



Optimization of an Optical Shutter using Machine Learning

Benjamin A. Jasperson, Michael G. Wood, Harley T. Johnson

Presented at:

Sandia Academic Alliance – Fall 2022 – University of Illinois LDRD Mini-Conference

September 15, 2022

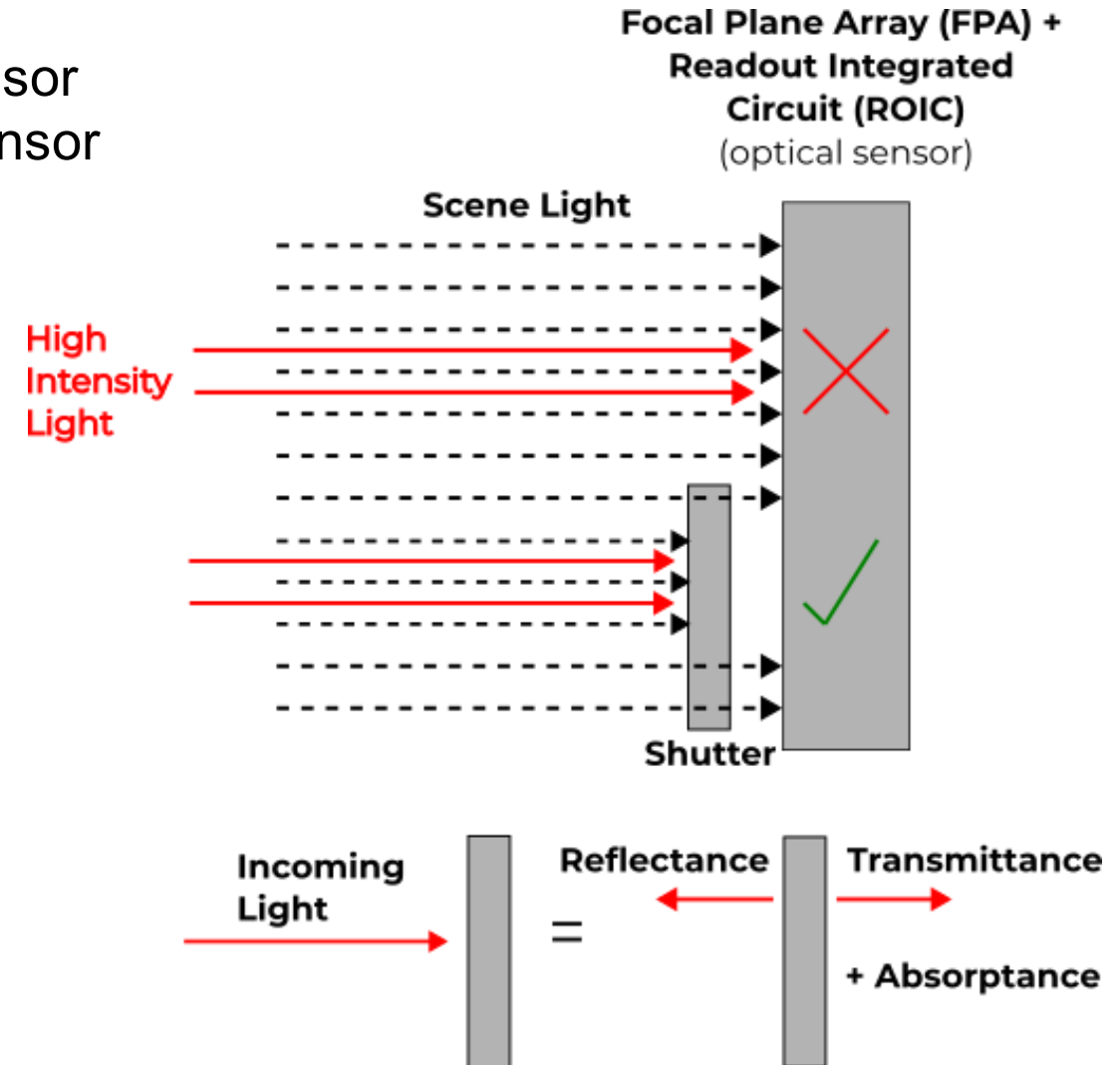
SAND #: X123456789

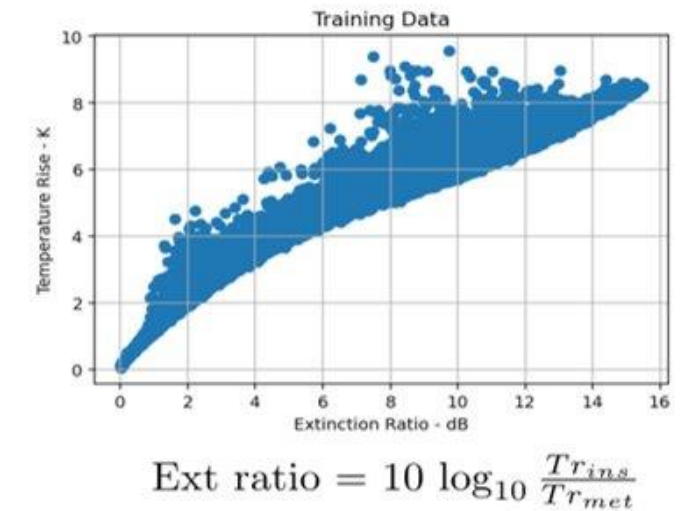
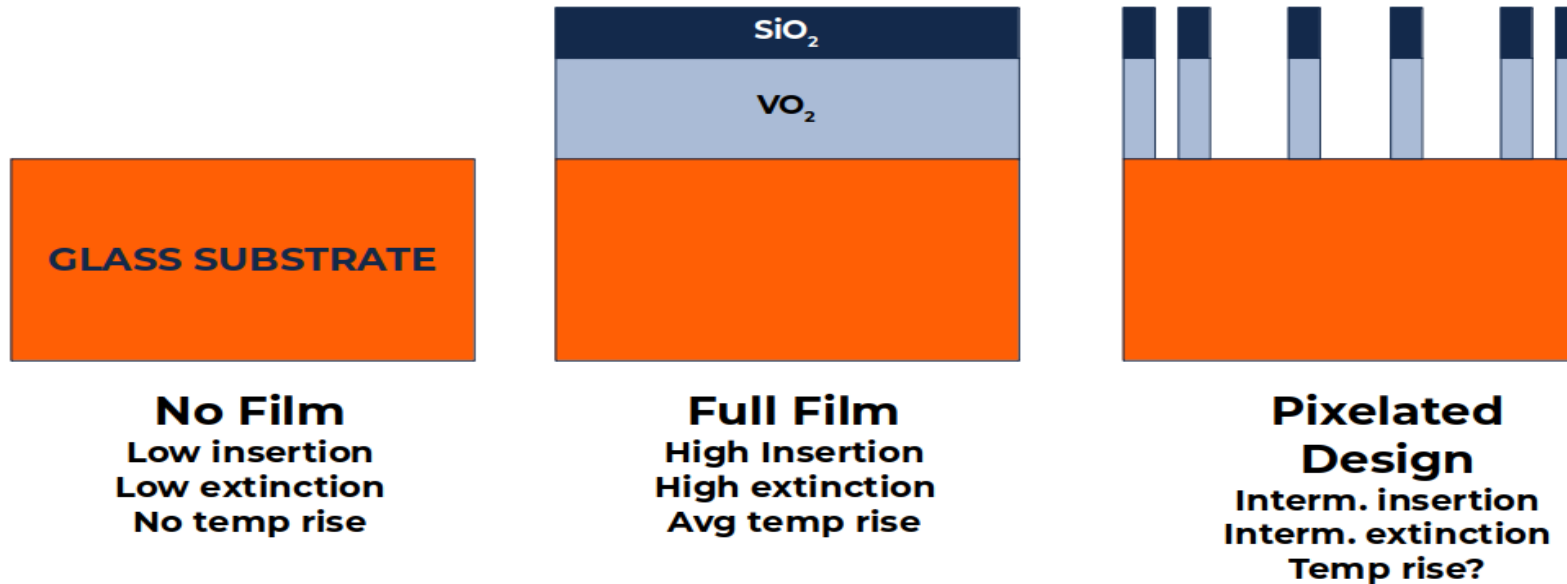
This material is based upon work supported by the
National Science Foundation under Grant No. 1922758

Acknowledgement. This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and 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-NA-0003525. 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.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and 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.

- **Purpose:** sensor protection using optical shutter
 - Normal operation: scene light reaches optical sensor
 - High intensity light: can overwhelm or damage sensor
- **Ideal scenario:** passively switch the shutter on and block/reflect the high intensity light
- Utilize **VO₂**:
 - Phase change material: thermally triggered
 - Insulating (monoclinic) phase: low-loss, semi-transparent
 - Metallic (rutile) phase: lossy, reflective
- Figures of merit
 - **Extinction ratio:**
 - Transmittance on / Transmittance off
 - Bigger is better
 - **Temperature rise:**
 - Efficiently switch on
 - Bigger is better

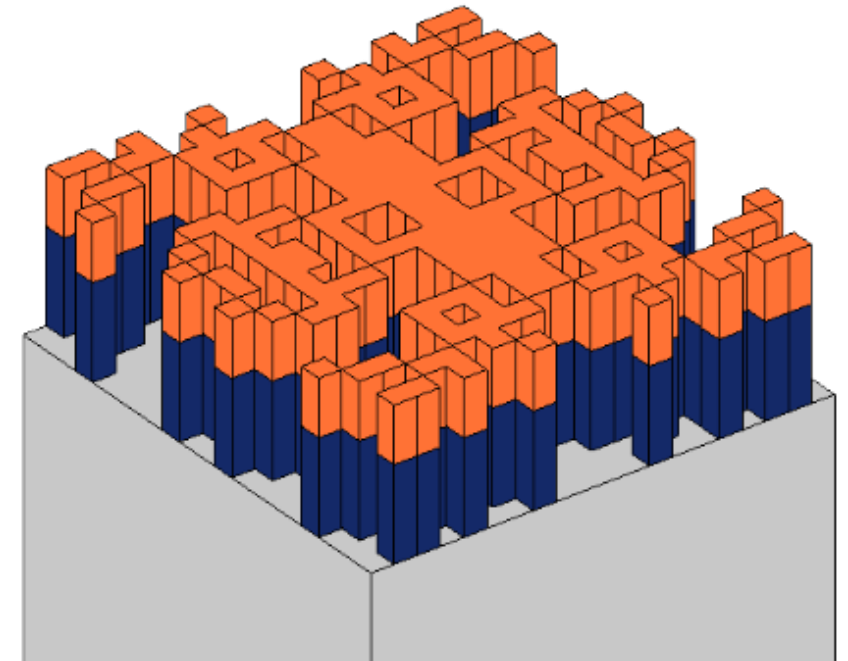




Can we find a pixelated design that maximizes temperature rise for a given extinction ratio?

Topology Optimization

- **Goal**: Optimization of optical switch using phase change material (VO_2) using machine learning
- **Plan**:
 - Perform simple modeling to generate data
 - Optimize using a completely machine learning (ML) approach
 - Check using FEA
 - Fabricate/test at Sandia National Lab



- Discretize problem:
 - Write governing equation, set boundary conditions, discretize domain
 - Finite element setup
- Allocate a given amount of material across the points
 - Density function (ρ)
 - $\rho = 0$ means no material, 1 means material
 - Discrete = Tough
 - Use continuous
- Determine objective (cost) function to minimize; e.g. compliance (structural) or band gap (EM)
 - In our case, extinction ratio and temperature rise targets
- Iterate, determine gradient, adjust, repeat
 - **Requires costly finite element solver calls each iteration**

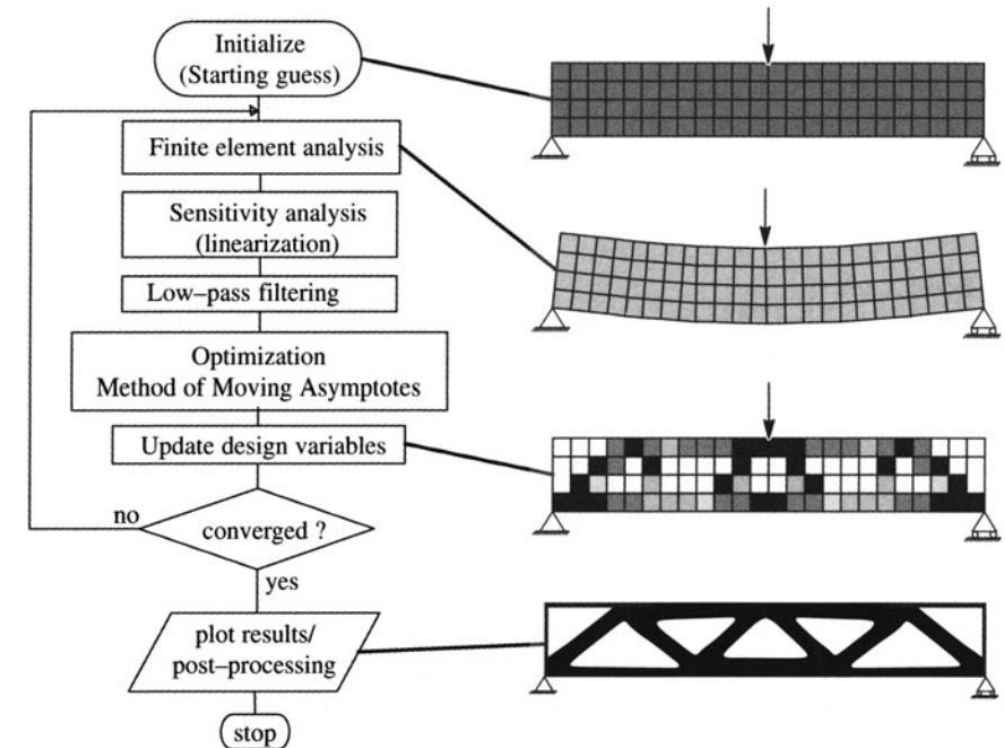


Fig. 1.5. The flow of computations for topology design using the material distribution method and the Method of Moving Asymptotes (MMA) for optimization. The low-pass filter step (filtering of sensitivities) is discussed in Sec. 1.3.1.

Source: Bense and Sigmund, "Topology Optimization: Theory, Methods, and Applications", 2003

- Neural Networks (NNs) for topology optimization:
 - Collection of variables that get changed to perform a task
 - Image classification, regression, etc.
 - Allow for accurate and cheap prediction of device performance
 - Can be trained to provide design performance (FEA) and density function (material distribution)
- Utilize Convolutional Neural Networks (CNNs) to bypass COMSOL model after training (Performance Neural Network - PerfNet)
 - Heavily used for image recognition
 - Scanning an image, looking for patterns
 - Excels at image/pattern recognition
 - Dot product between kernel (filter) and feature combine to create feature map
- Utilizing Pytorch, an open source ML package
- Train model using labeled data (supervised model)

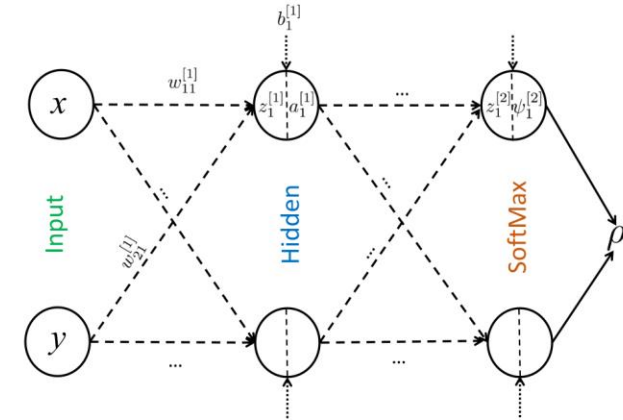
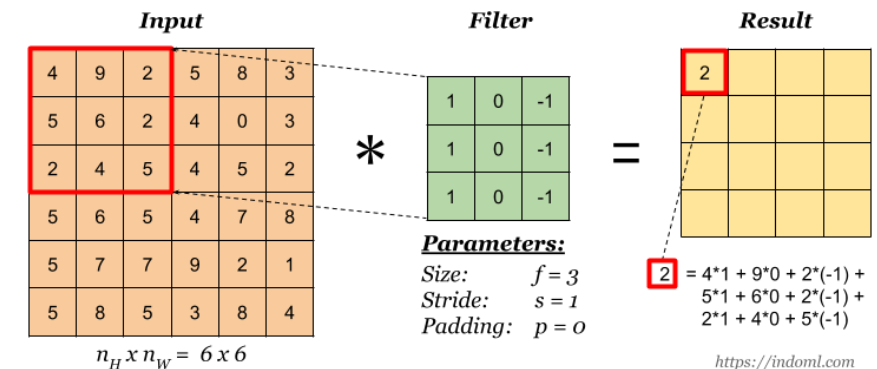


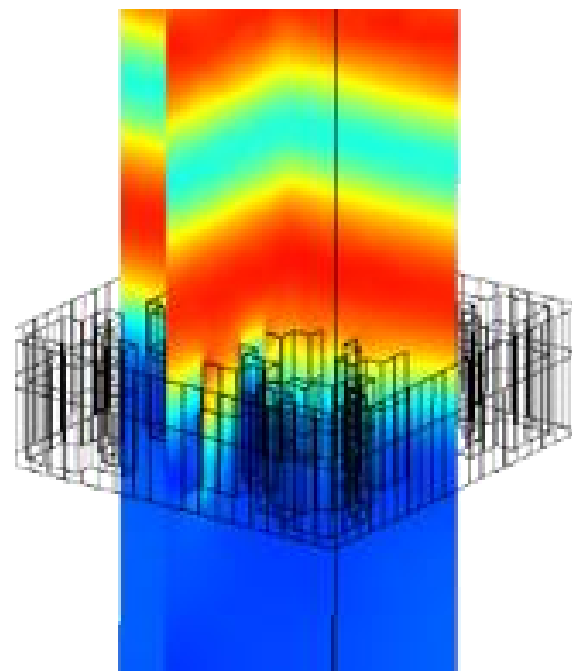
Fig. 4 Illustration of a simple network with one hidden layer of height 2

Source: Chandrasekhar and Suresh, "TOuNN: Topology Optimization using Neural Networks," <https://doi.org/10.1007/s00158-020-02748-4>



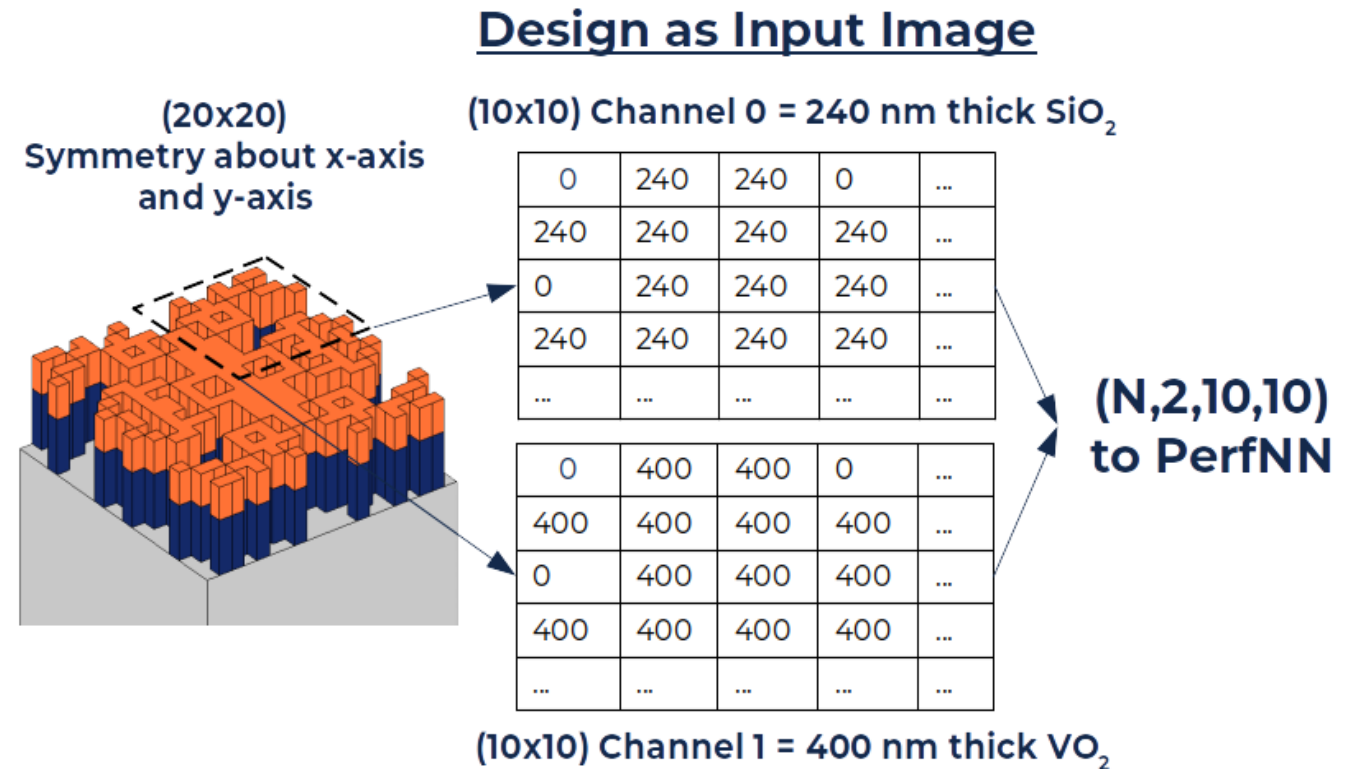
Source: <https://medium.com/analytics-vidhya/everything-you-need-to-know-about-convolutional-neural-networks-cnns-3a82f7aa29c5>

- Generate designs (symmetric about x and y axis)
- Run frequency domain model in insulating phase:
 - Tr_{ins}
- Using insulating absorptance (total power dissipation density), run time domain model:
 - $Temp\ rise$
- Run frequency domain model in metallic phase:
 - Tr_{met}
- Calculate Extinction Ratio



Variable	Value
Insulating $T_{ambient}$	273.15 K (0 deg C)
Metallic $T_{ambient}$	373.15 K (100 deg C)
Time	10 us
Incident power flux	1 kW/cm ²
Wavelength	2.7 um
Unit cell dimensions	2 x 2 um
Number of sub-pixels	20 x 20
Pixel dimensions	0.1 x 0.1 um
Stack-up	Substrate + 400 nm VO ₂ + 240 nm SiO ₂
Number of sims	~15K

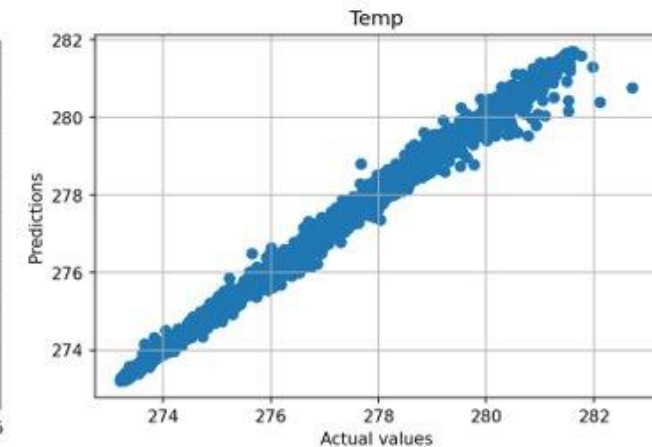
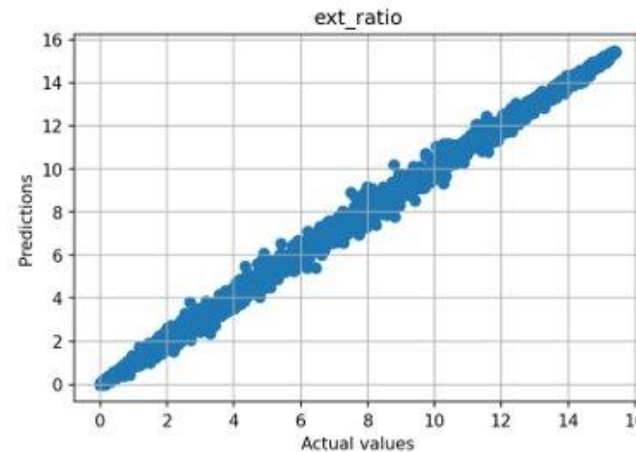
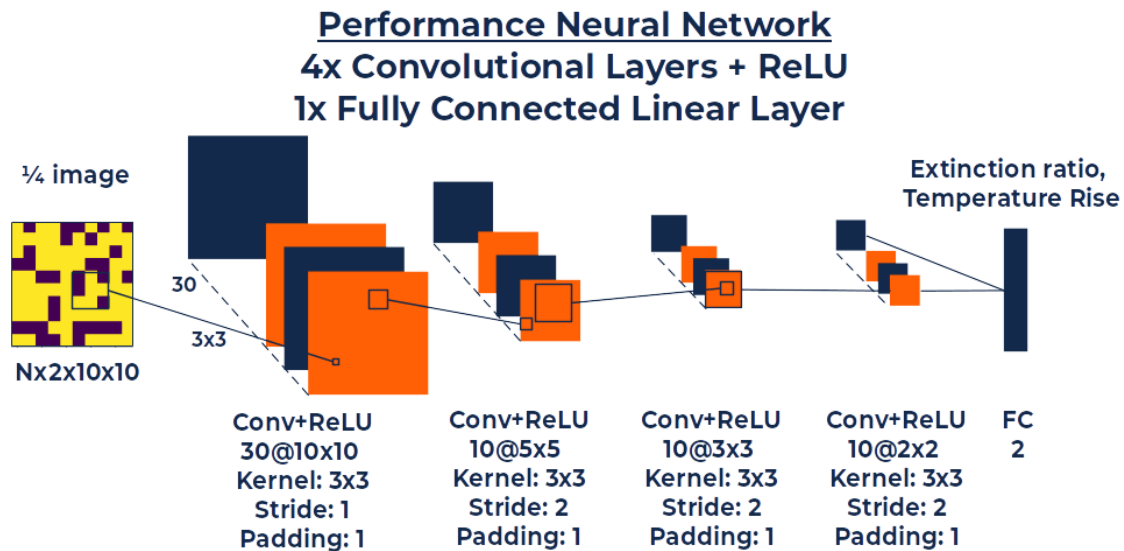
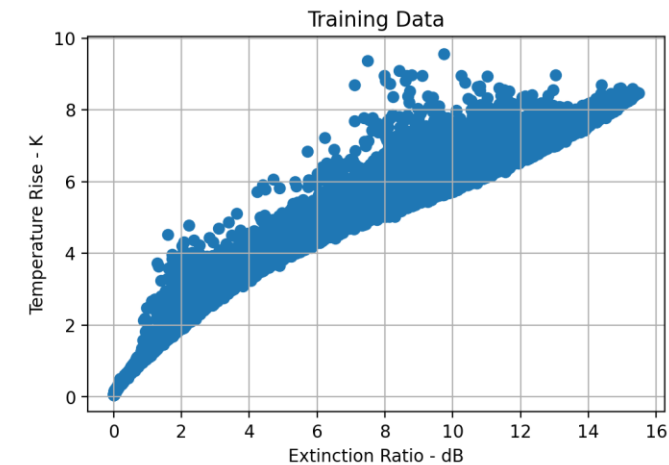
- Only need one corner of design (symmetry about horizontal and vertical axis)
- Height of layer [nm] at given point is image pixel value
- 2 channels = 2 layers ($\text{VO}_2 + \text{SiO}_2$)



Training the Performance Neural Network



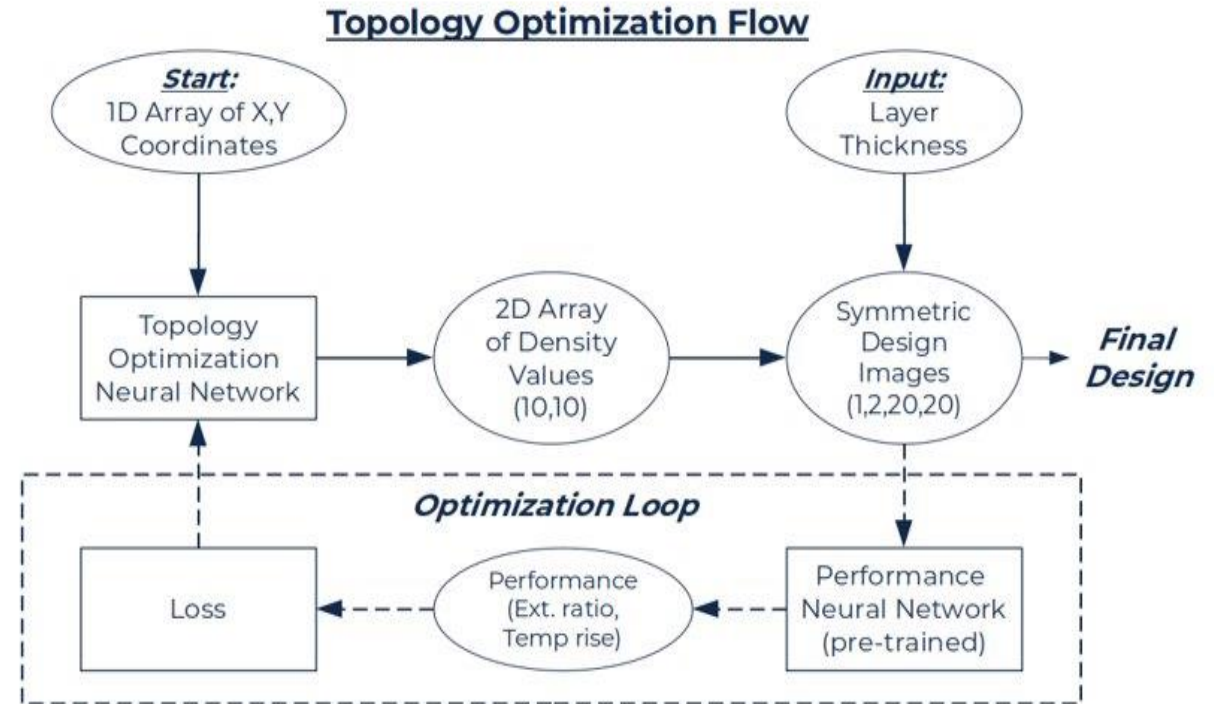
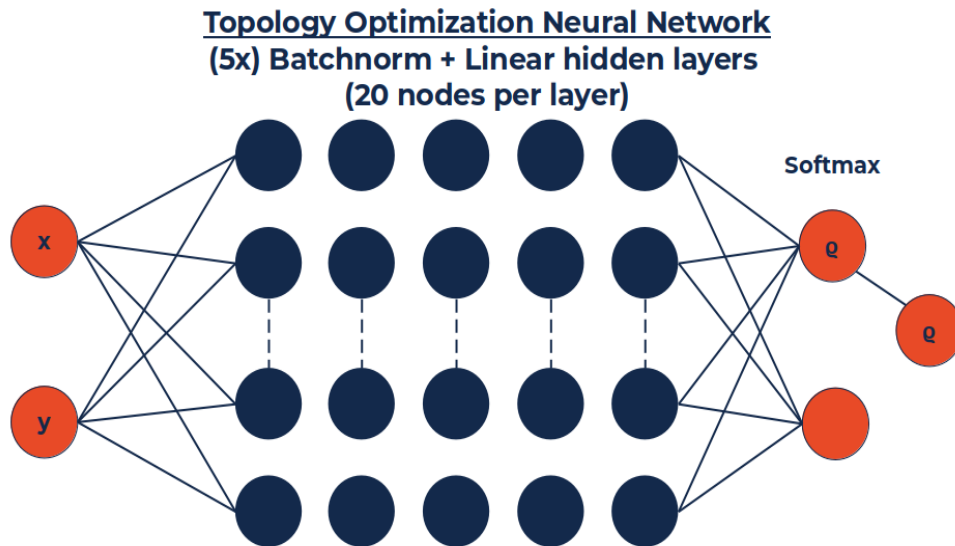
- Train performance neural network
 - Determining what filters to use to best predict performance
 - Backpropagation (automatic differentiation)
- Trained performance
 - Avg abs error: ~13% ext, ~.04% temp
 - Maximum difference: ~1.5 dB ext, ~1.6 K temp

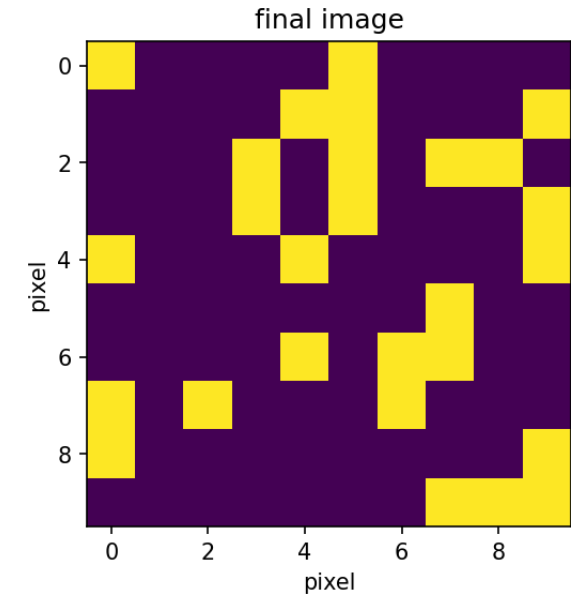
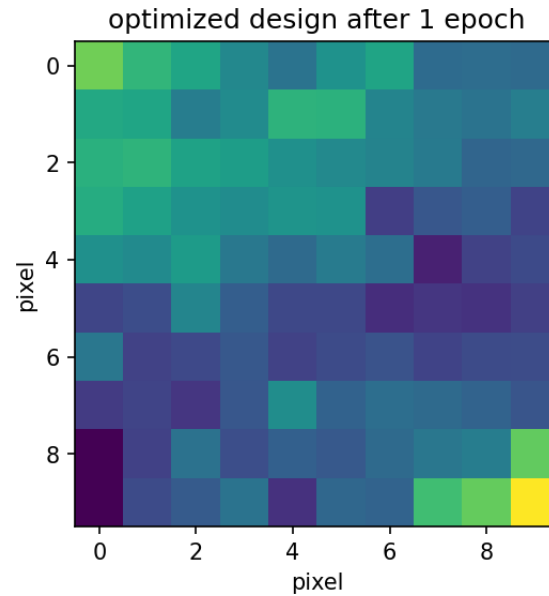
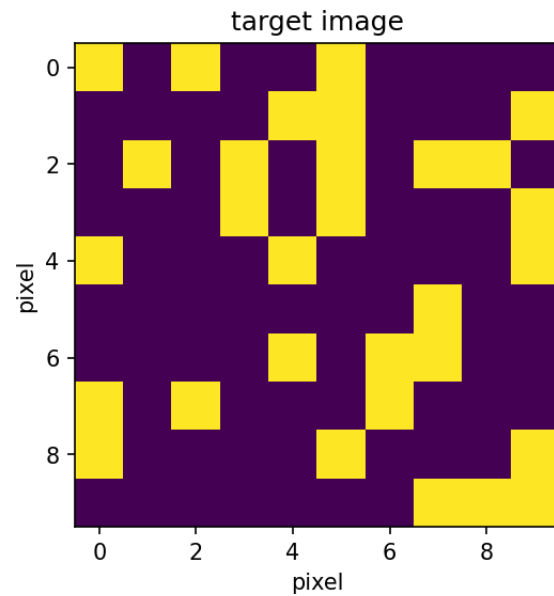


Topology Optimization Neural Network (TopOpt NN)



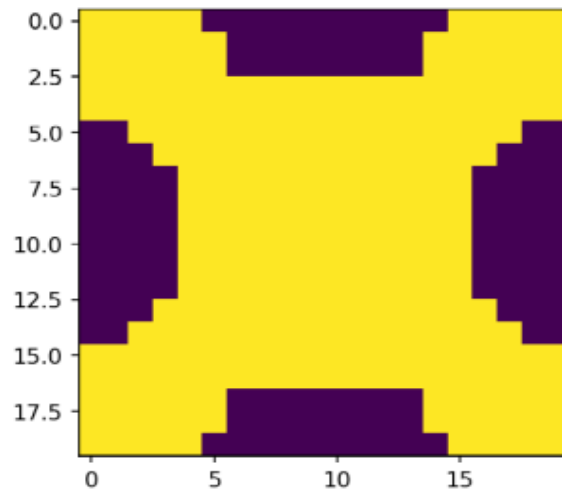
- Training TopOpt NN
- Each epoch adjusts weights to predict material density at each point



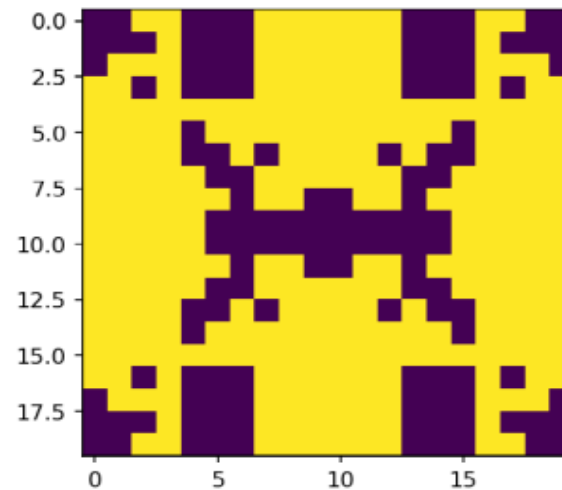


Test data generated with arbitrary cost function shows good performance

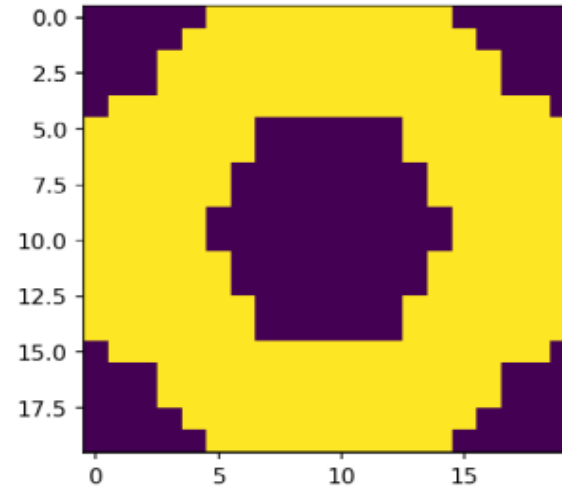
Sample Designs (Glass Substrate + 400 VO₂ + 240 SiO₂)



220818-0734
NN Predicted
Ext ratio: 10.01
Temp rise: 10.94
COMSOL
Ext ratio: 12.14
Temp rise: 13.77



220818-1035
NN Predicted
Ext ratio: 10.22
Temp rise: 11.49
COMSOL
Ext ratio: 8.96
Temp rise: 11.31



220818-1054
NN Predicted
Ext ratio: 10.03
Temp rise: 11.83
COMSOL
Ext ratio: 11.44
Temp rise: 13.86

- TopOpt NN minimizes loss function and provides a proposed (non-unique) solution
- COMSOL confirms that proposed design exceeds performance of training data

- Fabrication and testing of (3x) designs
- Transfer learning: use simple model to pre-train performance NN and use with more complex coupled EM/thermal time domain simulation
- Expand on use of NN's to solve the inverse design / optimization problem



The Grainger College of Engineering

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

