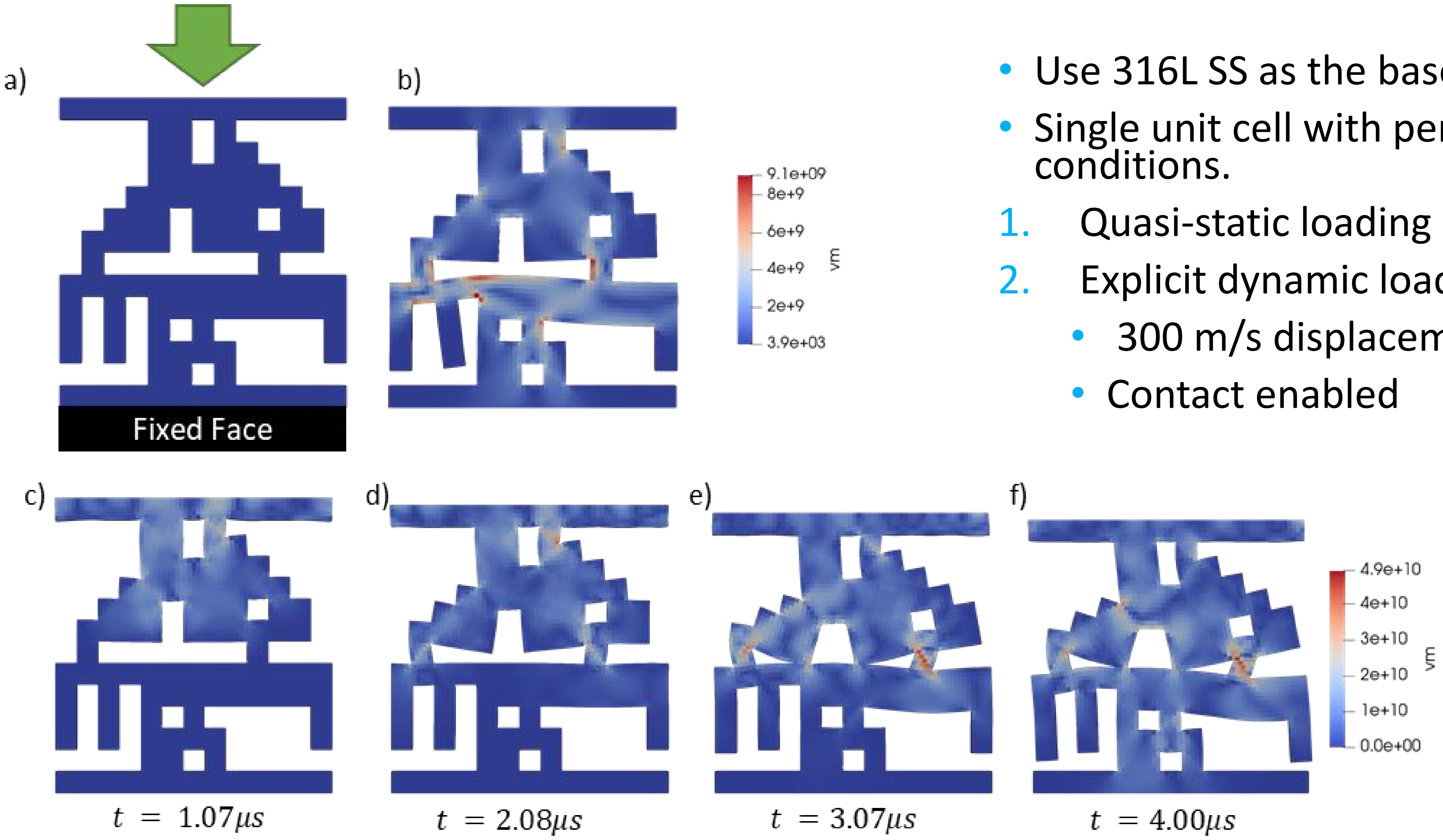


Bootstrap –Generate initial designs

- Generate 1000 random designs.
- Iteratively correct the design until they meet all the constraints.



Simulate



- Use 316L SS as the base material
- Single unit cell with periodic boundary conditions.

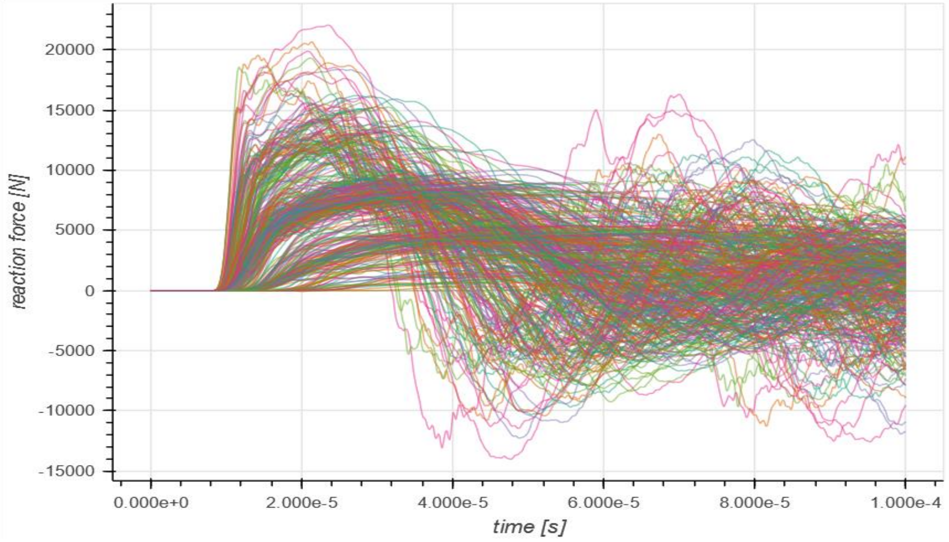
1. Quasi-static loading 3% strain
2. Explicit dynamic loading
    - 300 m/s displacement on top surface
    - Contact enabled

Extract

- Extract modulus from the quasi-static stress–strain curve
- Extract wave speed from the dynamic simulation force-time curve.

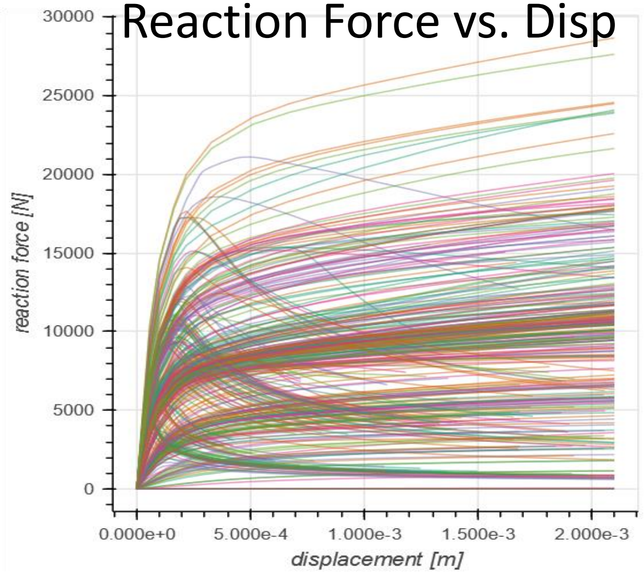
Dynamic

Reaction force vs. Time

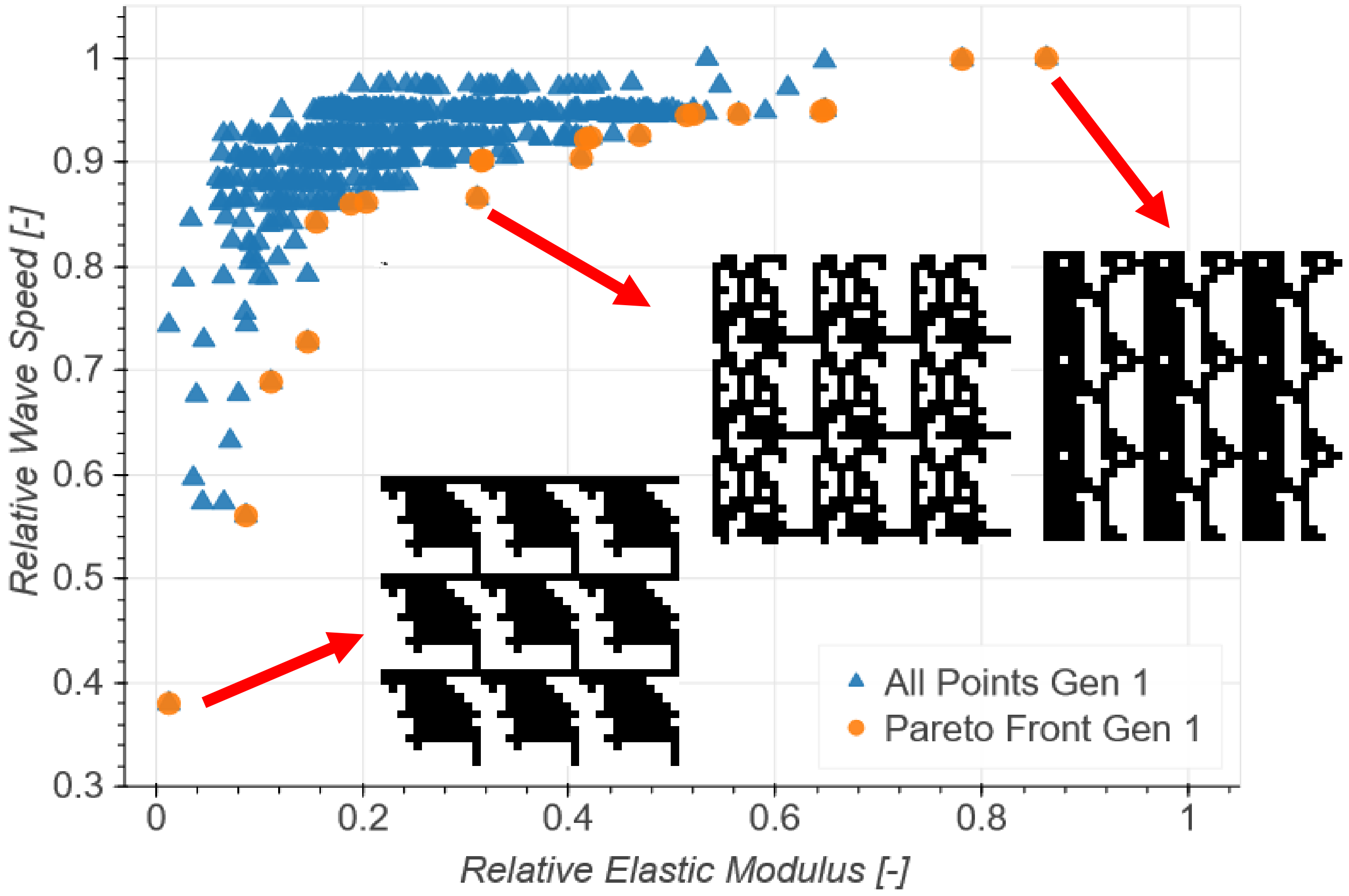


Quasi-static

Reaction Force vs. Disp



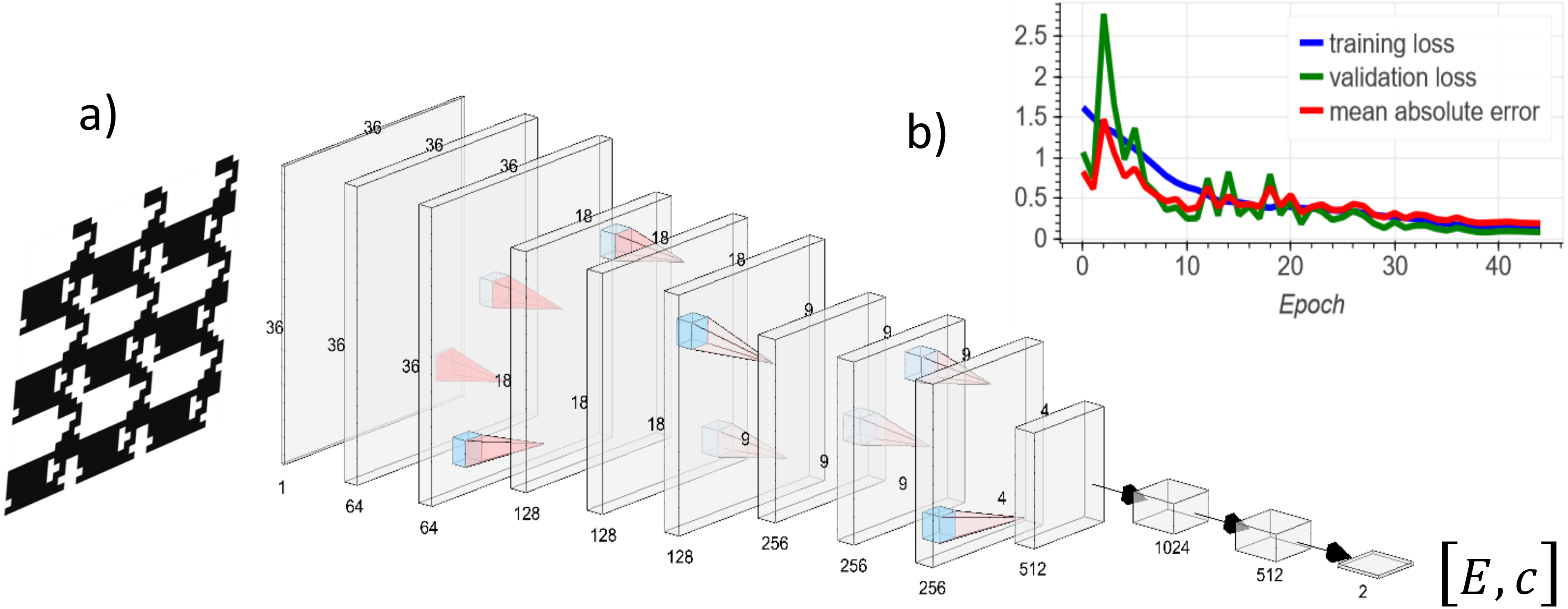
Extract II



A trade-off (Pareto Front) of designs exists.

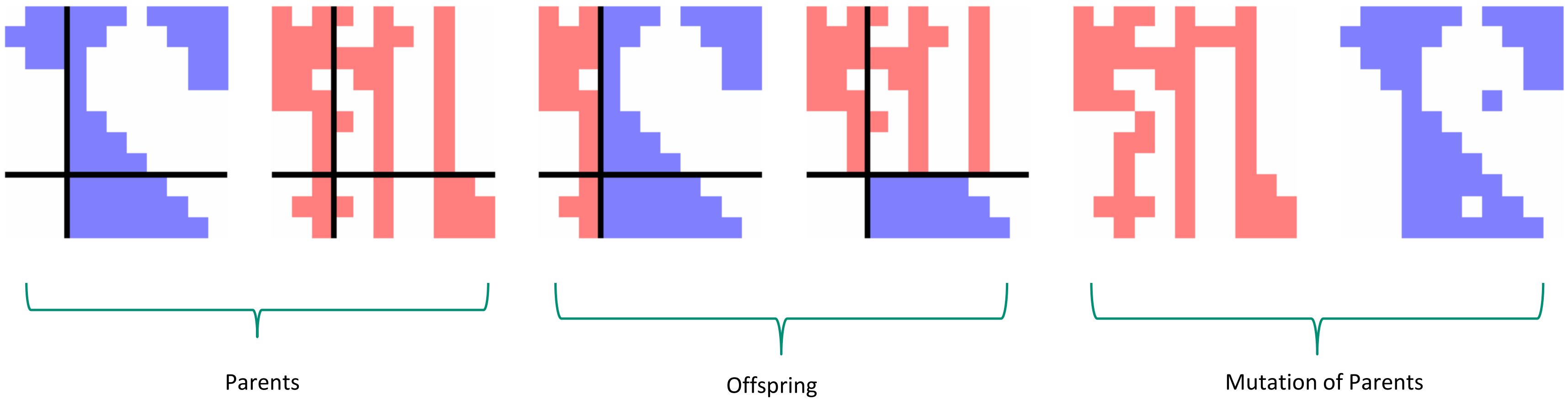
Train

- A Convolutional Neural Network (CNN) is trained to predict modulus and wave-speed based on the unit cell.



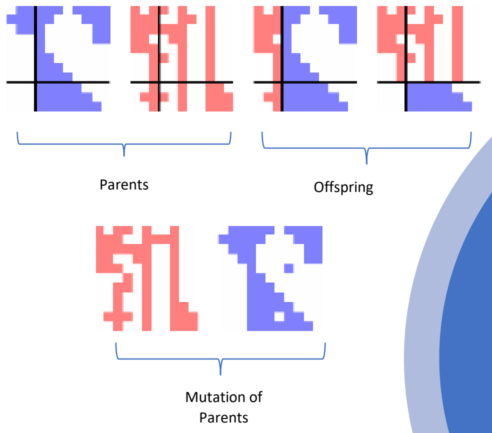
Generate

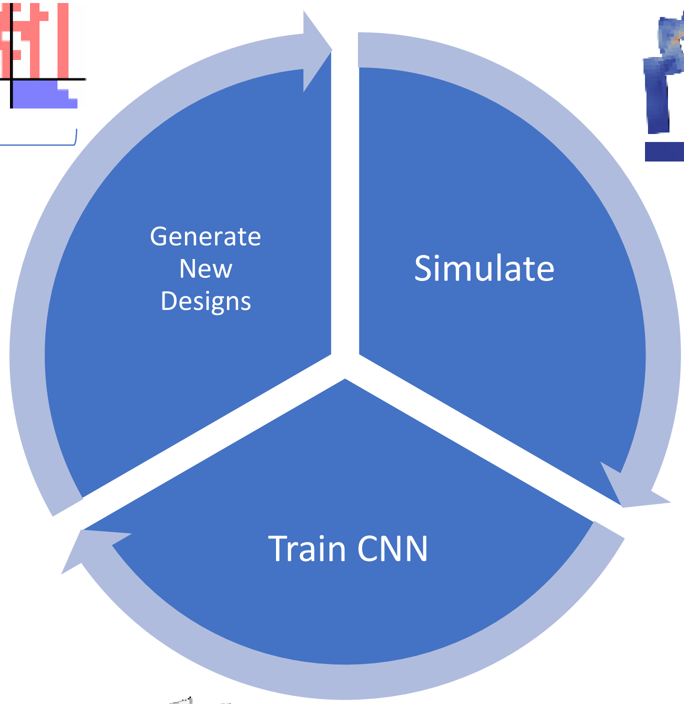
- Genetic Algorithm generates new designs.
- Uses the CNN as the evaluation function
- NSGA-II – multi-objective GA attempts to build a well distributed pareto front
- Designs which don't meet design constraints are discarded

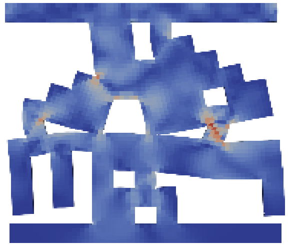


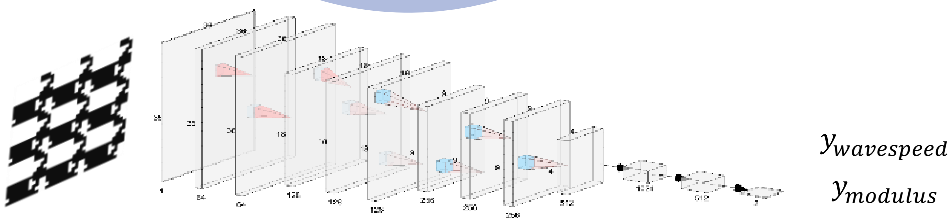
Active Learning

- The GA generates/picks the next set of designs to simulate
- Active Learning
  - Taking an active part in your own learning
  - e.g. Picking its own training data





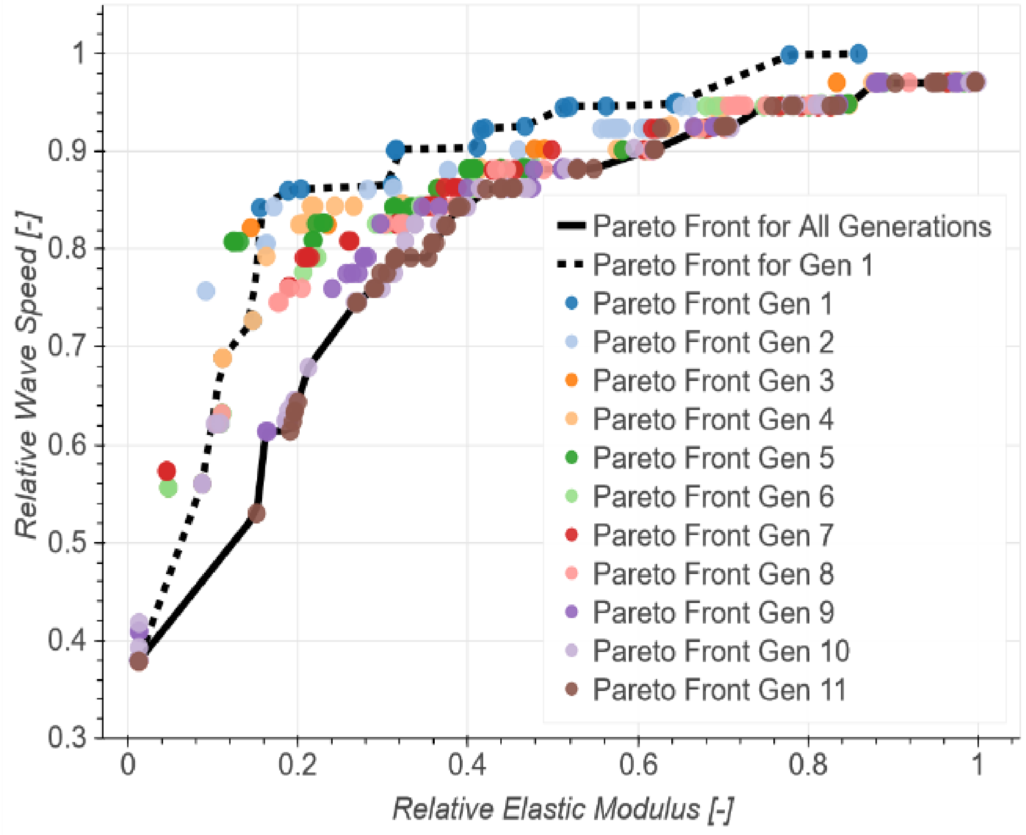




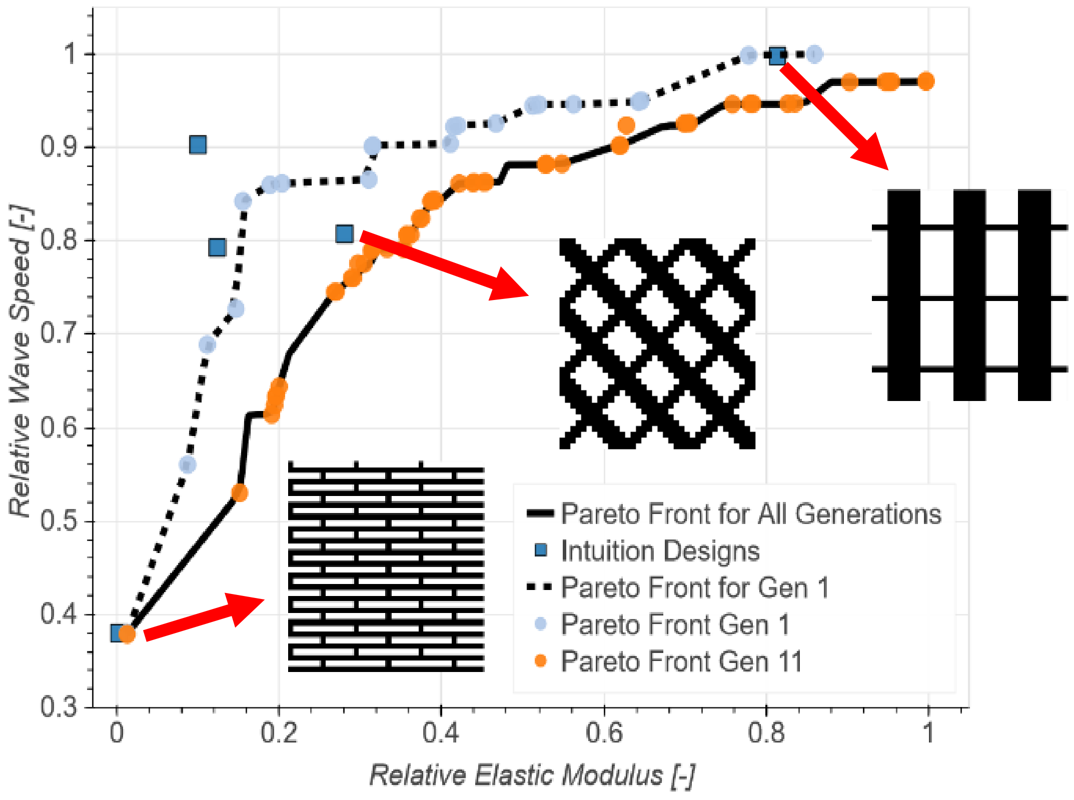
Run for 11 generations (loops)

Results

a) Progression of Pareto Front

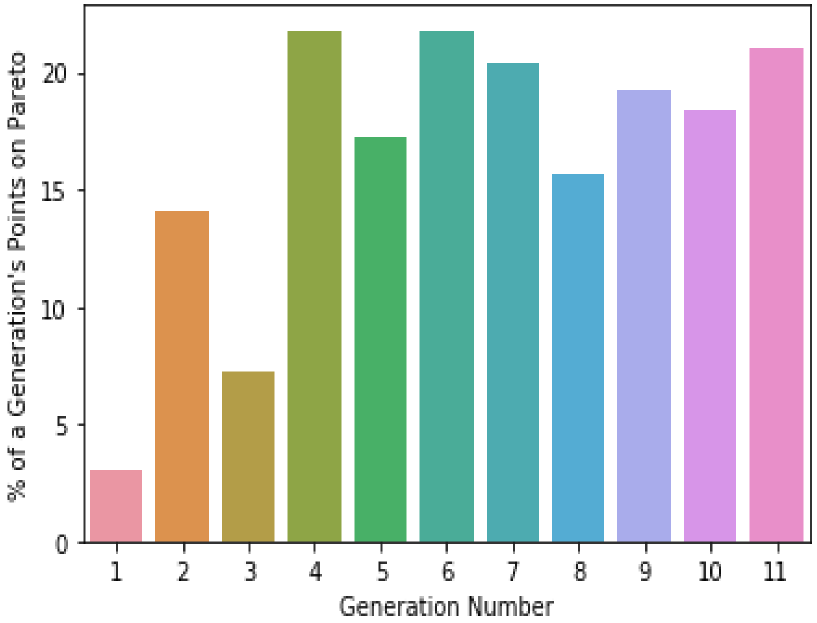


b) Comparison to intuition based designs



Results II

c)



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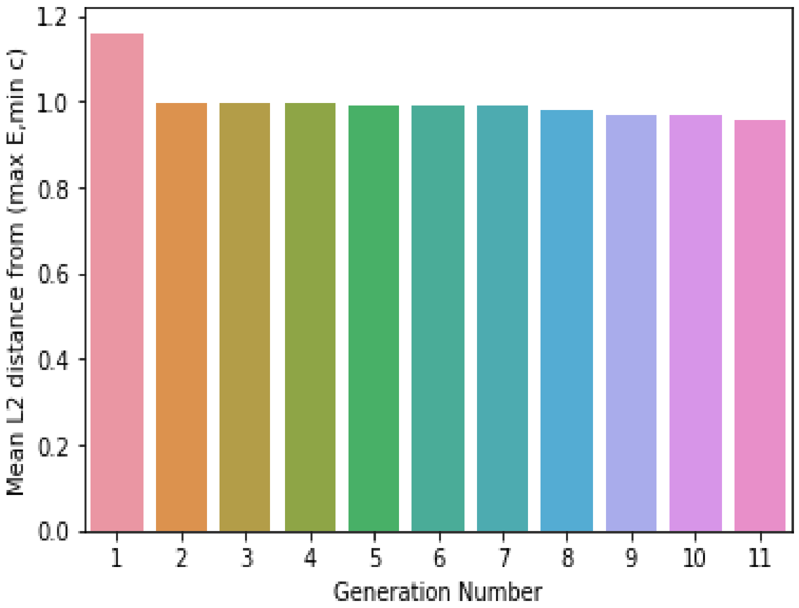

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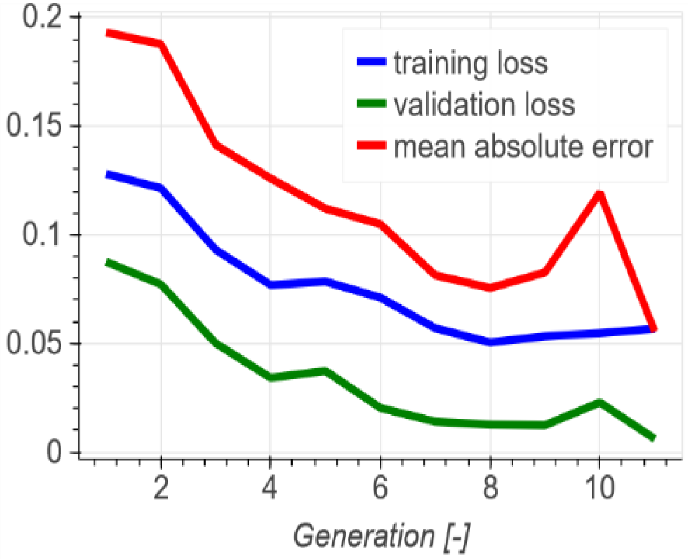
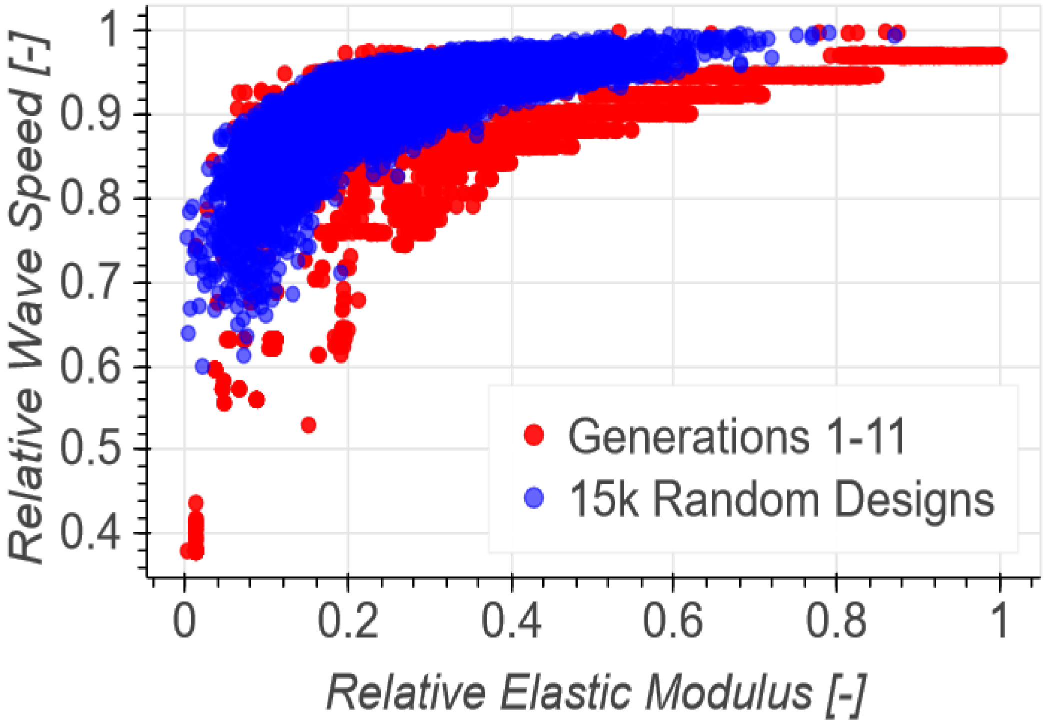
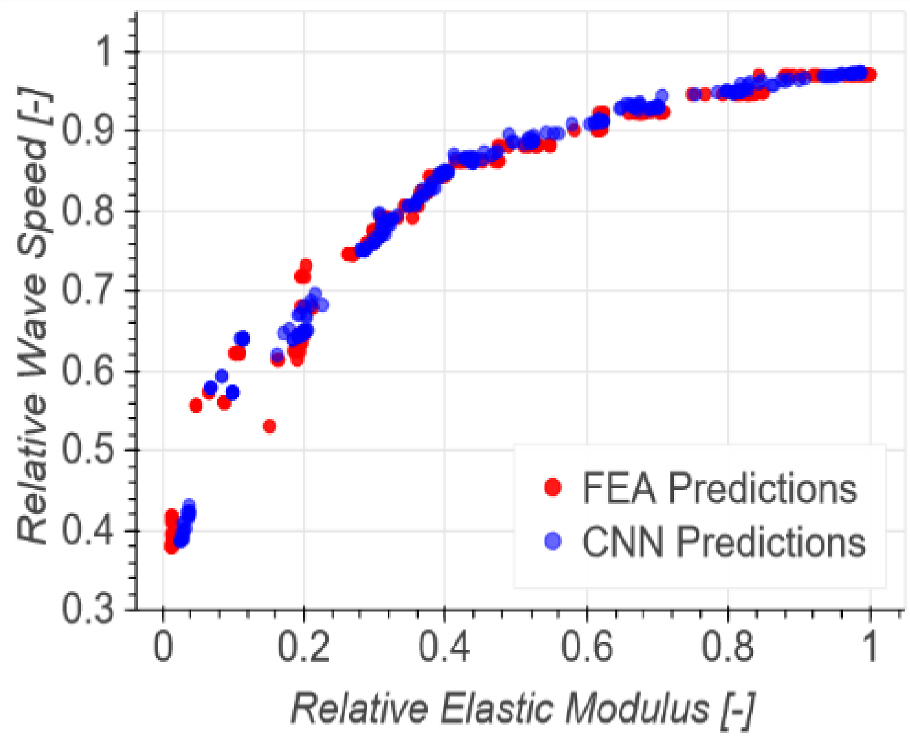


Results III

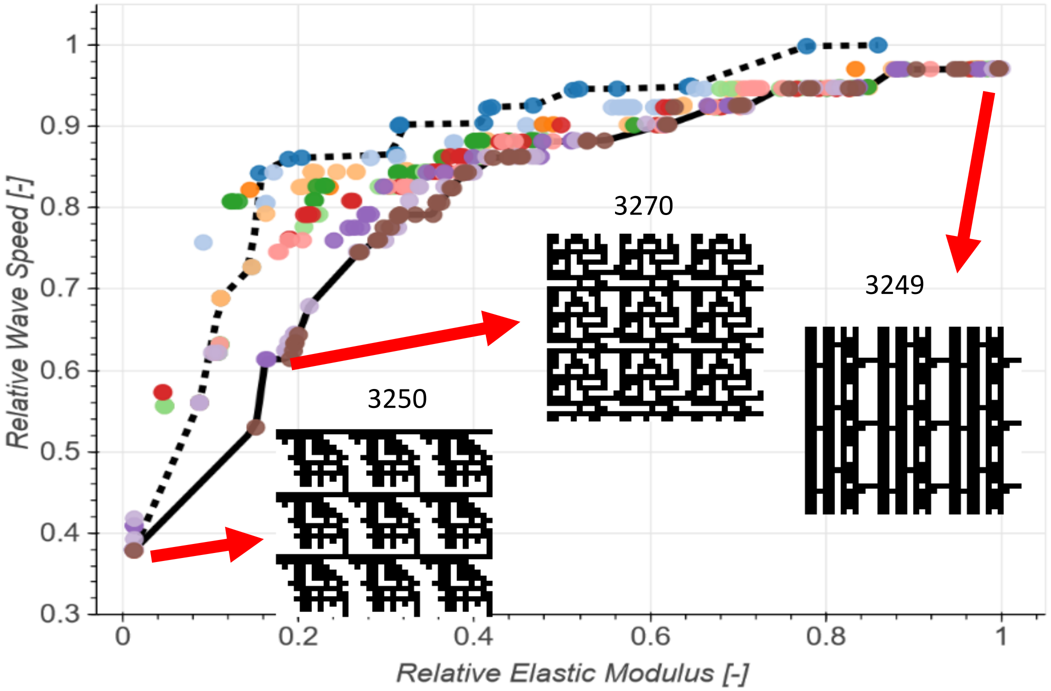
a) Design Results vs 15k Random Designs

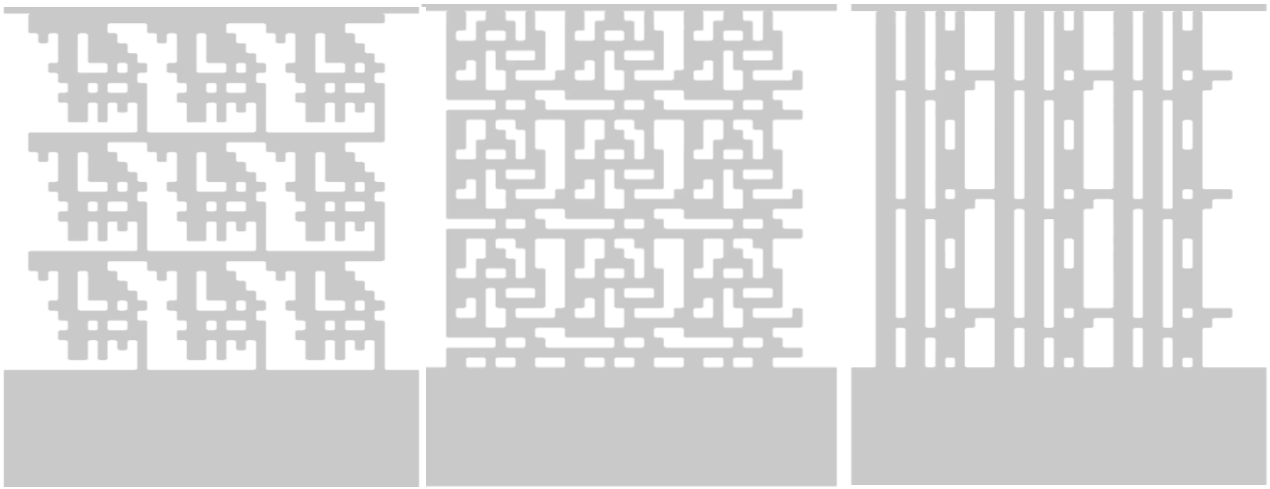


b) CNN vs FEA Predictions



Validation





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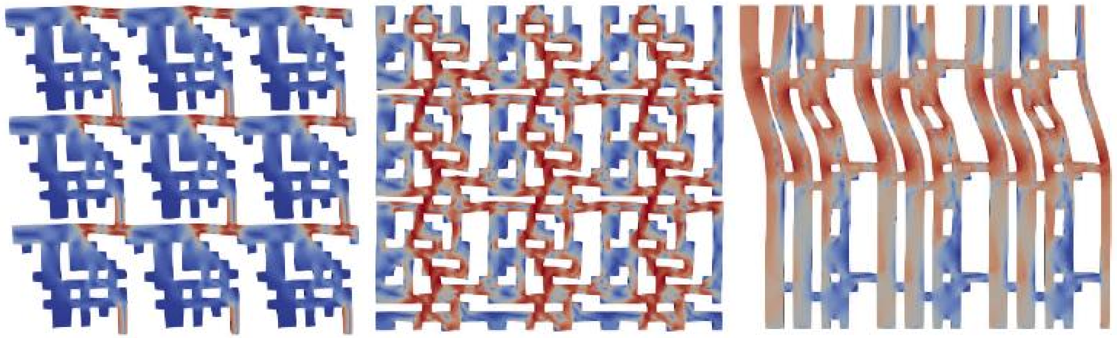

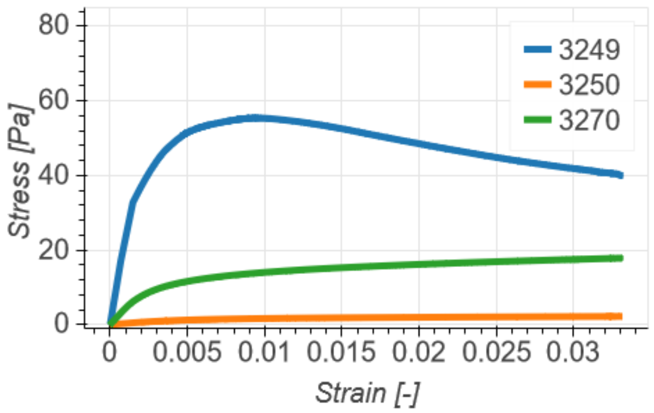

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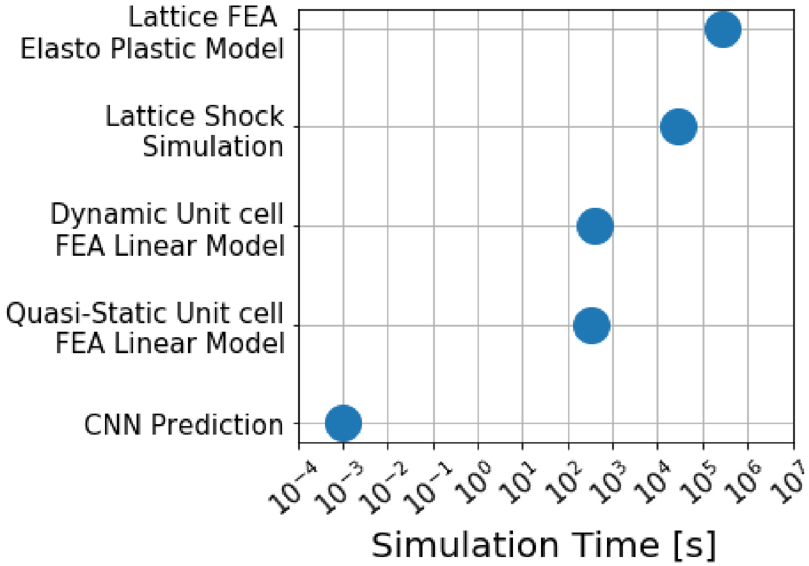

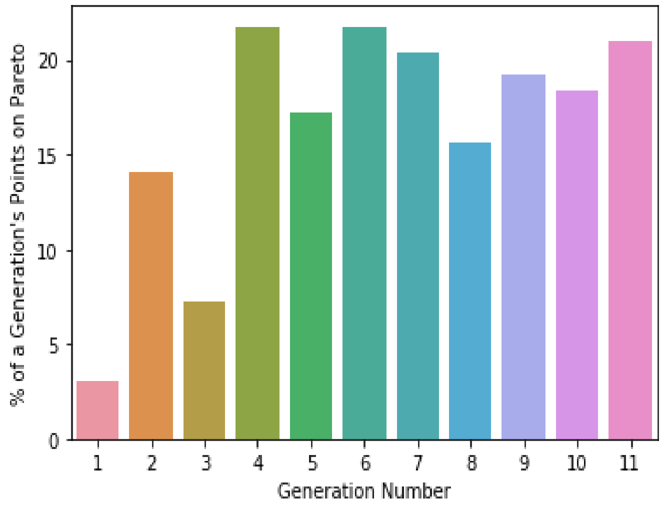

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