Inverse Design Methods for Novel, High-Performance and Manufacturable Components for Photonic Integrated Circuits

Presented by:

OSA Optoelectronics Technical Group

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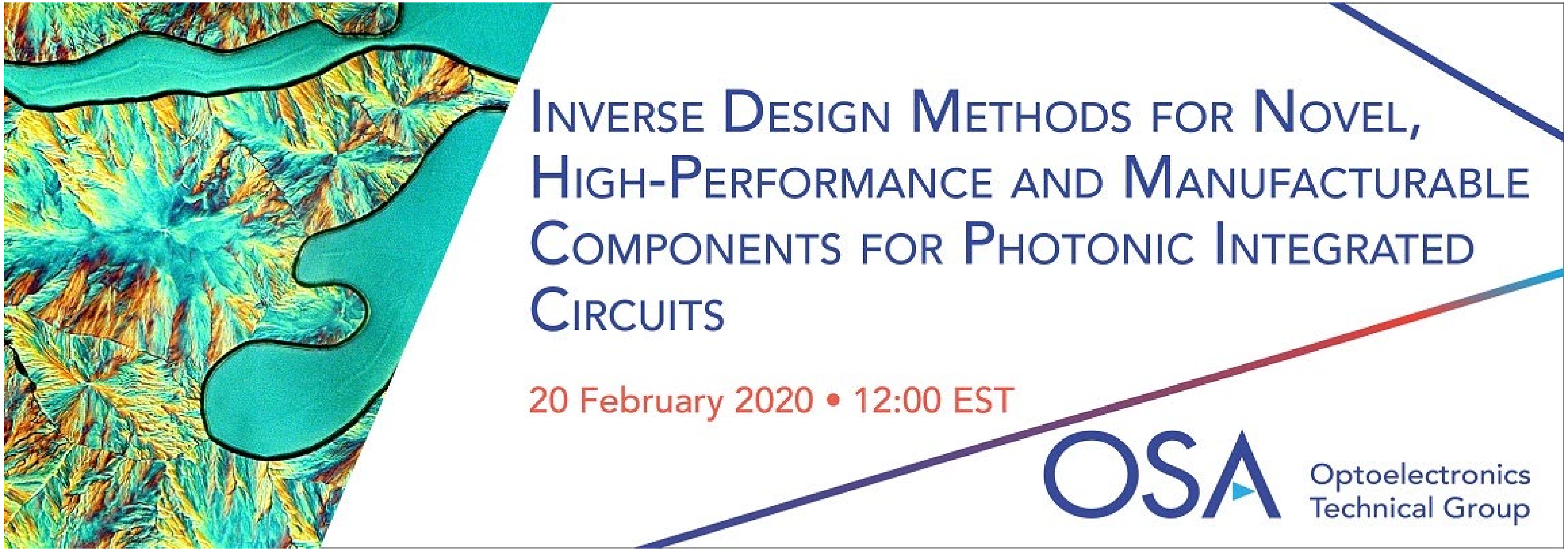

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Optoelectronics
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Technical Group at a Glance

- Focus
  - The OP TG focuses in the field of semiconductor lasers, amplifiers, LEDs and super luminescent diodes, and other areas related to optoelectronics
  - Over 4,500 members within OSA
- Mission
  - To benefit *YOU*
  - Webinars, e-Presence, publications, technical events, business events, outreach
  - Interested in presenting your research? Have ideas for TG events? Contact winnie.ye@carleton.ca
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Today’s Webinar

Inverse Design Methods for Novel, High-Performance and Manufacturable Components for Photonic Integrated Circuits

Dr. James Pond is the CTO and co-founder of Lumerical Inc. and is a driving force behind the company’s core software algorithms, technology, and advanced photonic modeling capabilities. He has almost two decades of experience in optical and photonic simulation, and is the author of numerous papers, patents and conference presentations.Prof. Benjamin Eggleton is the Director of The University of Sydney Nano Institute. He also currently serves as the co-Director of the NSW Smart Sensing Network (NSSN).

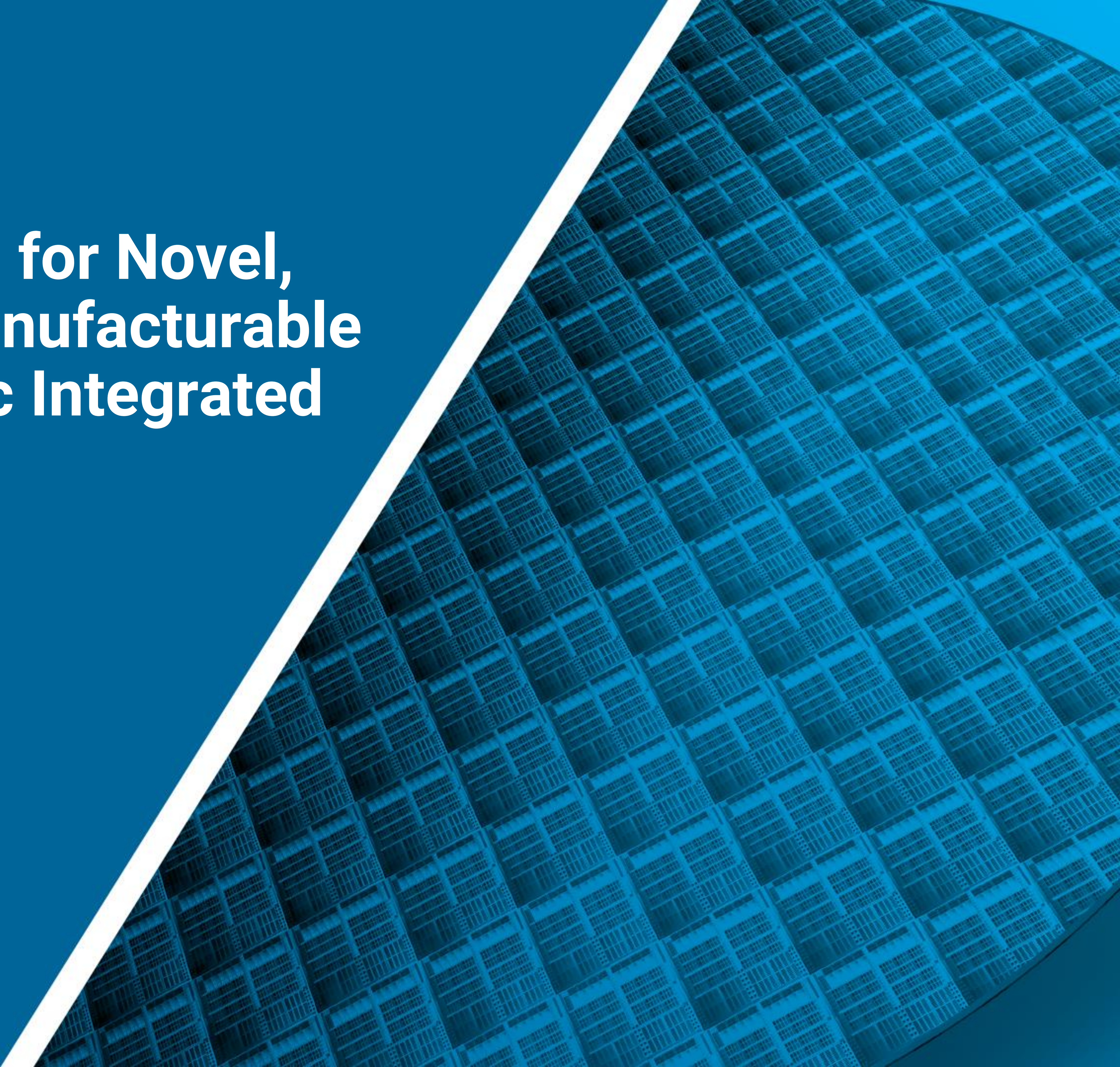
Dr. Jens Niegemann received his PhD in theoretical physics in 2008 from the University of Karlsruhe, Germany. In 2015 he became Principal Scientist at Lumerical Inc. where he focuses on the development and implementation of efficient algorithms for photonic simulations. Dr. Niegemann has contributed to more than 50 peer-reviewed publications and conference presentations.

Please join me to welcome **Dr. Pond** and **Dr. Niegemann**.

Question & Answer

Inverse Design Methods for Novel, High-Performance and Manufacturable Components for Photonic Integrated Circuits

Lumerical Inc.
February 20th, 2020



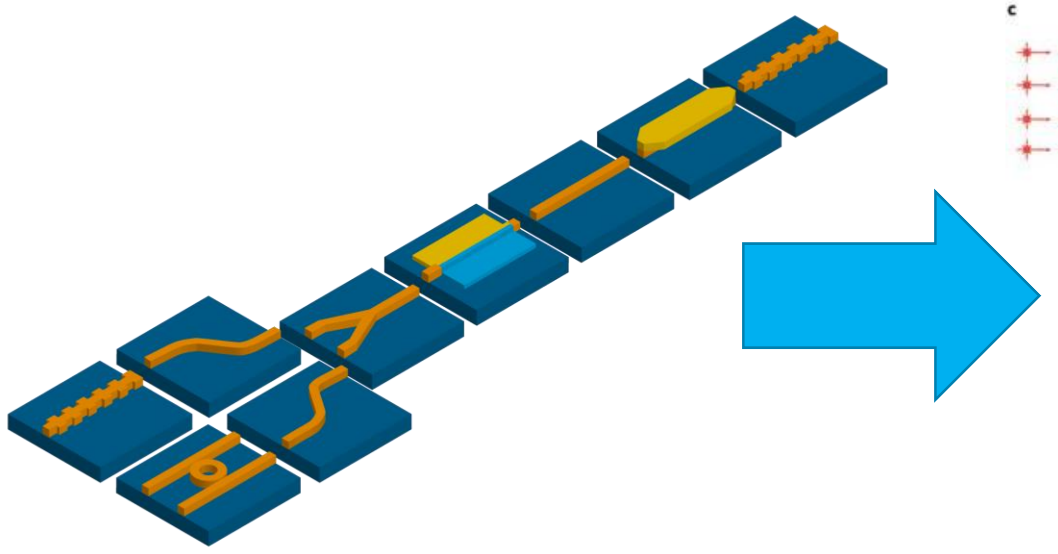
Outline

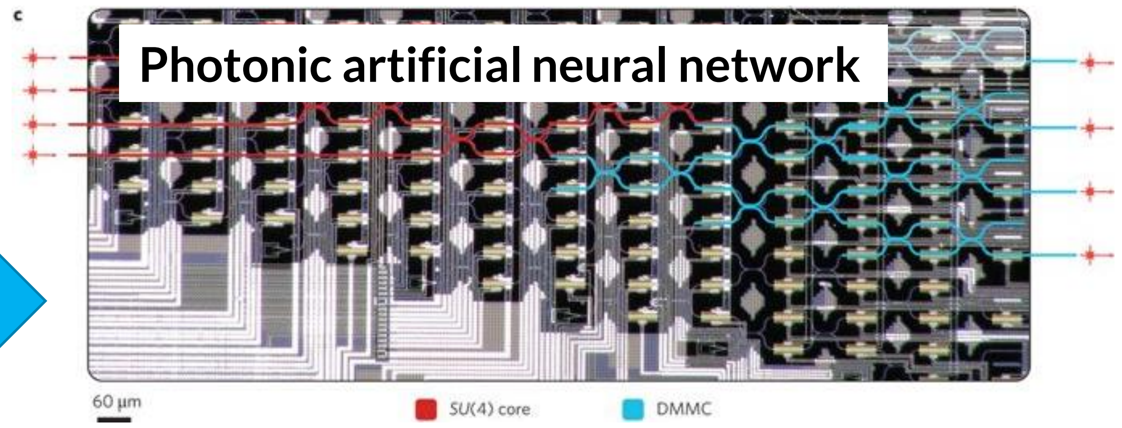
- Motivation and Introduction
- Parametric Shape Optimization
- Topology Optimization
- Summary
- Q&A

Motivation and Introduction

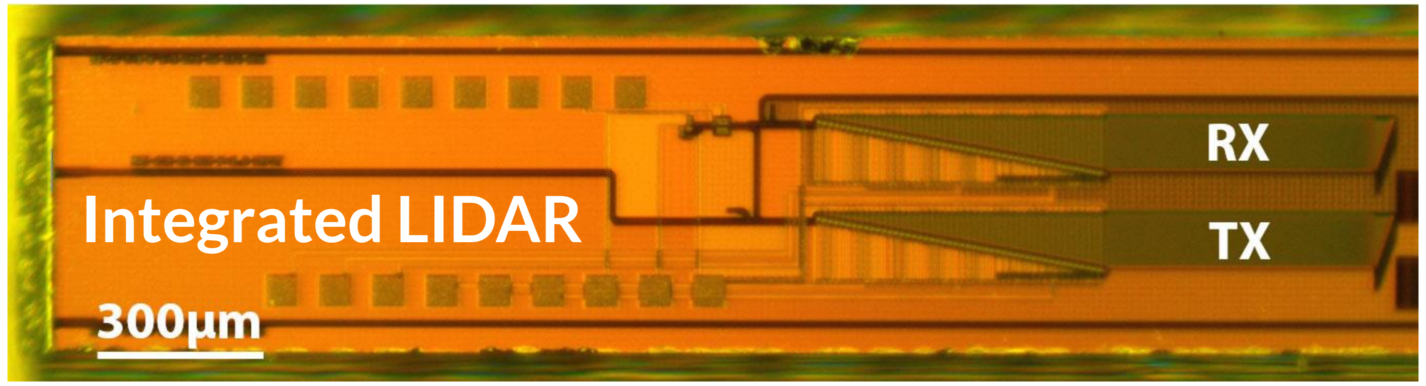
Motivation

Photonic integrated circuits (PICs) are becoming increasingly more complex





Y. Shen et al. Deep learning with coherent nanophotonic circuits, Nature Photonics, https://doi.org/10.1038/nphoton.2017.93

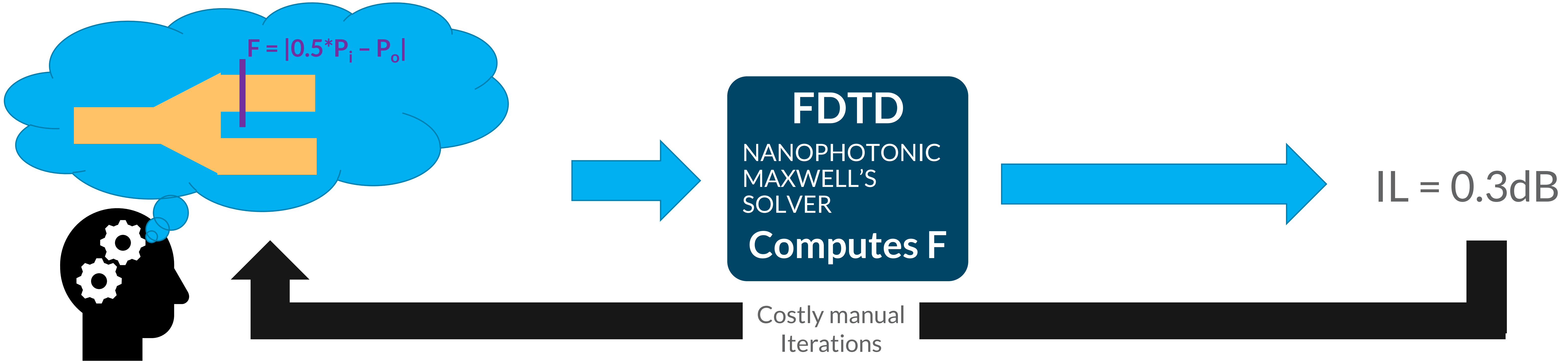


MIT and DARPA Pack Lidar Sensor Onto Single Chip
https://spectrum.ieee.org/tech-talk/semiconductors/optoelectronics/mit-lidar-on-a-chip
Image: Christopher V. Poulton

Individual photonic components need to become:

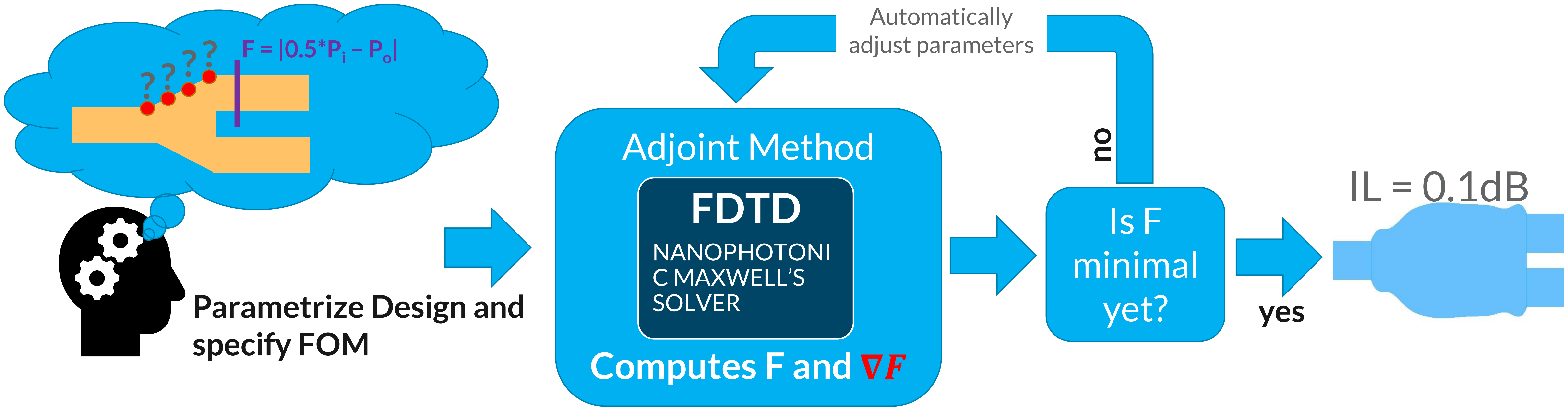
- more efficient
- more tolerant against manufacturing defects or variations
- more compact

Traditional Forward Design



- Traditional design often guided by physical insight
- Might use parameter sweeps or optimization in a small (e.g. 2-5) number of parameters
- Has produced a large library of template devices over the past decades
- But: Time-consuming and often difficult to generalize (e.g. to broad-band devices)

Photonic Inverse Design



- User can target an arbitrary figure of merit (FOM)
- Still allows to use physical insight (or an existing design) to seed the process
- Efficient optimizers allow a much larger number of design parameters
- Here: gradient based algorithms which use the adjoint method to efficiently compute ∇F

The general building blocks of a PID method

Parametrization
- Shape
- Topology
- Level-Set
- …

EM-Solver
- FDTD
- DGTD
- FDFD
- FEM
- RCWA
- …

Time Domain

Frequency Domain

Optimizer
- Genetic Algorithms
- Bayesian Regression
- L-BFGS
- MMA
- SLSQP
- …

Gradient based

Gradient Calculation
- Adjoint Method
  - Continuous-first approach
  - Discrete-first approach
  - Born approximation
- Automatic Differentiation
- …

- Many combinations have been studied in literature over the past decade or so
- They each have their own advantages and disadvantages

The general building blocks of a PID method

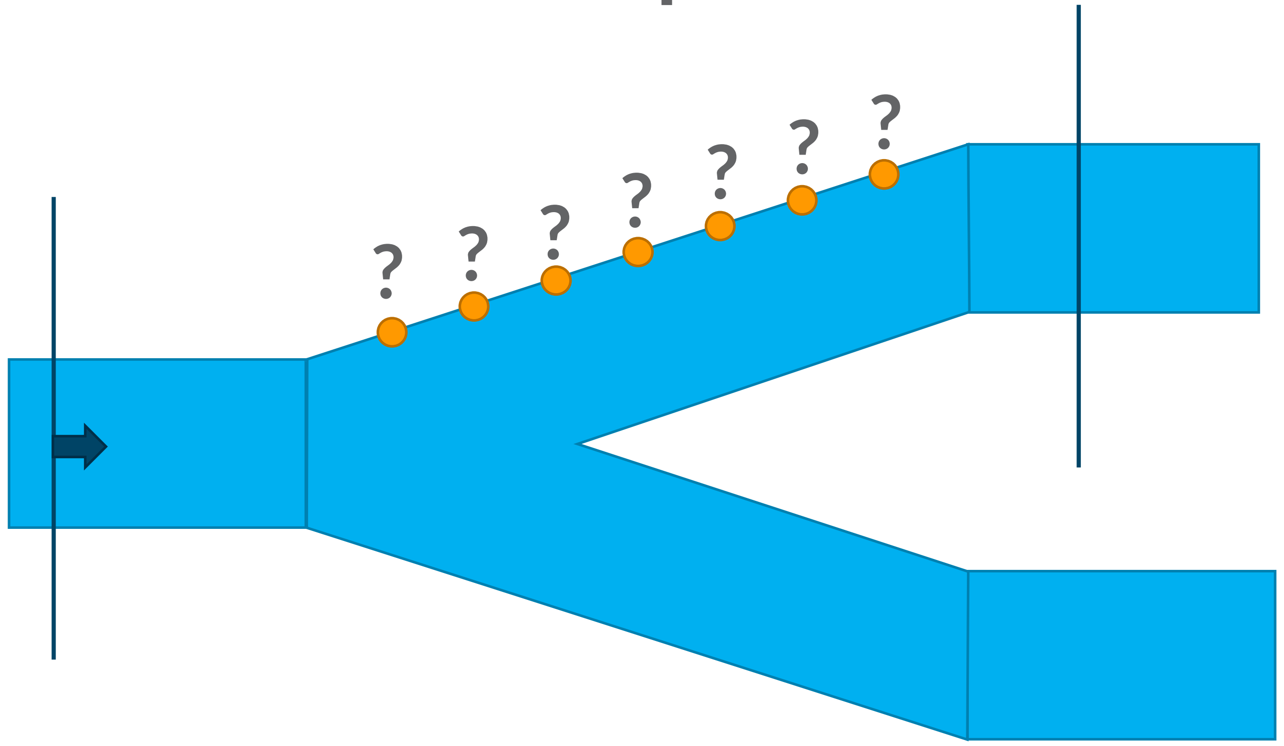
Parametrization	EM-Solver	Optimizer	Gradient Calculation

• Shape
• Topology
• Level-Set
• …
	• FDTD
	• DGTD
	(Time Domain)
	• FDFD
	• FEM
	• RCWA
	(Frequency Domain)
	• …
		• Genetic Algorithms
		• Bayesian Regression
		• L-BFGS
		• MMA
		• SLSQP
		(Gradient based)
		• …
			• Adjoint Method
			  • Continuous-first approach
			  • Discrete-first approach
			  • Born approximation
			• Automatic Differentiation
			• …

- Many combinations have been studied in literature over the past decade or so
- They each have their own advantages and disadvantages
- Here, we focus on a specific combination
- For more details on PID, see review articles (and references therein):
  - "Topology optimization for nano-photonics", Jensen, J. and Sigmund, O. Laser & Photon. Rev. 5, 308-321. (2011)
  - "Inverse design in nanophotonics", Molesky, S. et al., Nat. Photon. 12, 659–670 (2018)

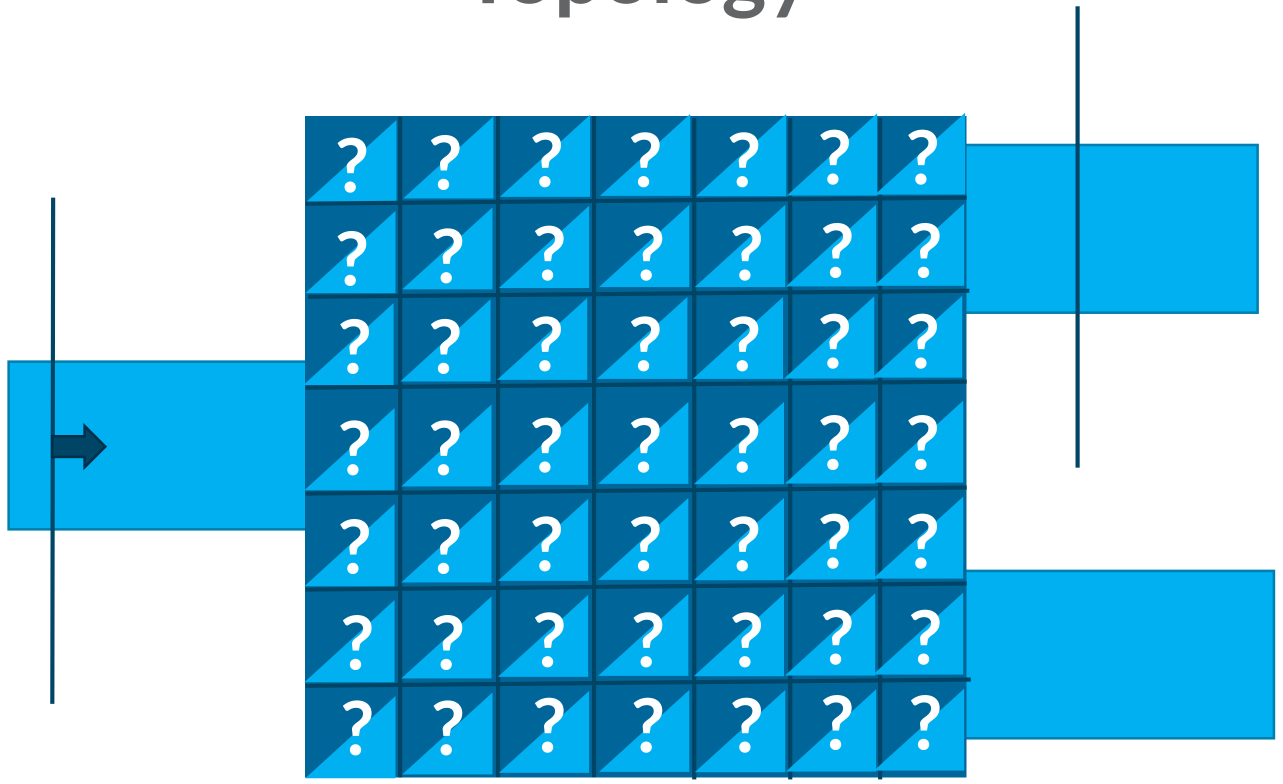
Parametrization: Shape/Topology

Shape



- ☺ Allows to quickly optimize existing designs
- ☺ Manufacturing constraints can be built into parametrization
- 😐 Requires good initial design
- 😐 Parametrization may still be too restrictive

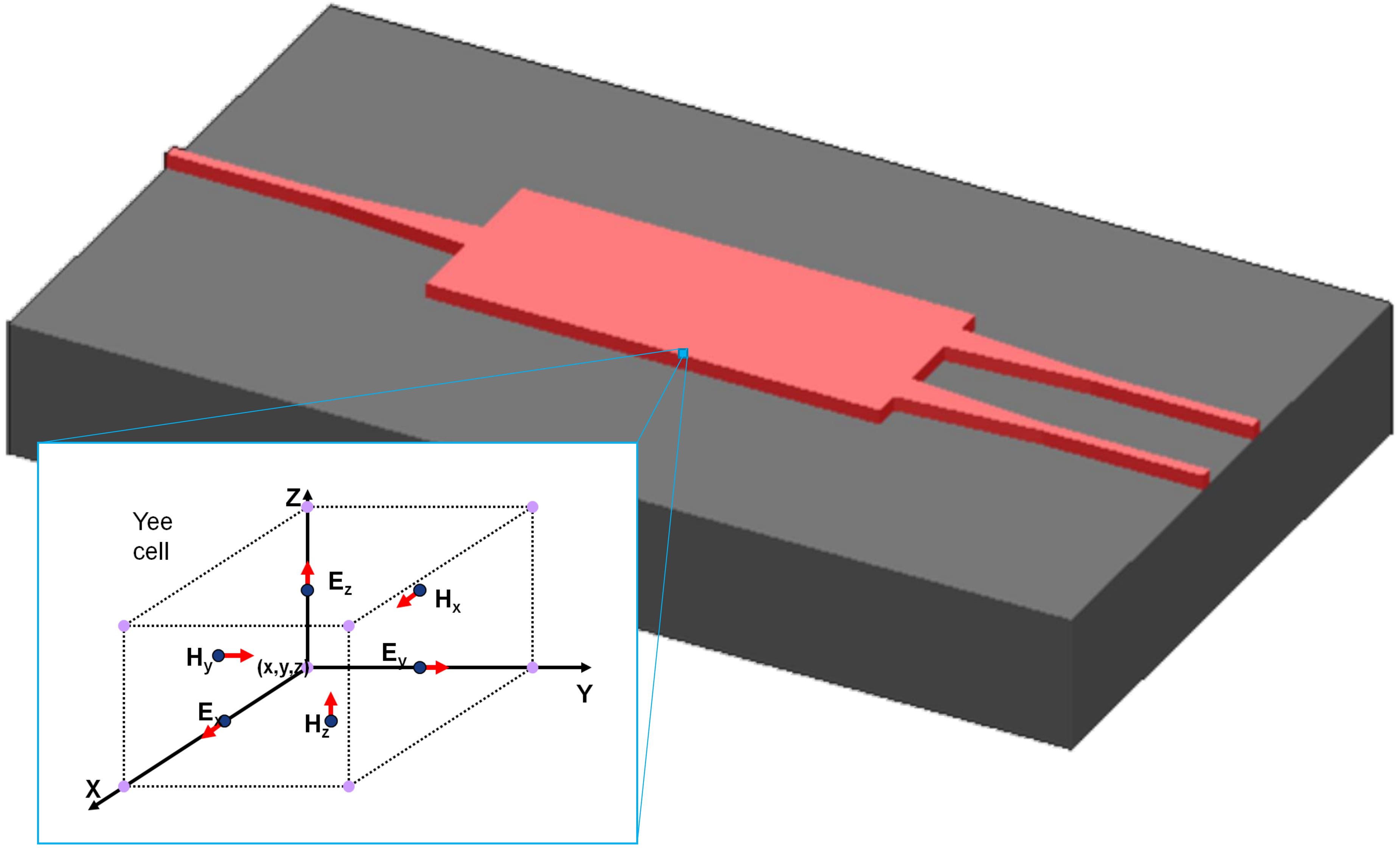
Topology



- ☺ User only specifies footprint and materials
- ☺ Often yields very high-performance
- 😐 Manufacturing constraints more difficult to enforce
- 😐 Design often unintuitive and not easy to generalize

EM-Solver: FDTD

- Robust, well-established method based on the Yee grid
- Very fast, especially for low/medium accuracy requirements
- Broadband optimization is easy and cheap
- Scales well to large 3d systems
- For Topology Optimization: rectilinear grid matches parametrization

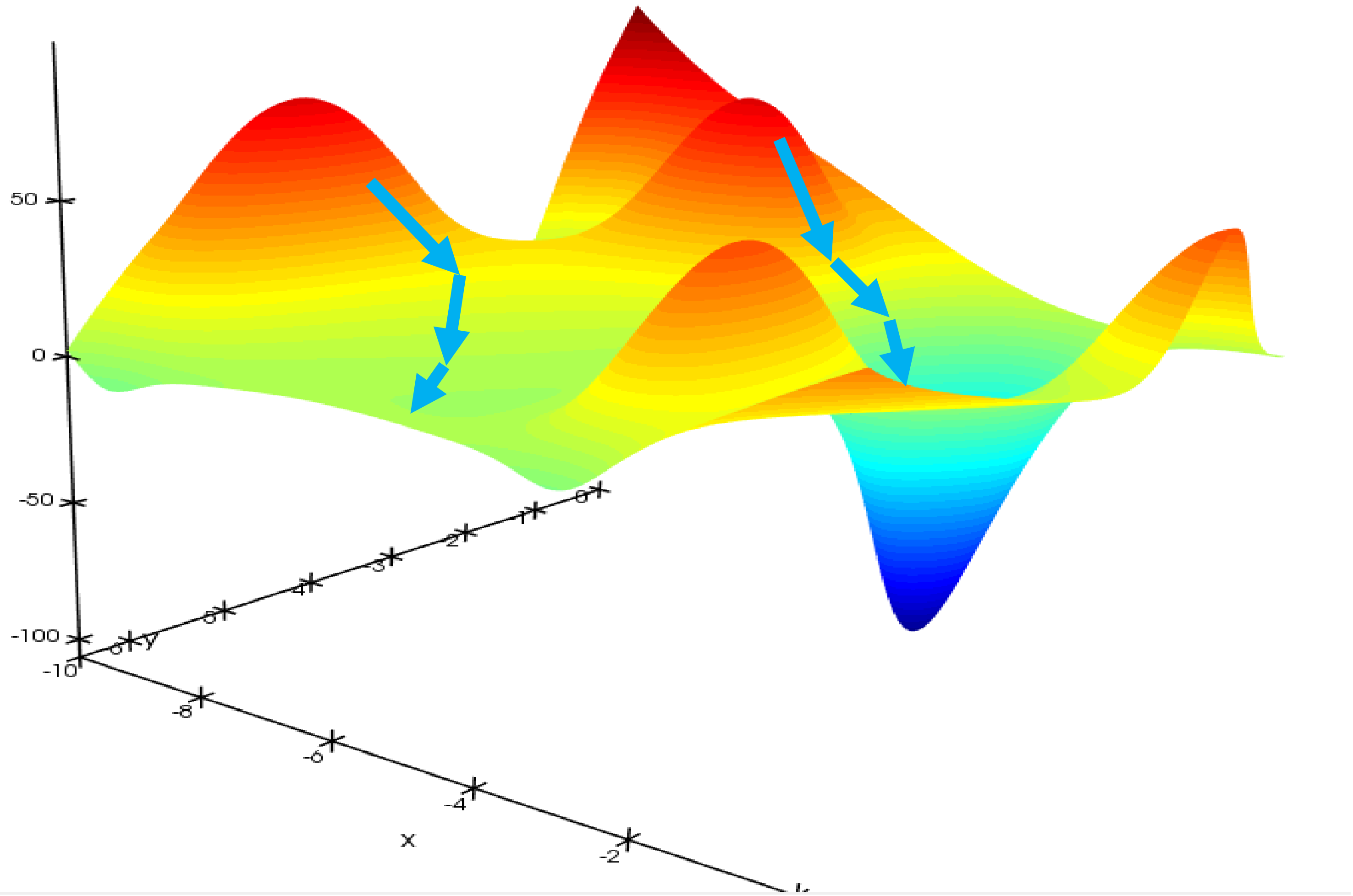


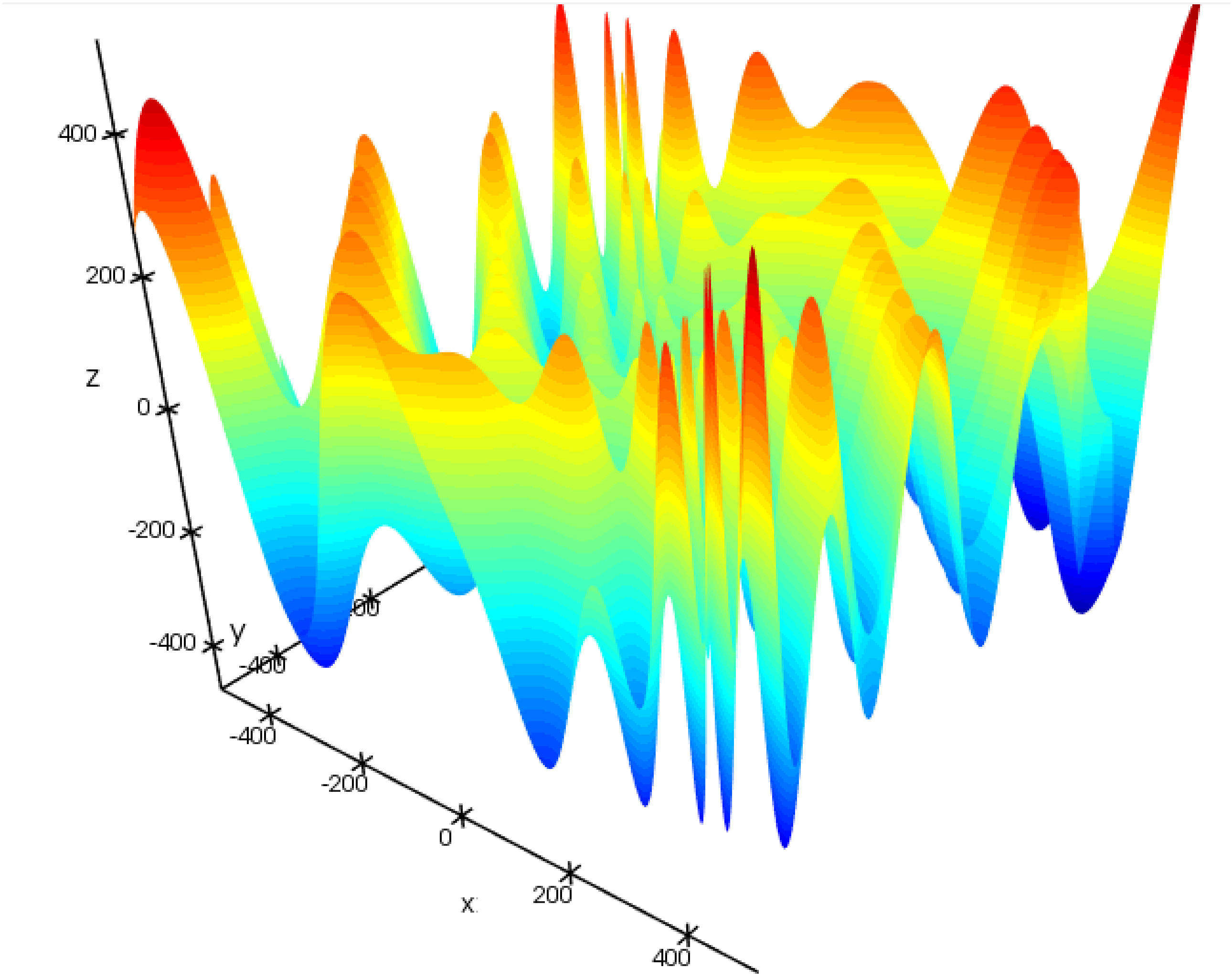
Optimizer: Gradient Based

- Running simulations to evaluate figure-of-merit F is generally expensive.
- Gradient methods find local solutions very quickly.
- They require an estimate of the gradient:

$$\nabla_p F = \left(\frac{\partial F}{\partial p_1}, \cdots, \frac{\partial F}{\partial p_N} \right)$$

- The gradient determines the direction of steepest descent:





Gradient Calculation: Adjoint sensitivity analysis, a long history

A long history over many decades in many fields including atmospheric science, fluid dynamics, electromagnetics, structural mechanics and more

Some examples of early work:

- Hall, M. C. G., D. G. Cacuci, and M. E. Schlesinger, 1982: Sensitivity analysis of a radiative convective model by the adjoint method. J. Atmos. Sci., 39, 2083–2050
- J. W. Bandler, Qi-Jun Zhang and R. M. Biernacki, "A unified theory for frequency-domain simulation and sensitivity analysis of linear and nonlinear circuits," in IEEE Transactions on Microwave Theory and Techniques, vol. 36, no. 12, pp. 1661-1669, Dec. 1988.
- O. Sigmund "A 99 line topology optimization code written in MATLAB", Structural and Multidisciplinary Optimization 21(2), 2001, pp. 120-127
- …

Not a comprehensive literature review!

Early use with FDTD simulation

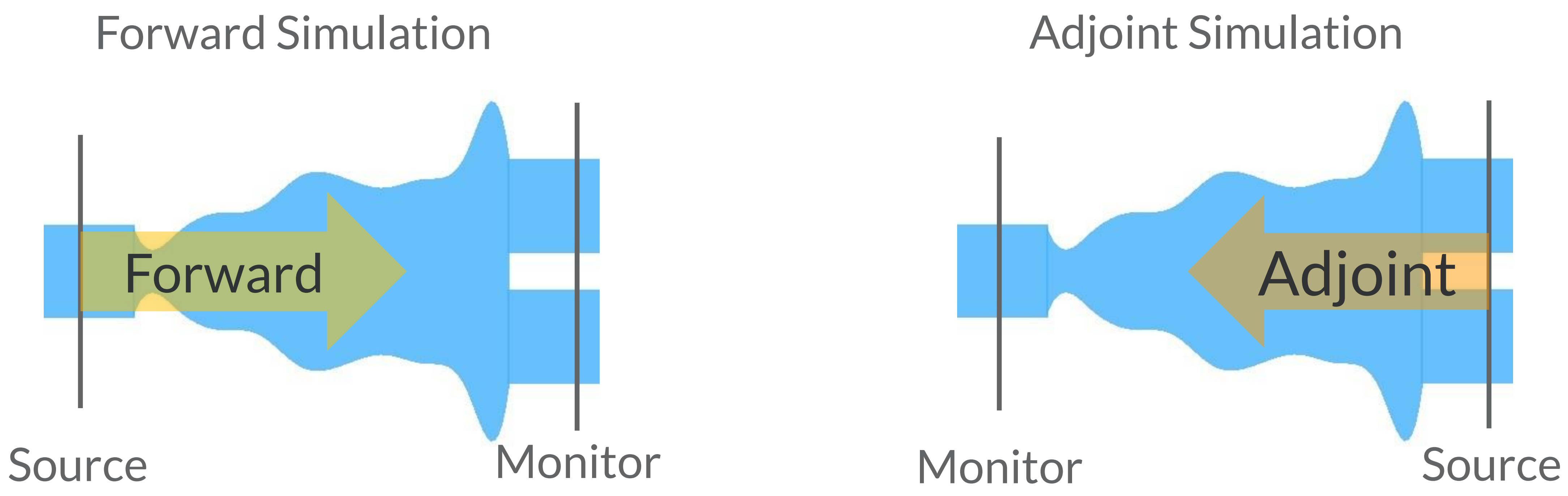
- N. K. Nikolova, H. W. Tam and M. H. Bakr, "Sensitivity analysis with the FDTD method on structured grids," in IEEE Transactions on Microwave Theory and Techniques, vol. 52, no. 4, pp. 1207-1216, April 2004.
- M. A. Swillam, M. H. Bakr, and X. Li, "Accurate sensitivity analysis of photonic devices exploiting the finite- difference time-domain central adjoint variable method," J. Applied Optics, vol. 46 , no. 9, pp. 1492 – 1499, March 2007
- …

Use in integrated photonics

- J. Jensen and O. Sigmund, "Topology optimization for nano-photonics," Laser & Photon. Rev., 5: 308-321 (2011)
- Alexander Y. Piggott, Jesse Lu, Konstantinos G. Lagoudakis, Jan Petykiewicz, Thomas M. Babinec & Jelena Vučković, "Inverse design and demonstration of a compact and broadband on-chip wavelength demultiplexer", Nature Photonics volume 9, pages 374–377 (2015).
- Christopher M. Lalau-Keraly, Samarth Bhargava, Owen D. Miller, and Eli Yablonovitch, "Adjoint shape optimization applied to electromagnetic design," Opt. Express 21, 21693-21701 (2013).
- …

Gradient Calculation: The Adjoint Method

- Adjoint method allows for **efficient** evaluation of F and its gradient
- Only **two simulations (independent of the number of parameters)** are required:



Gradient Calculation: The Adjoint Method for FDTD

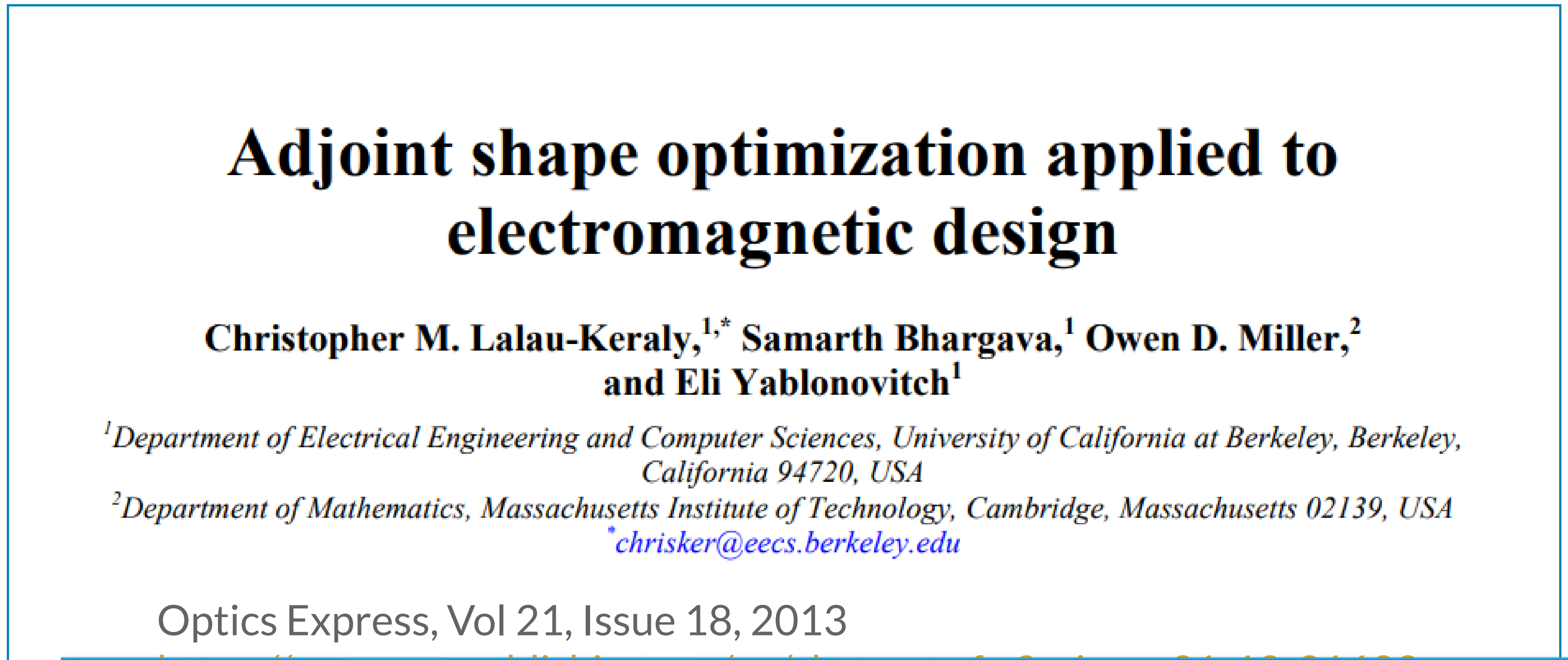
- Here, we use an approach based on Green's functions/the Born approximation

- Requires no change to the solver

- Our implementation started as a collaboration with Christopher Keraly from Eli Yablonovitch's group (UCB)

- (Almost) Everything we present here today is freely available in an open-source project called "lumopt"

- Hosted on github under a MIT license at https://github.com/chriskeraly/lumopt

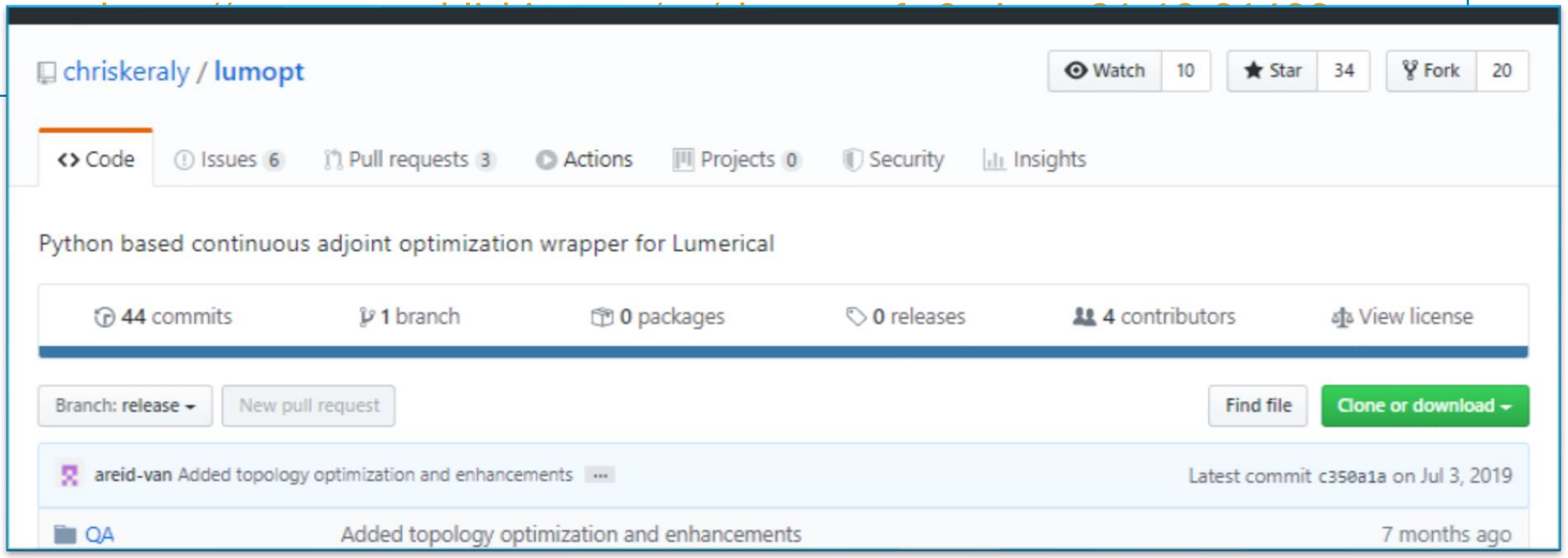


Adjoint shape optimization applied to electromagnetic design

Christopher M. Lalau-Keraly,[1,*] Samarth Bhargava,[1] Owen D. Miller,[2] and Eli Yablonovitch[1]

[1]Department of Electrical Engineering and Computer Sciences, University of California at Berkeley, Berkeley, California 94720, USA
[2]Department of Mathematics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
[*]chrisker@eecs.berkeley.edu

Optics Express, Vol 21, Issue 18, 2013

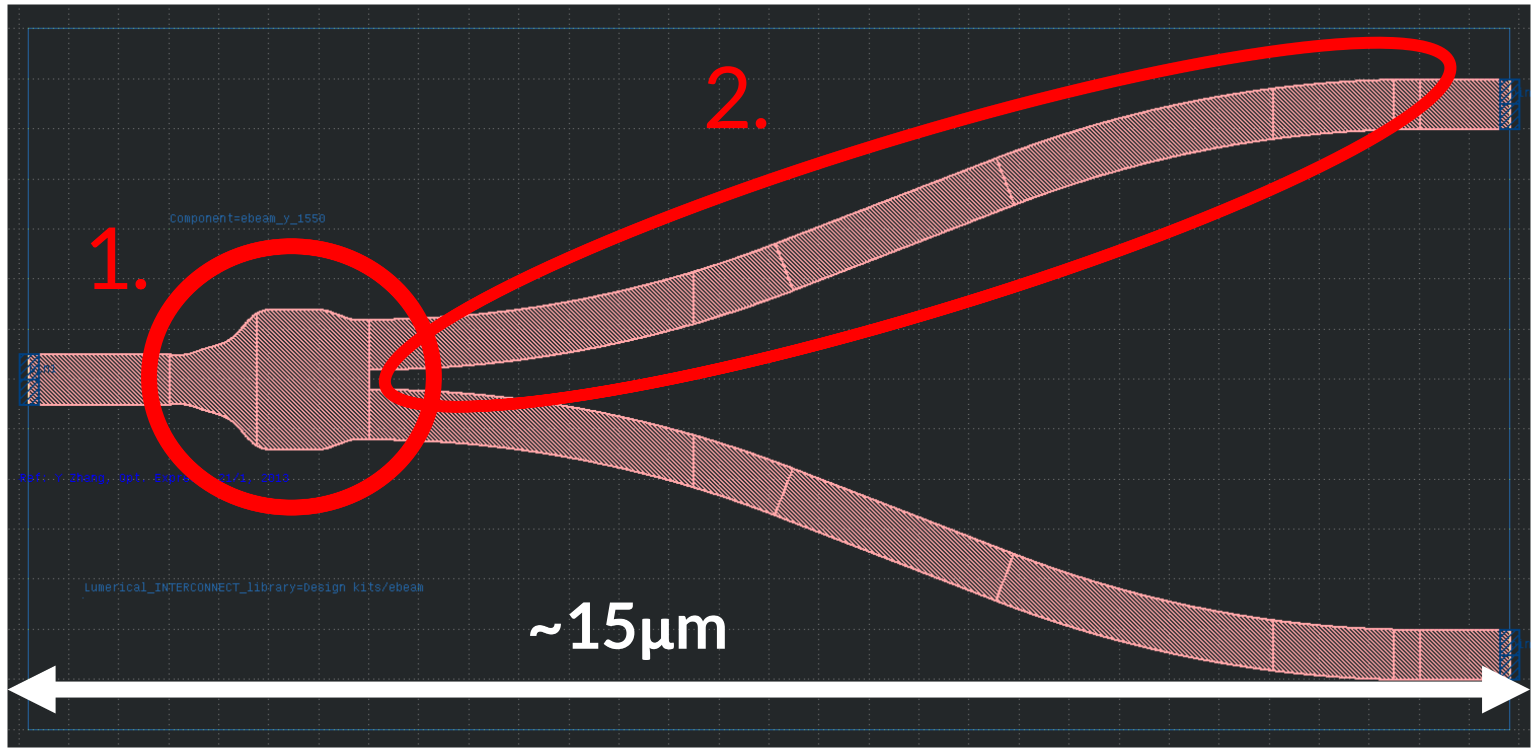


Parametric Shape Optimization

Y-splitter example: Designing a smaller splitter

Prior art

1. Inverse design using particle swarm optimization
2. Output waveguides added post optimization

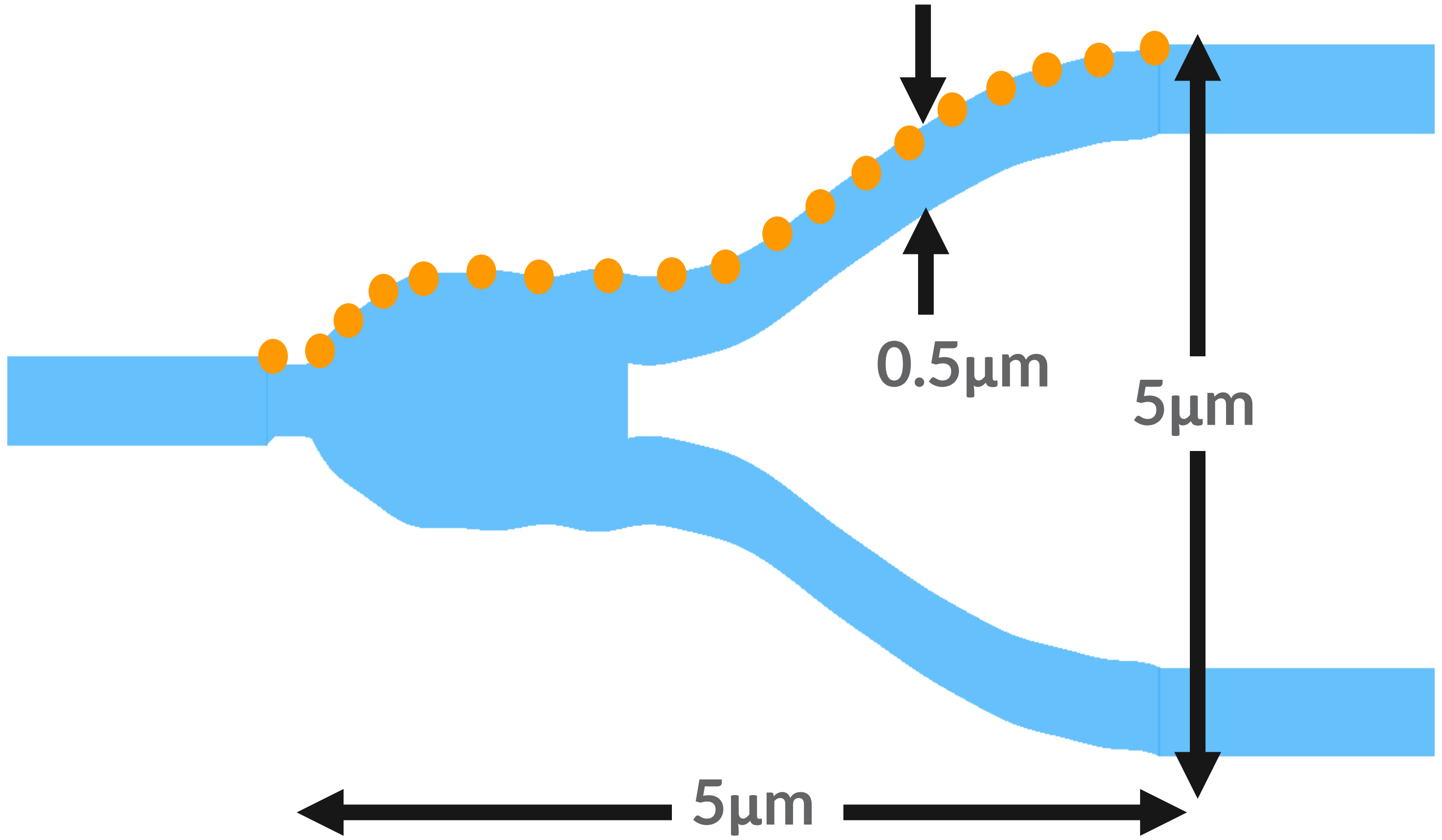


https://github.com/lukasc-ubc/SiEPIC_EBeam_PDK

A compact and low loss Y-junction for submicron silicon waveguide
Yi Zhang, et al, Optics Express Vol. 21, Issue 1, pp. 1310-1316 (2013)

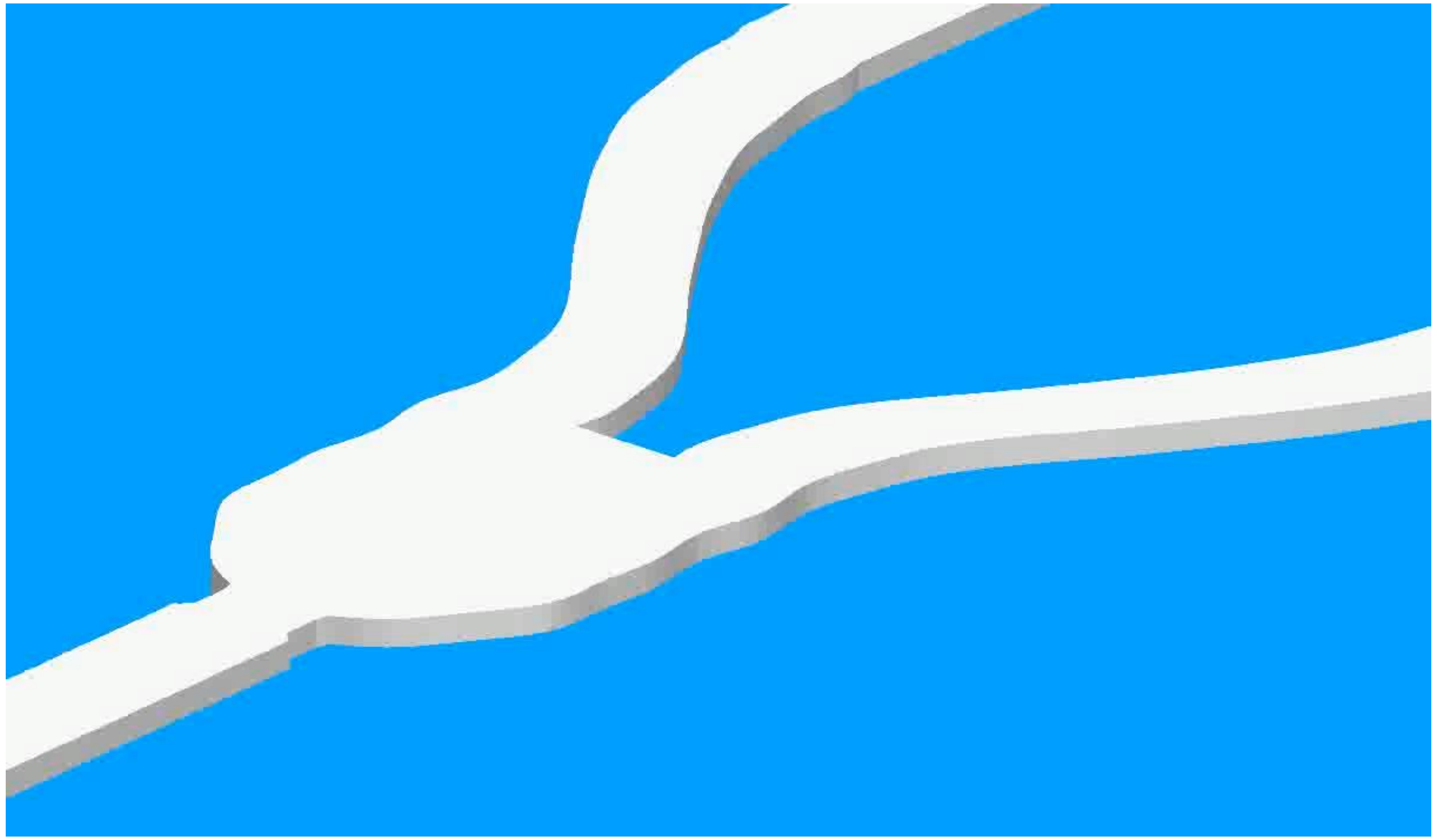
Example splitter

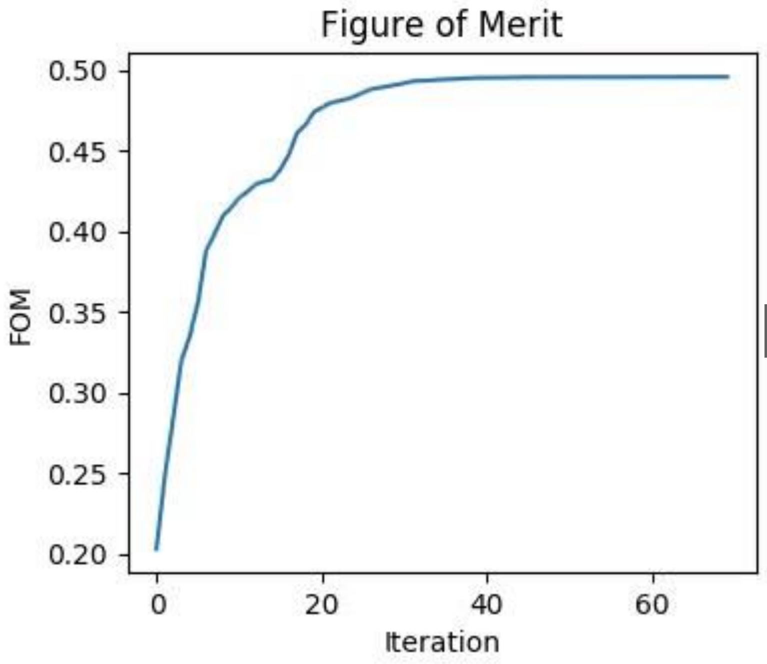
- Parametric shape includes output waveguides
- 20 parameters
- Smaller footprint



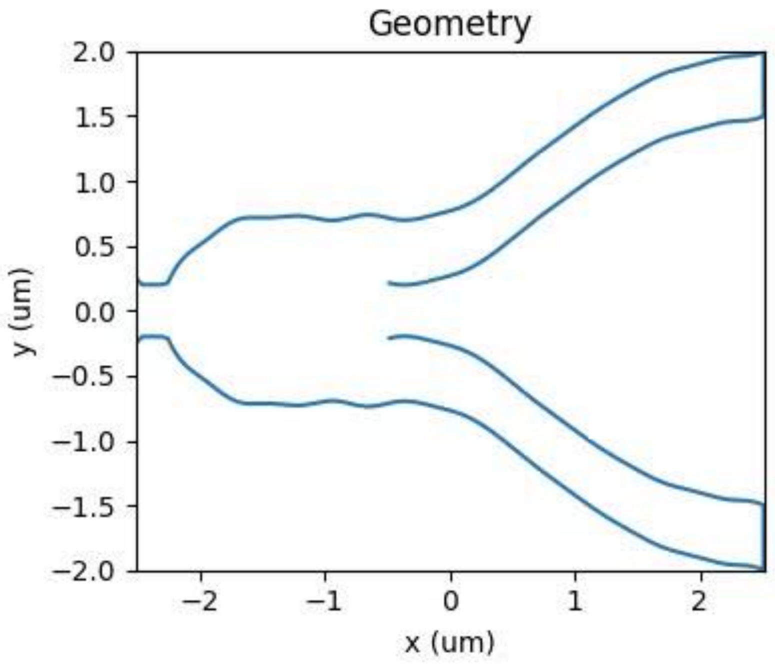
Y-splitter example: Run fast 2D optimization

This example takes < 60 minutes to run:



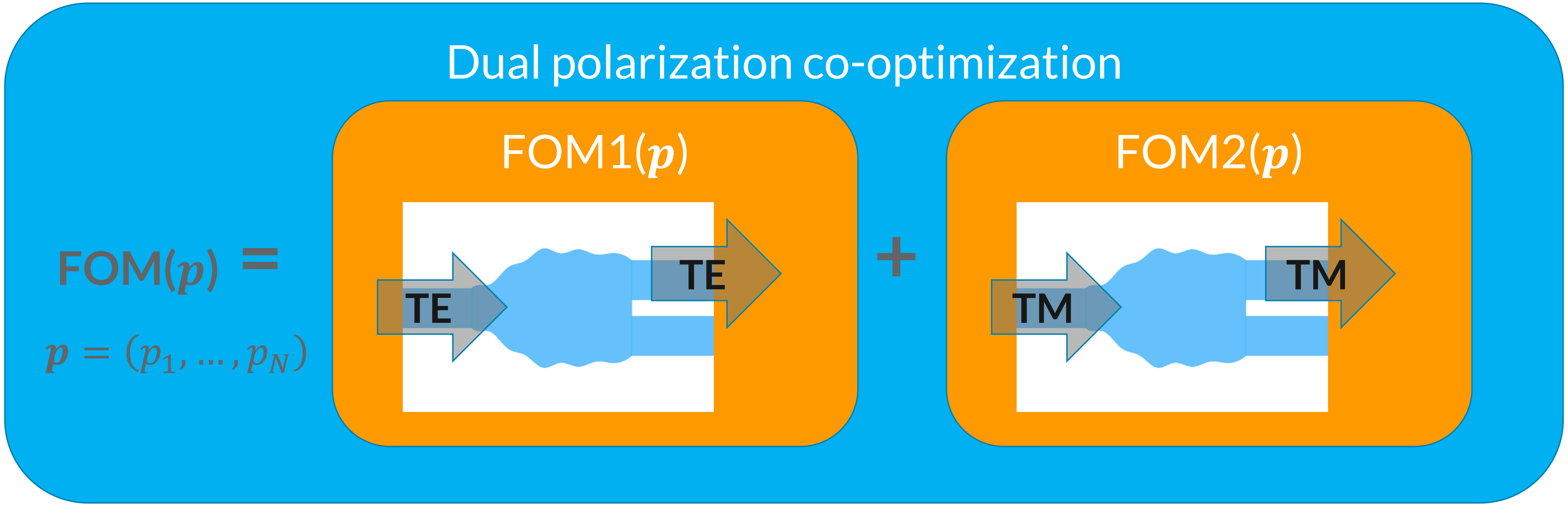


FOM = 0.5 = ideal




```
FINAL FOM = [0.49560308]
FINAL PARAMETERS = [0.2        0.26701897 0.48560055 0.67317026 0.69742398 0.727
36151
 0.69563423 0.74014193 0.69735868 0.7383804  0.82057129 0.99880643
 1.21080748 1.40641413 1.58424313 1.72710327 1.84192843 1.90636349
 1.96069338 1.99607748]
>>>
```

Co-Optimization



Co-optimization:

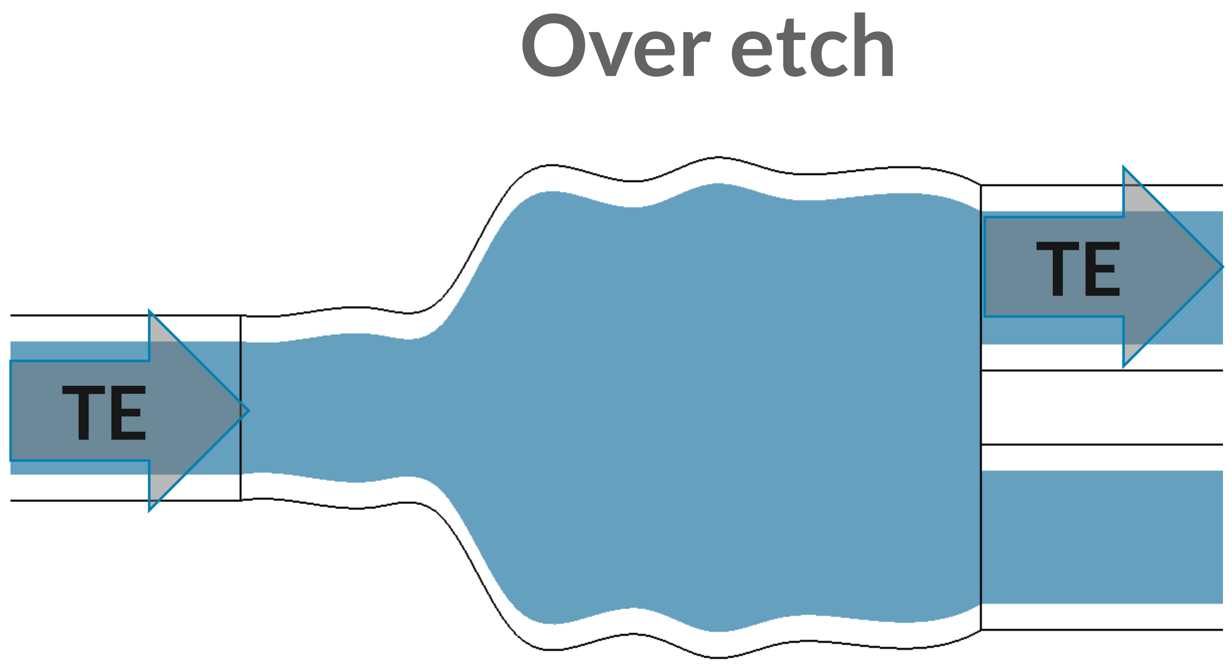
- Run multiple optimizations concurrently
- Optimizations share same parameters
- Figure of merit or structure can be different

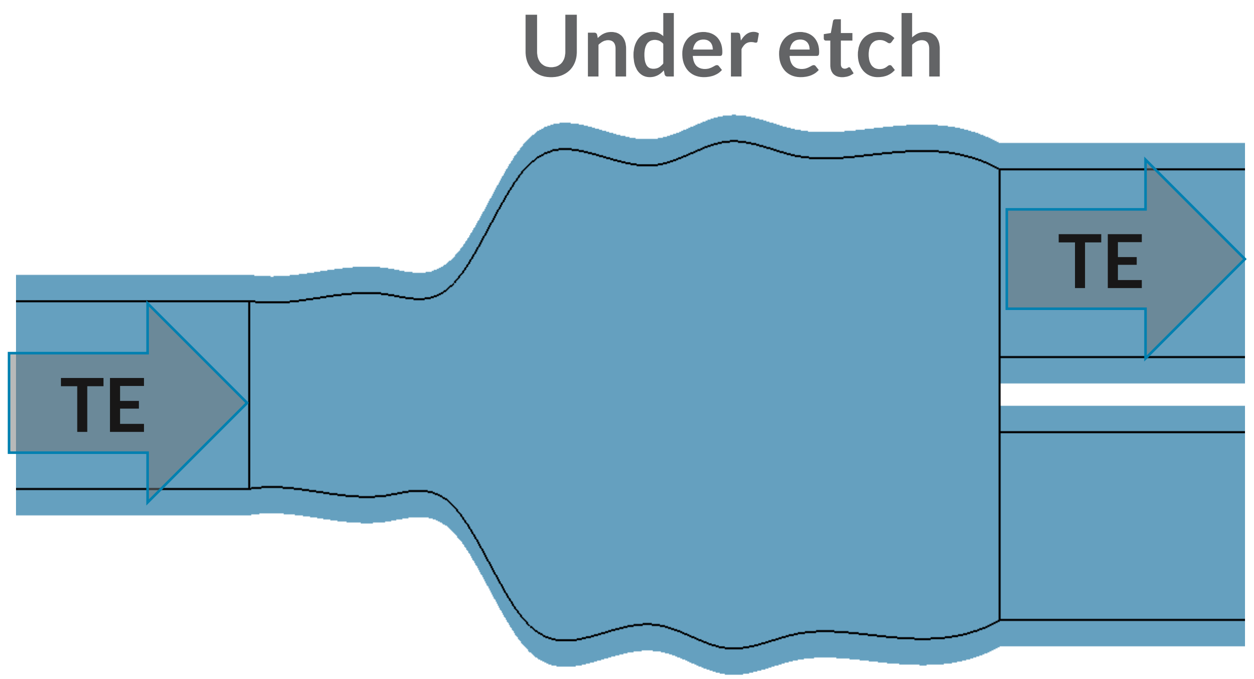
Example uses:

- Dual polarization devices (different FOM)
- Unequal splitting ratio (different FOM)
- De-multiplexing (different FOM)
- Optimize process corners (different geometry)

Co-optimization: Robust splitter

- Build a splitter tolerant to manufacturing error
- Co-optimize 2 different shapes (same parameters)
- “Over etch” slightly smaller than nominal
- “Under etch” slightly larger than nominal
- Same FOM function

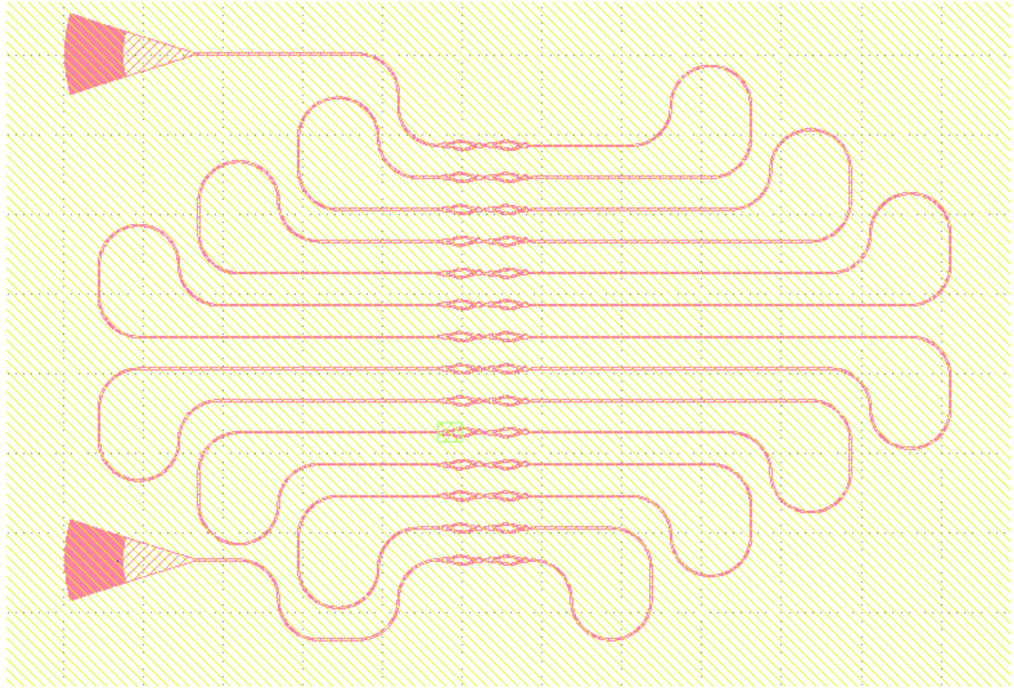


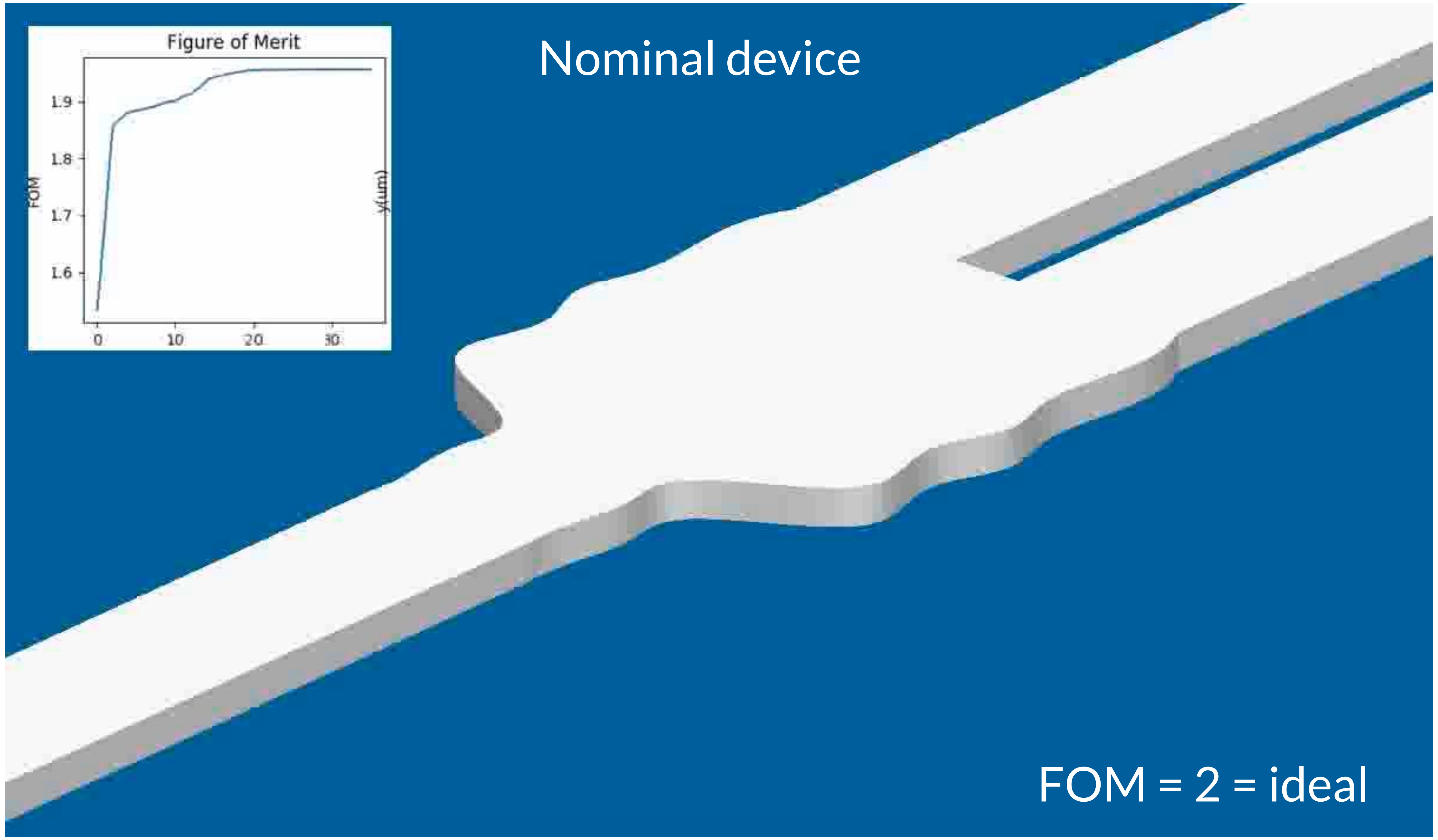


Co-optimization: Robust splitter

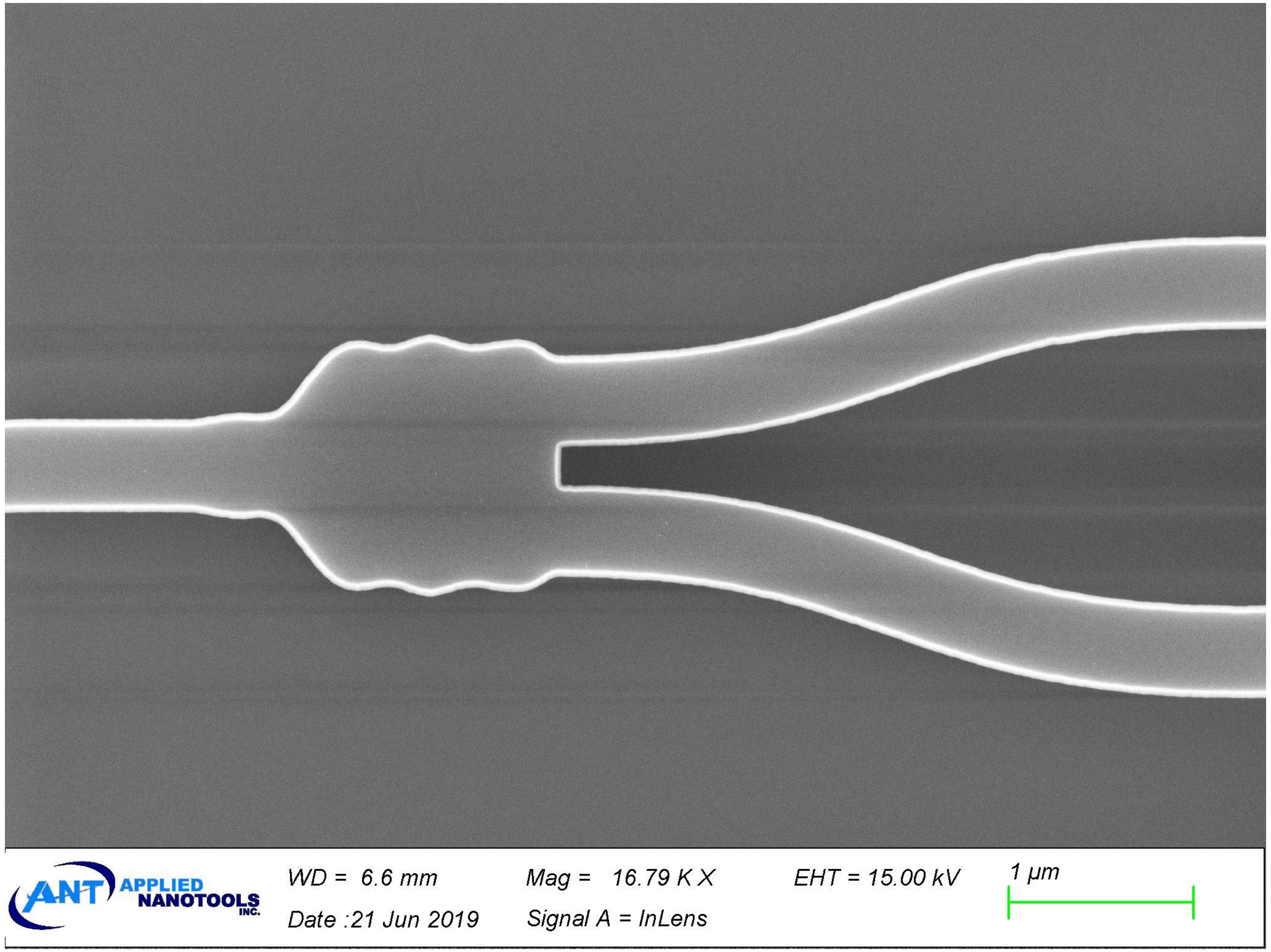
Co-optimization of +/- 14nm on edge position

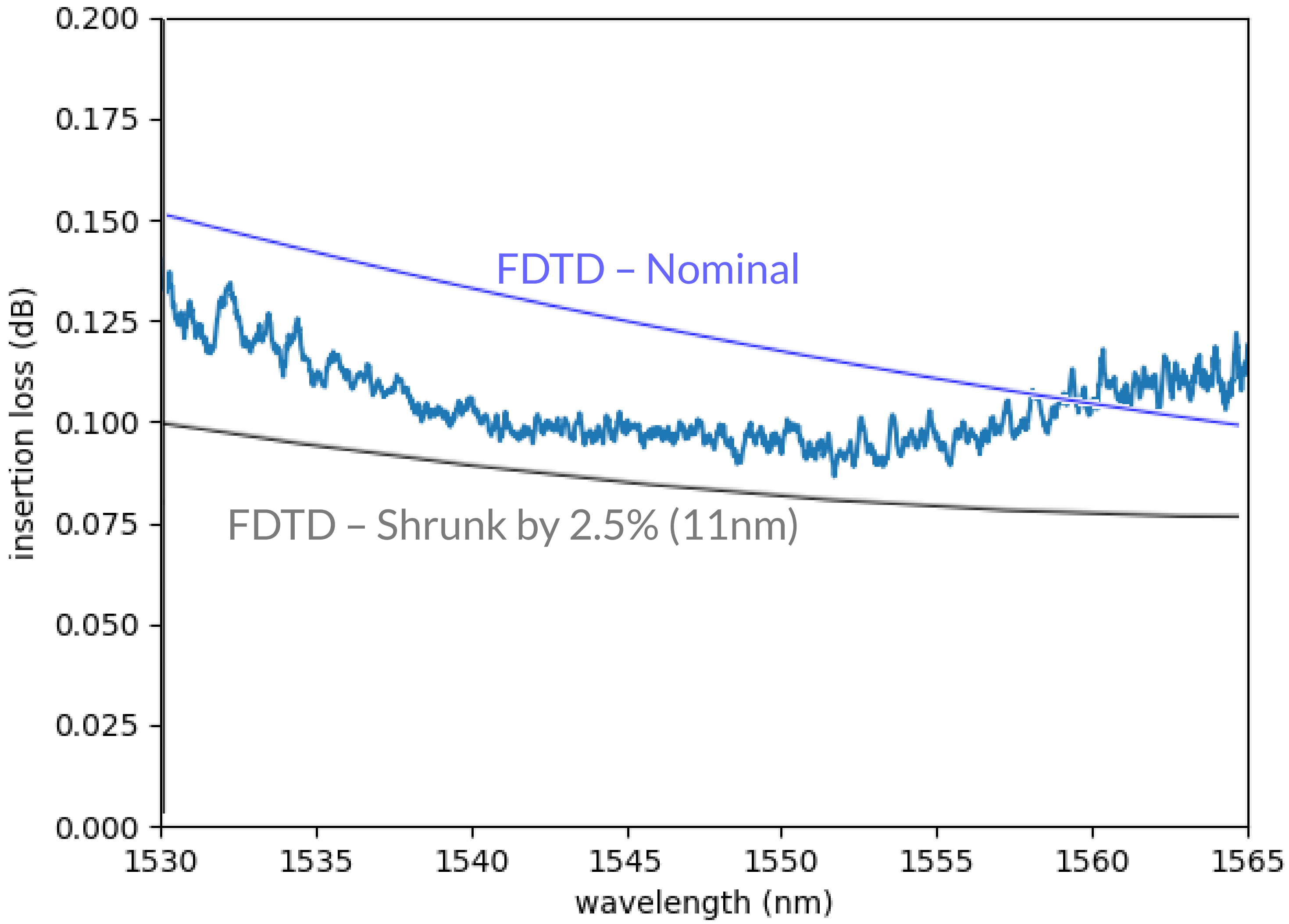
- Problem setup similar to before
- Setup 2 optimizations
- Sum the figures of merit
- 2 FDTD simulations/FOM/iteration





Measured Results of Devices Designed with Lumopt



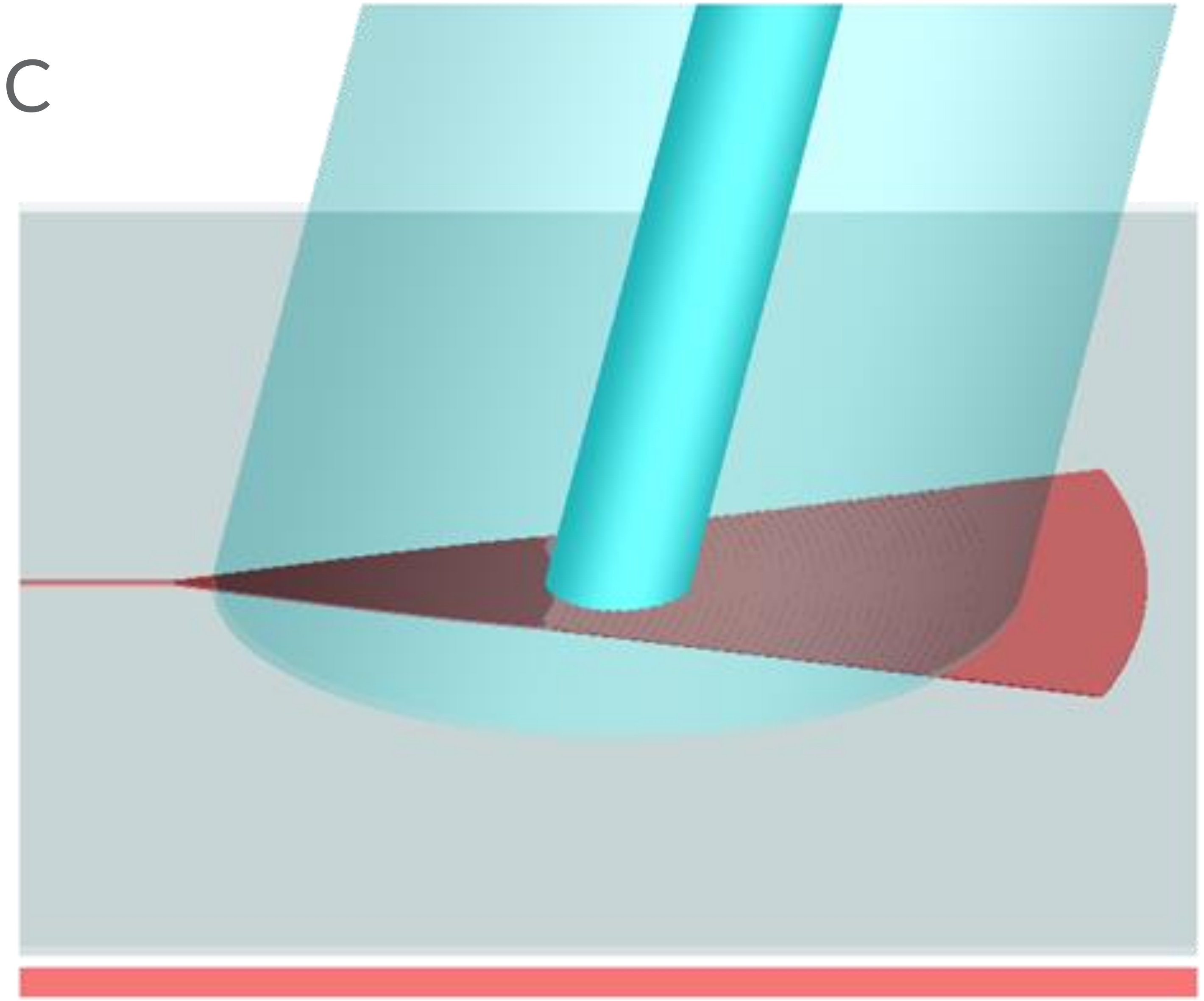


Designed and fabricated during the "SiEPIC-Passives workshop with Applied Nanotools fabrication“, Organized by Lukas Chrostowski at UBC (siepic.ubc.ca)

lumerical

Example: Grating Couplers

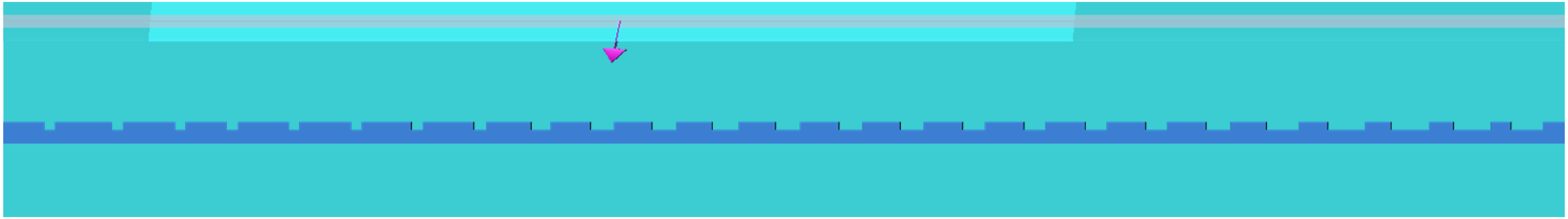
- Grating Couplers (GCs) are important devices for PIC
  - Don't require additional process steps
  - In/out-coupling anywhere on the chip
  - Allow for automatic wafer-scale testing
  - Alignment easier than alternative coupling techniques



- But they have challenges as well:
  - Not trivial to get high coupling efficiencies
  - Not intrinsically broad-band
  - Constrained by manufacturing capabilities
  - Large design space (50+ parameters) makes optimization challenging

Systematic Optimization of Grating Couplers

- A single-etch GC in 2d has ≈ 50 parameters

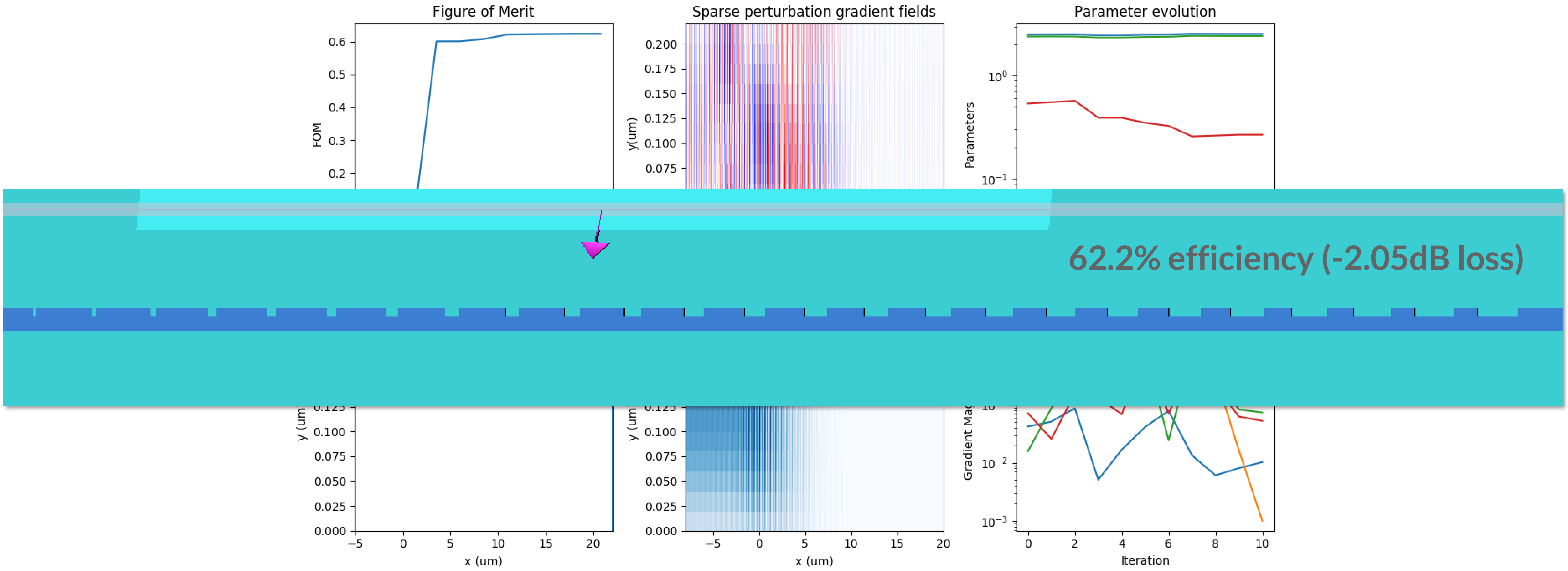


- We assume fiber angle (10 deg), Si layer thickness (220nm), BOX thickness (2um) as fixed
- Outcome of optimization strongly depends on initial guess

- **Systematic Approach to design highly efficient GCs**
  - Physical knowledge or analytic solutions provide a good initial guess
  - Use sequence of optimizations which gradually increase complexity

Optimization of basic partial-etch GC

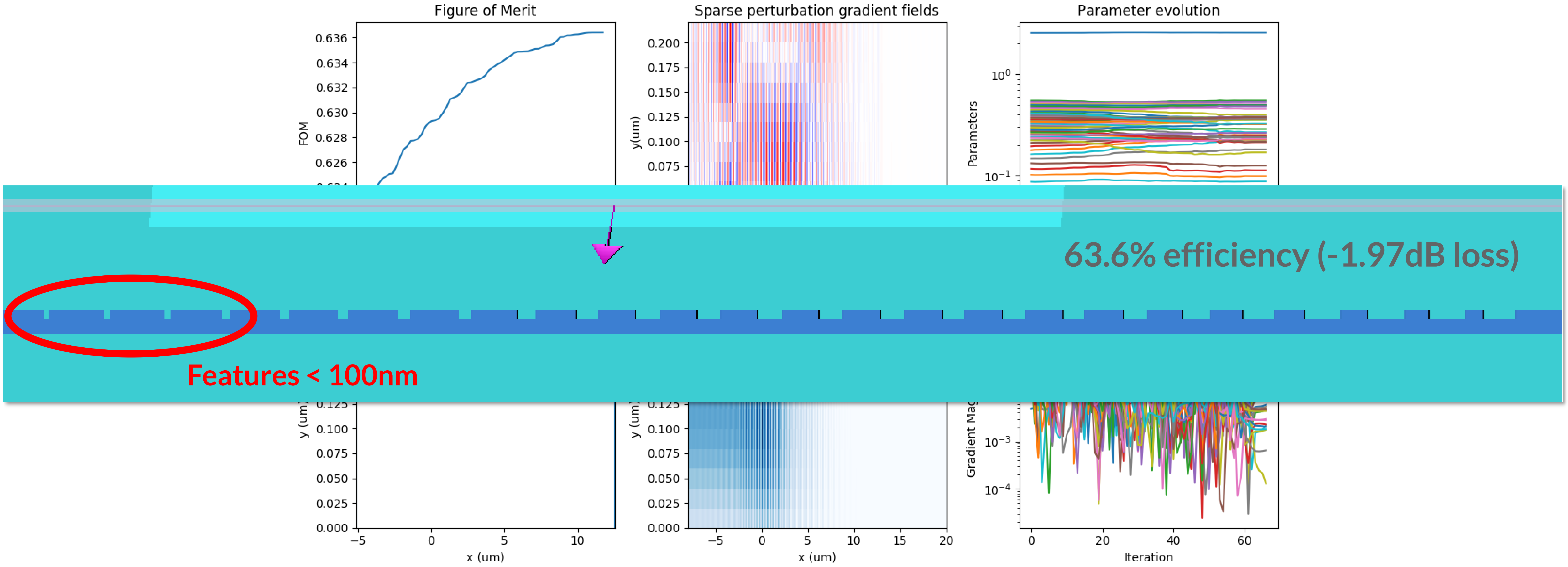
1. Use physical insight [1] to design **linearly apodized** coupler (only 4 parameters)



[1] R. Marchetti et al., “High-efficiency grating-couplers: demonstration of a new design strategy”, Scientific Reports 7, 16670 (2017), https://www.nature.com/articles/s41598-017-16505-z

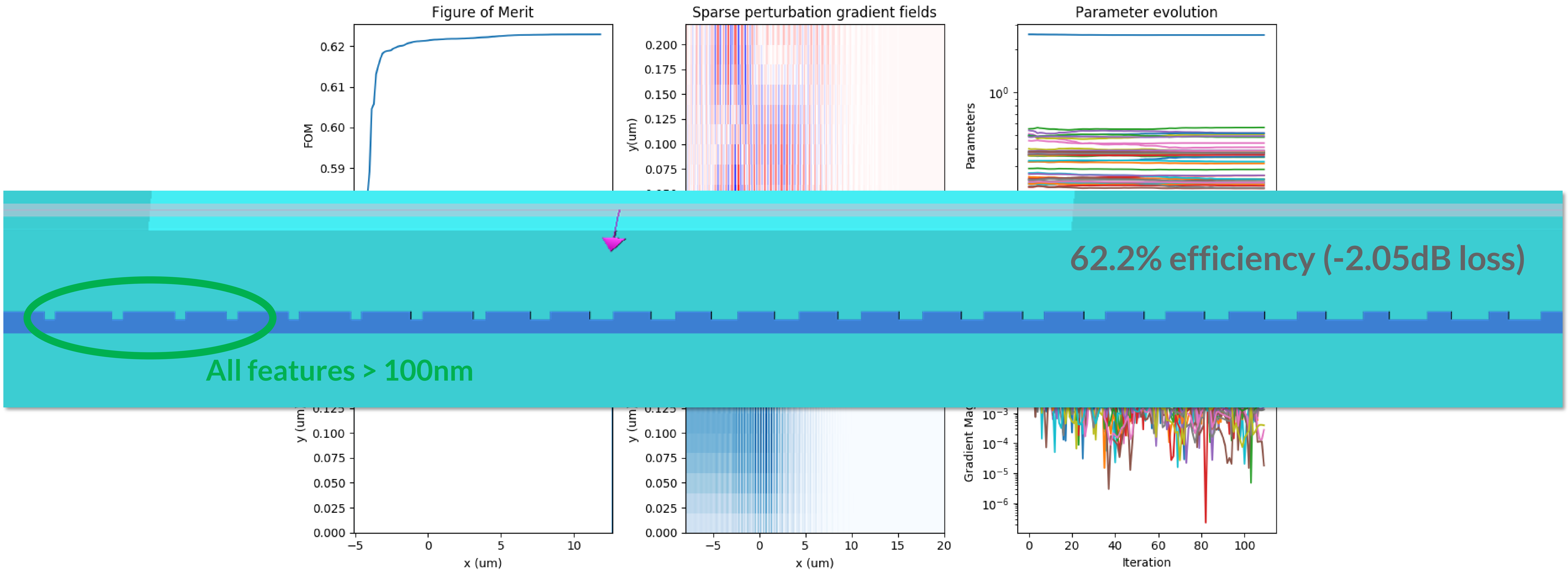
Optimization of basic partial-etch GC

2. Use previous result as initial guess for a full optimization (each wall position is free to move)



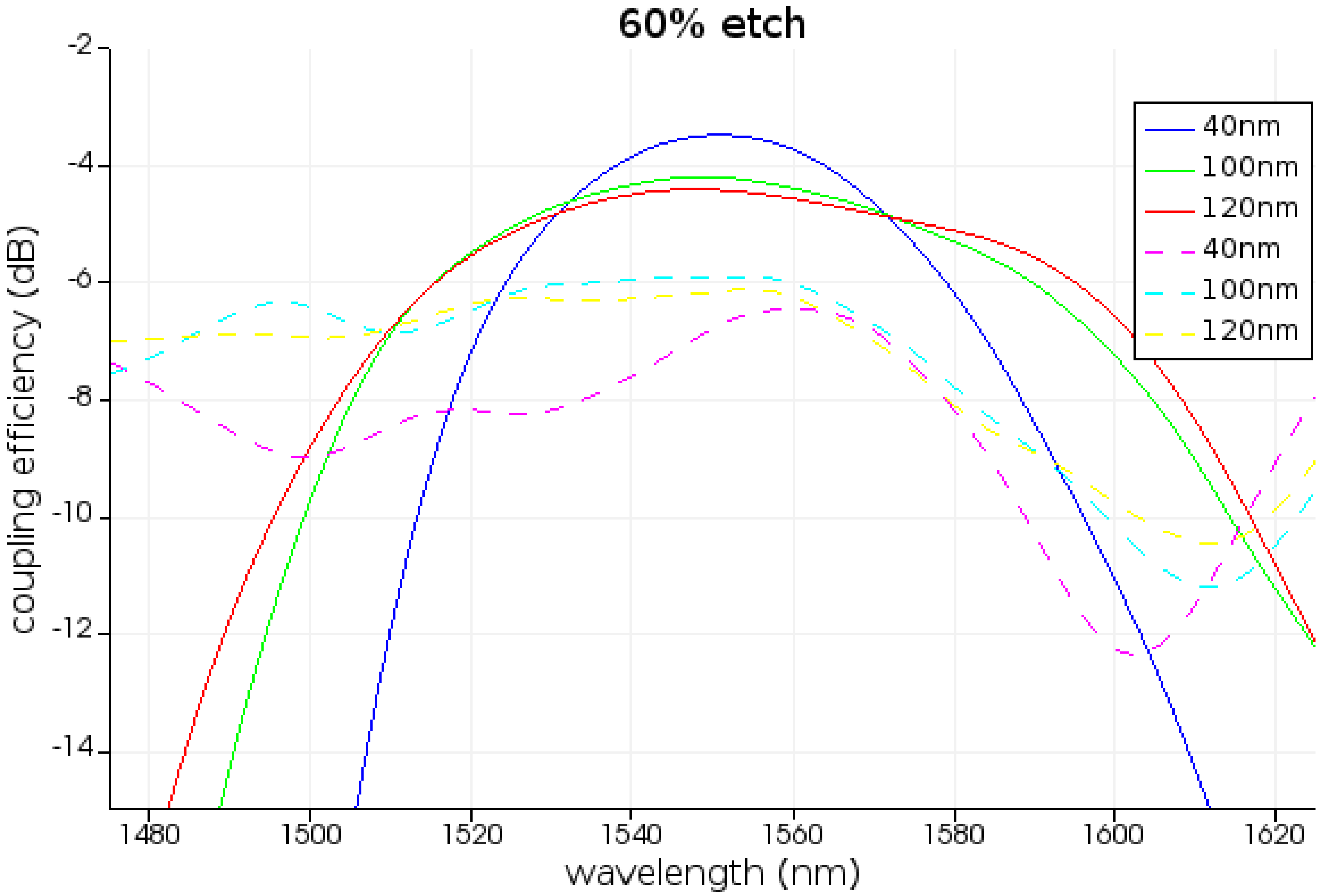
Introducing manufacturing constraints

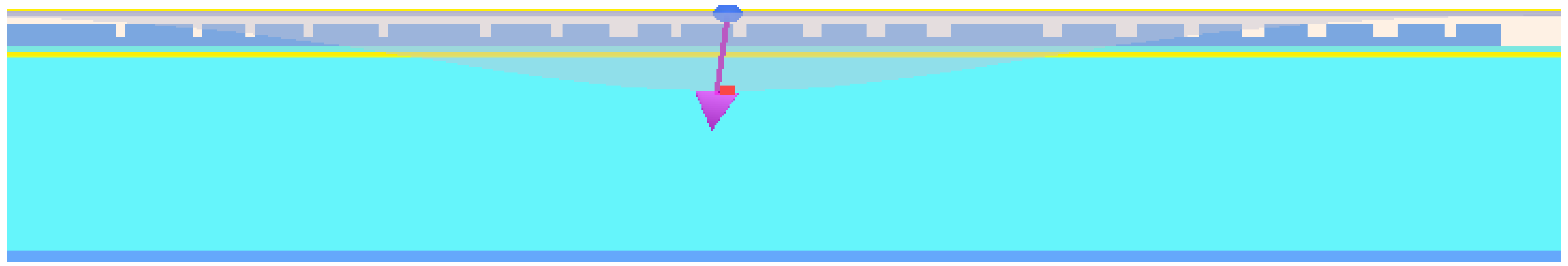
3. Re-run with a **minimal feature size constraint** of 100nm



Broadband Grating Coupler

- Starting with a grating optimized for C-band (40nm bandwidth)
- Re-optimize targeting 100nm and 120nm



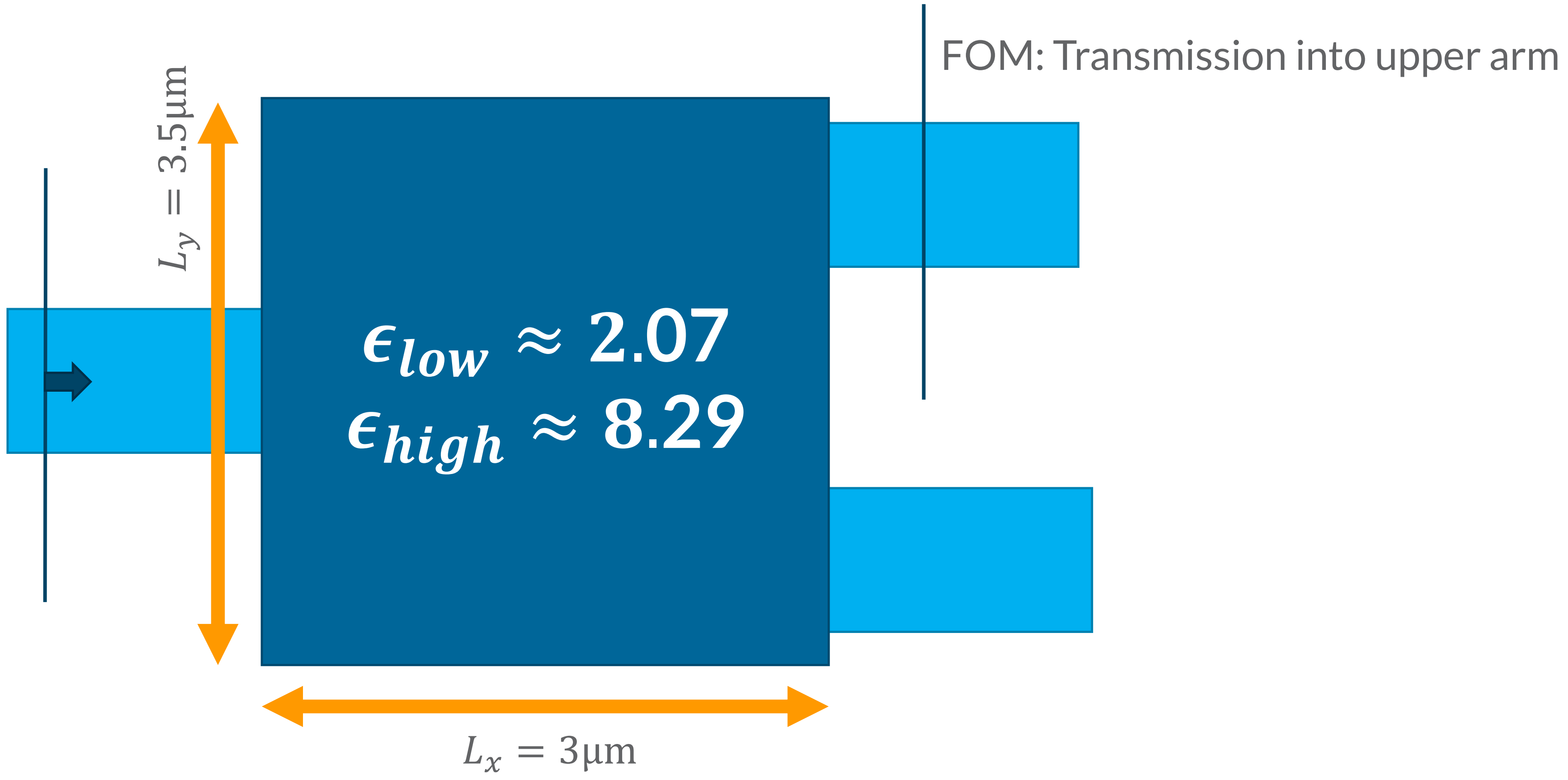


https://kx.lumerical.com/t/broadband-grating-coupler-design-bandwidth-vs-peak-efficiency/40954

Topology Optimization

Topology Optimization

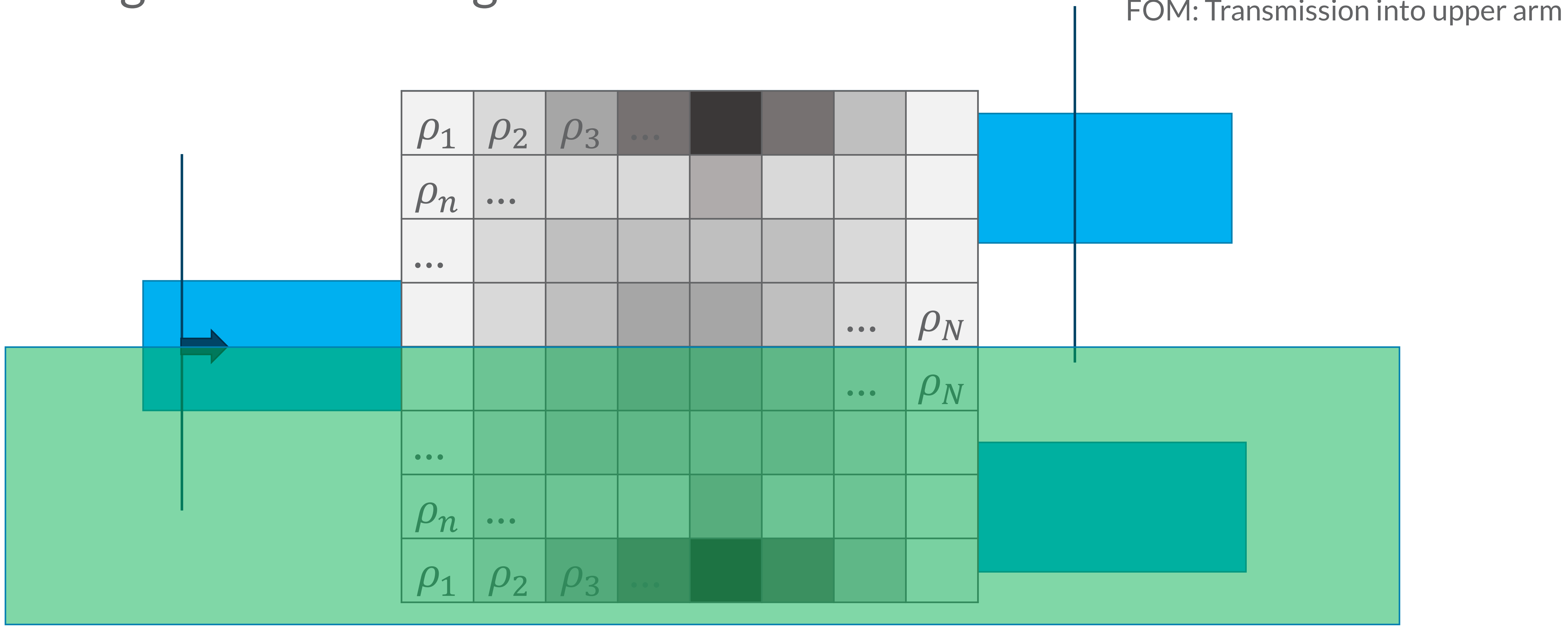
- Providing a parametrization can be difficult or overly restrictive
- With topology optimization, the user only provides **footprint**, **material parameters** and **FOM**



- Solver automatically discretizes the domain and tries to find best solution
- Challenge is to ensure that the resulting structure can be manufactured

Parametrization

- Use a rectilinear grid for the design area.



- Each cell is an optimization parameter $\rho_i \in [0,1]$ (typically $N > 10000$)
- Parameter maps directly to permittivity: $\epsilon_i = \epsilon_{low} + \rho_i(\epsilon_{high} - \epsilon_{low})$

General procedure

Our topology optimization method uses a two-phase approach:

Greyscale

- Allows any material in $[\epsilon_{low}, \epsilon_{high}]$
- Continuously smoothens the design

Binarization

- Gradually pushes material to either ϵ_{low} or ϵ_{high}

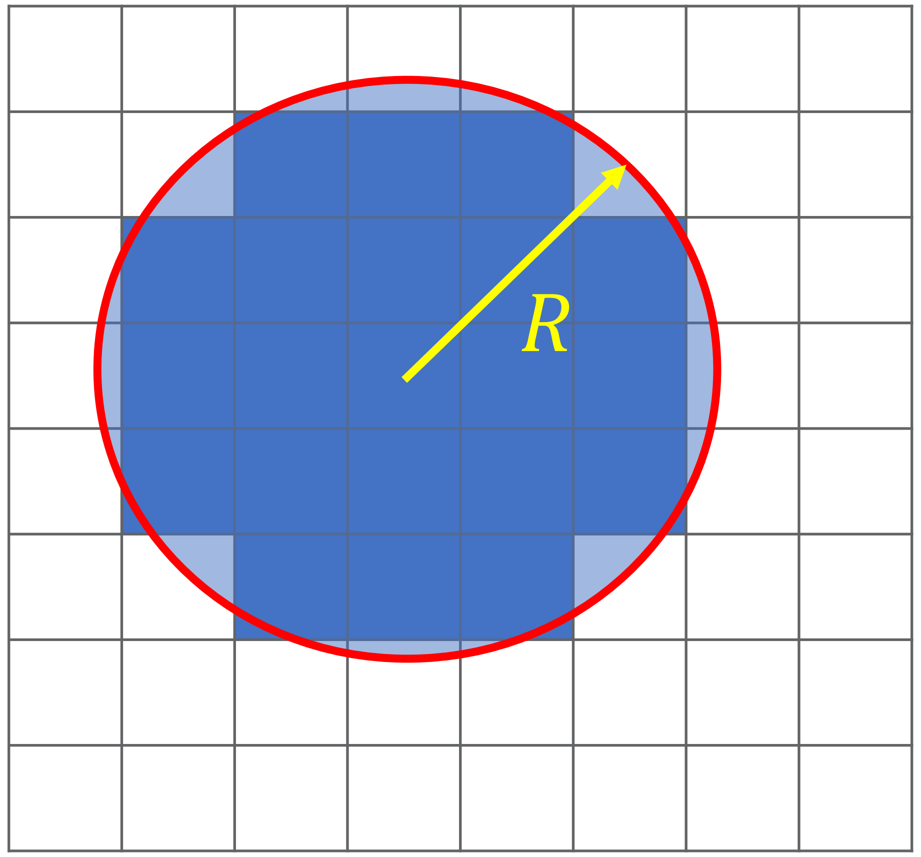
Jensen, J. and Sigmund, O., "Topology optimization for nano-photonics", Laser & Photon. Rev. 5, 308-321 (2011)

Greyscale Phase: Ensure Manufacturability

- Employ smoothing with a **user-specified radius *R***

$$\bar{\rho}_j = \frac{1}{N}\sum_j \rho_j w(x_i - x_j)$$

- Typical values: $R = 50 - 200\text{nm}$
- Leads to smooth designs that are "lithography-friendly"
- Also a first step in reducing small features
- **Instead of simple filter, we can also use transfer function of a specific lithography system**



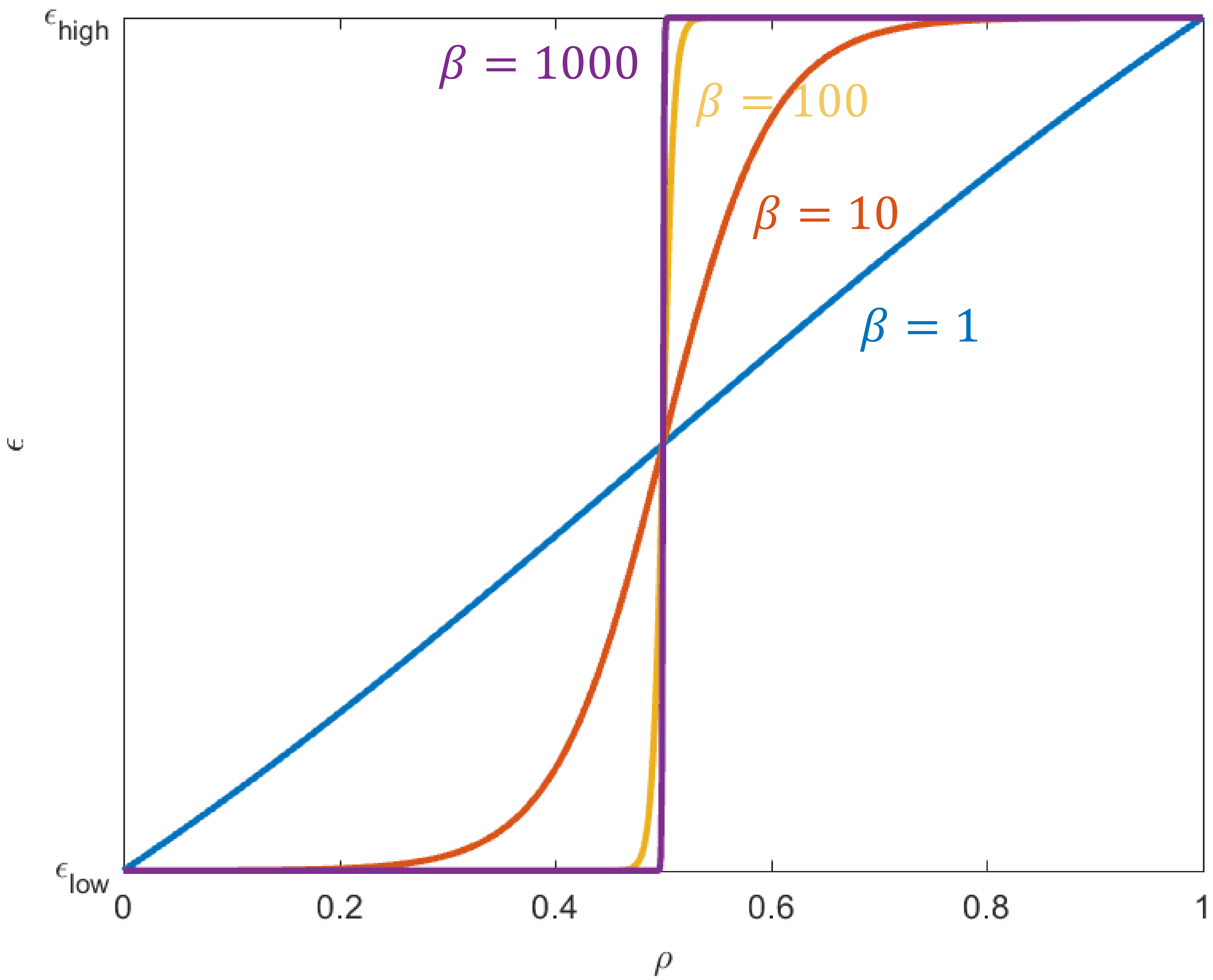
Mapping to Permittivities: Heaviside Filter

- Employ Heaviside filter:

$$\tilde{\rho} = \frac{\tanh(\beta\eta) + \tanh\big(\beta(\bar{\rho}_i - \eta)\big)}{\tanh(\beta\eta) + \tanh\big(\beta(1-\eta)\big)}$$

- Continuously increases β from 1 to around 1000

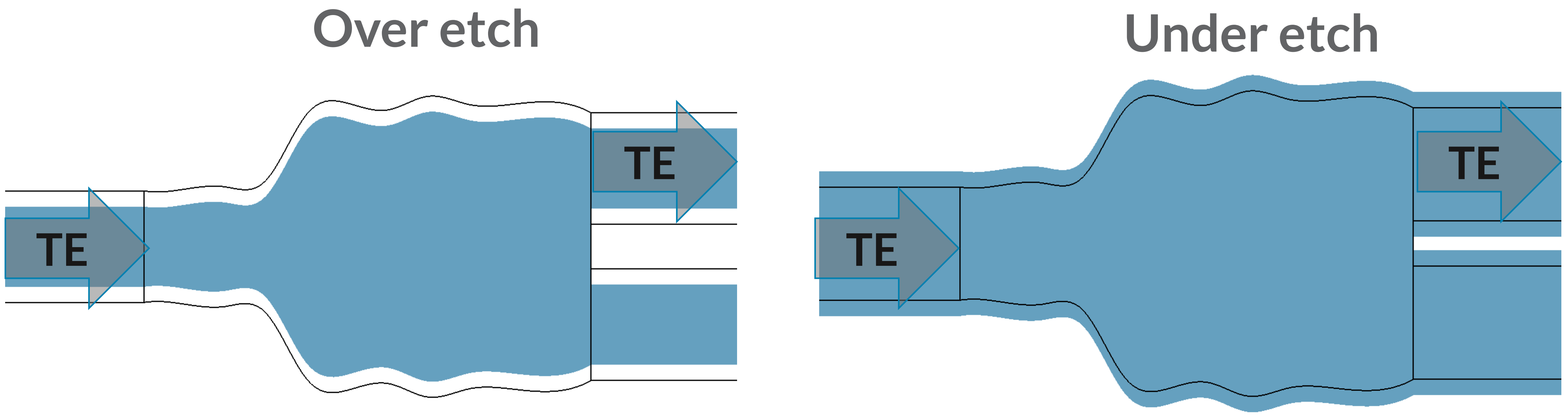
- Terminates once the design is sufficiently binary



Simple Example – Y-Splitter

Robust Design

- As with parametric shape optimization, we can co-optimize 3 different shapes:
    - "Nominal"
    - "Over etch" slightly smaller than nominal
    - "Under etch" slightly larger than nominal



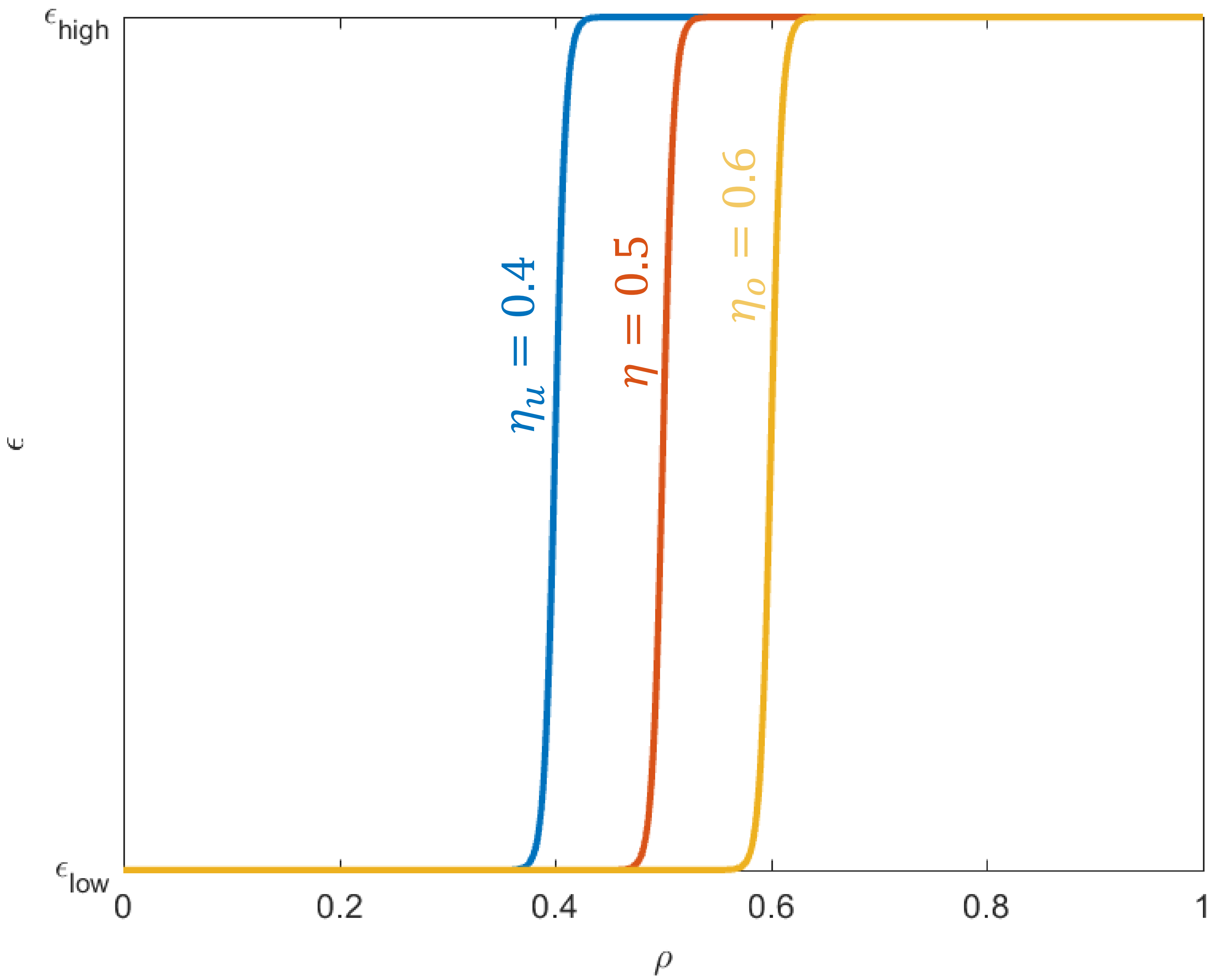
Binarization Phase: Heaviside Filter

- Heaviside filter:

$$\tilde{\rho}_i = \frac{\tanh(\beta\eta) + \tanh\left(\beta(\bar{\rho}_i - \eta)\right)}{\tanh(\beta\eta) + \tanh\left(\beta(1 - \eta)\right)}$$

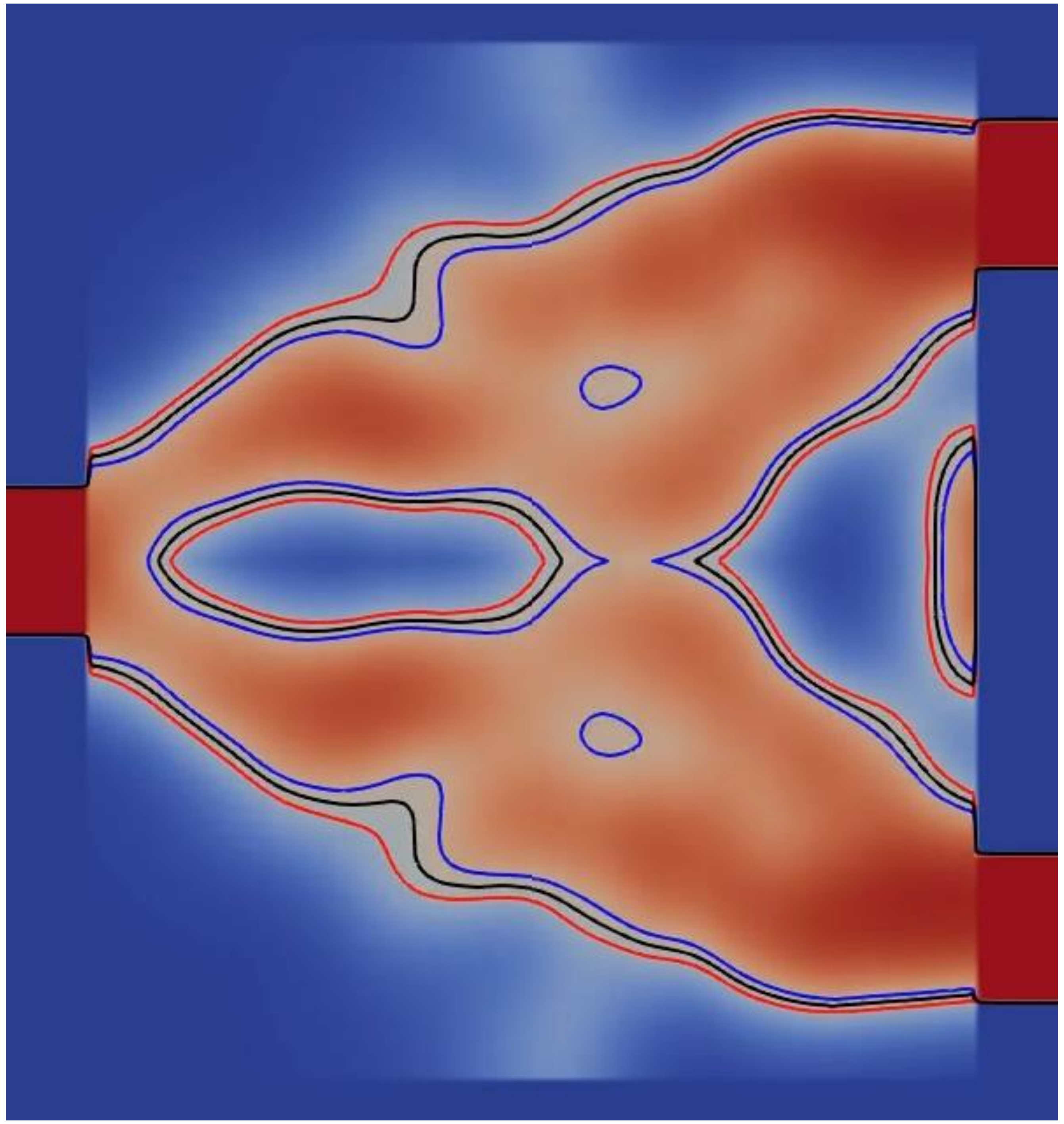
- Parameter η shifts the binarization threshold

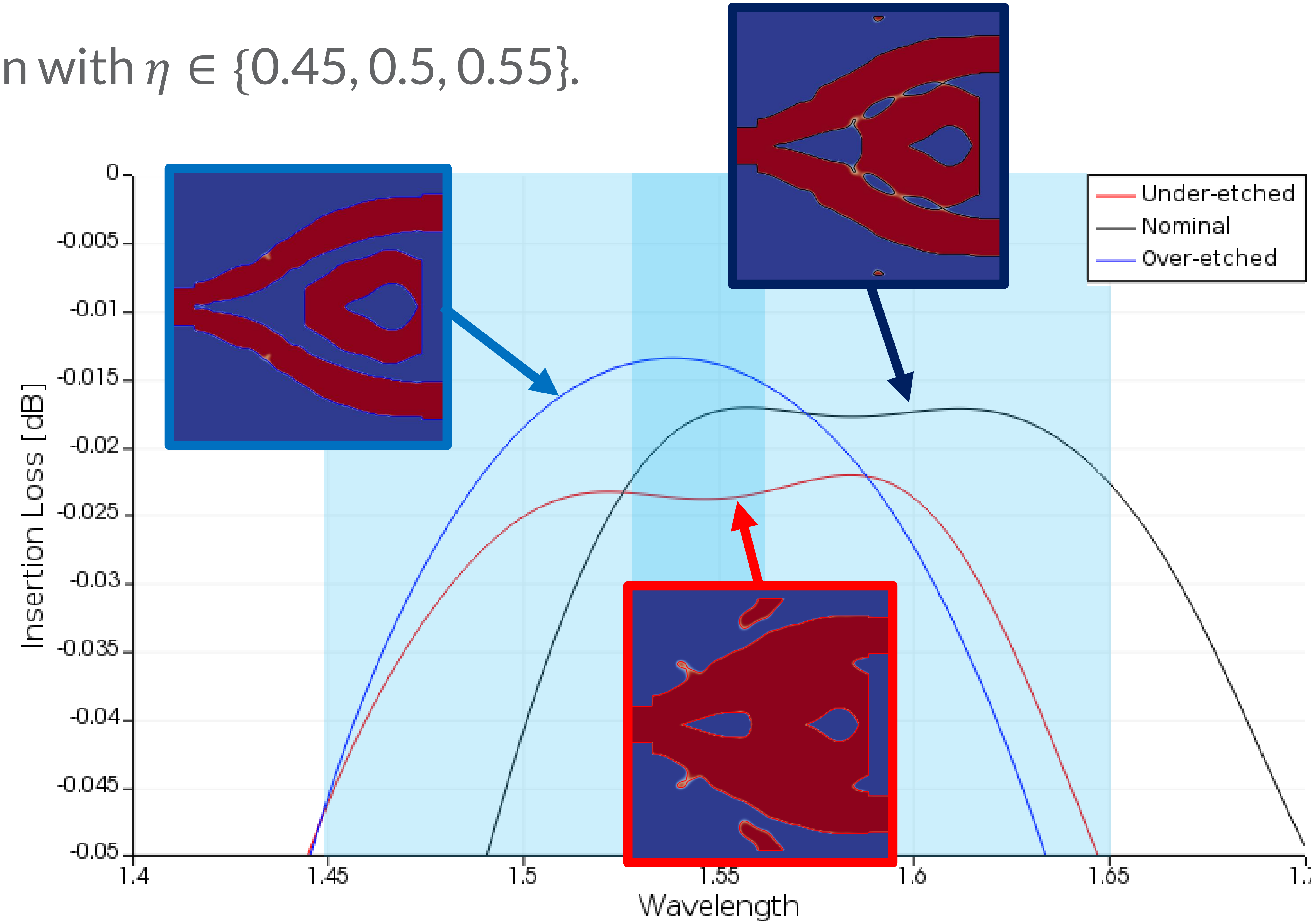
- In combination with the smoothing, this effectively moves the boundaries



Robustness to Manufacturing Tolerances ($\pm 20\mathrm{nm}$)

- Filter radius: 400nm, co-optimization with $\eta \in \{0.45, 0.5, 0.55\}$.





Enforcing Minimum Feature Size Constraints

- Even with filtering, topology optimization often yields structures that contain small features which are challenging to manufacture.

- To make structures manufacturable, we need to explicitly enforce constraints

- Here, we implement an algorithm originally proposed for structural mechanics in

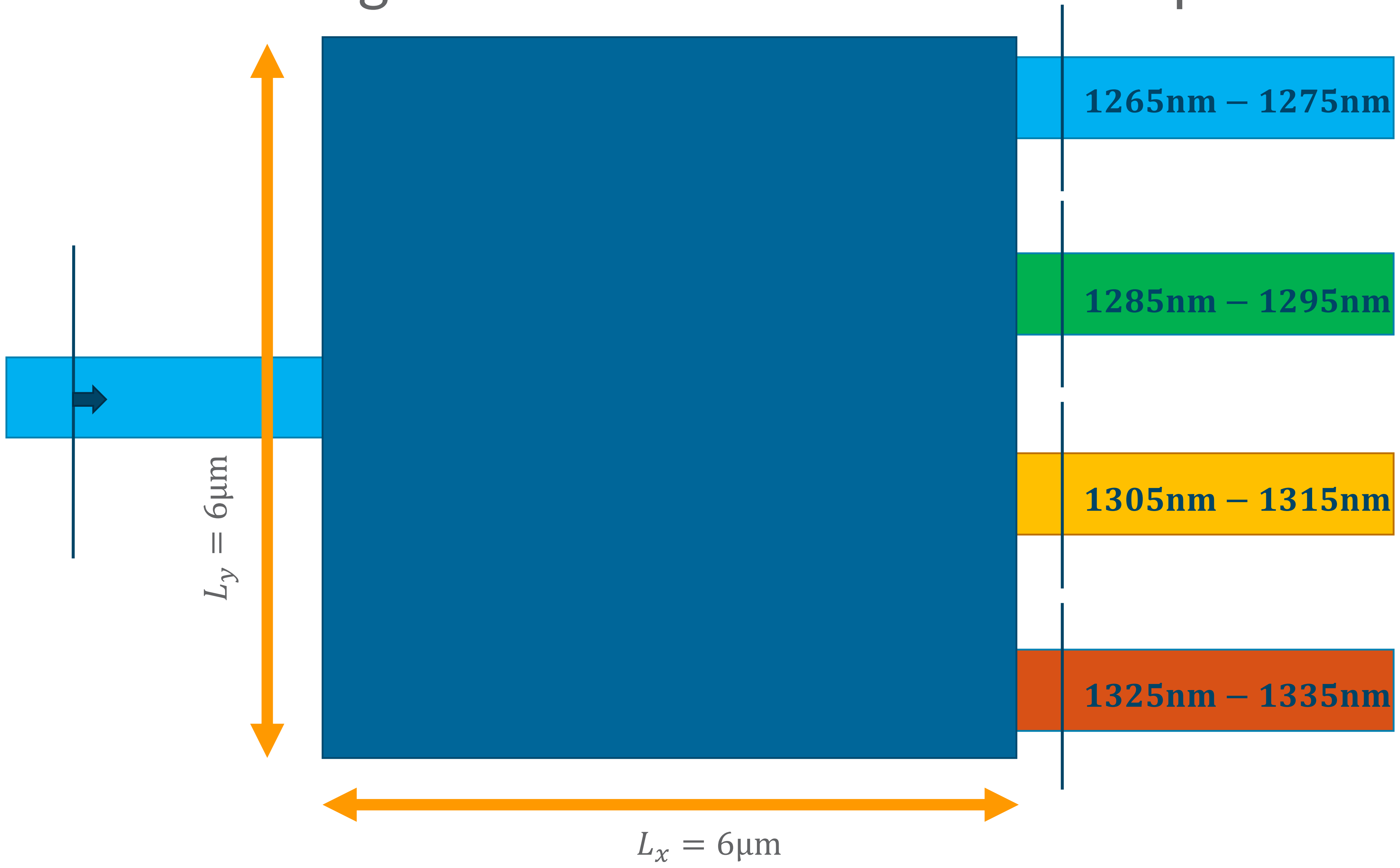
  Zhou, M. et al. "Minimum length scale in topology optimization by geometric constraints“, Comput. Methods in Appl. Mech. Eng 293, 266-282 (2015)

- It does not require additional simulations and is cheap to calculate

- Adds a simple constraint/penalty term to the optimization

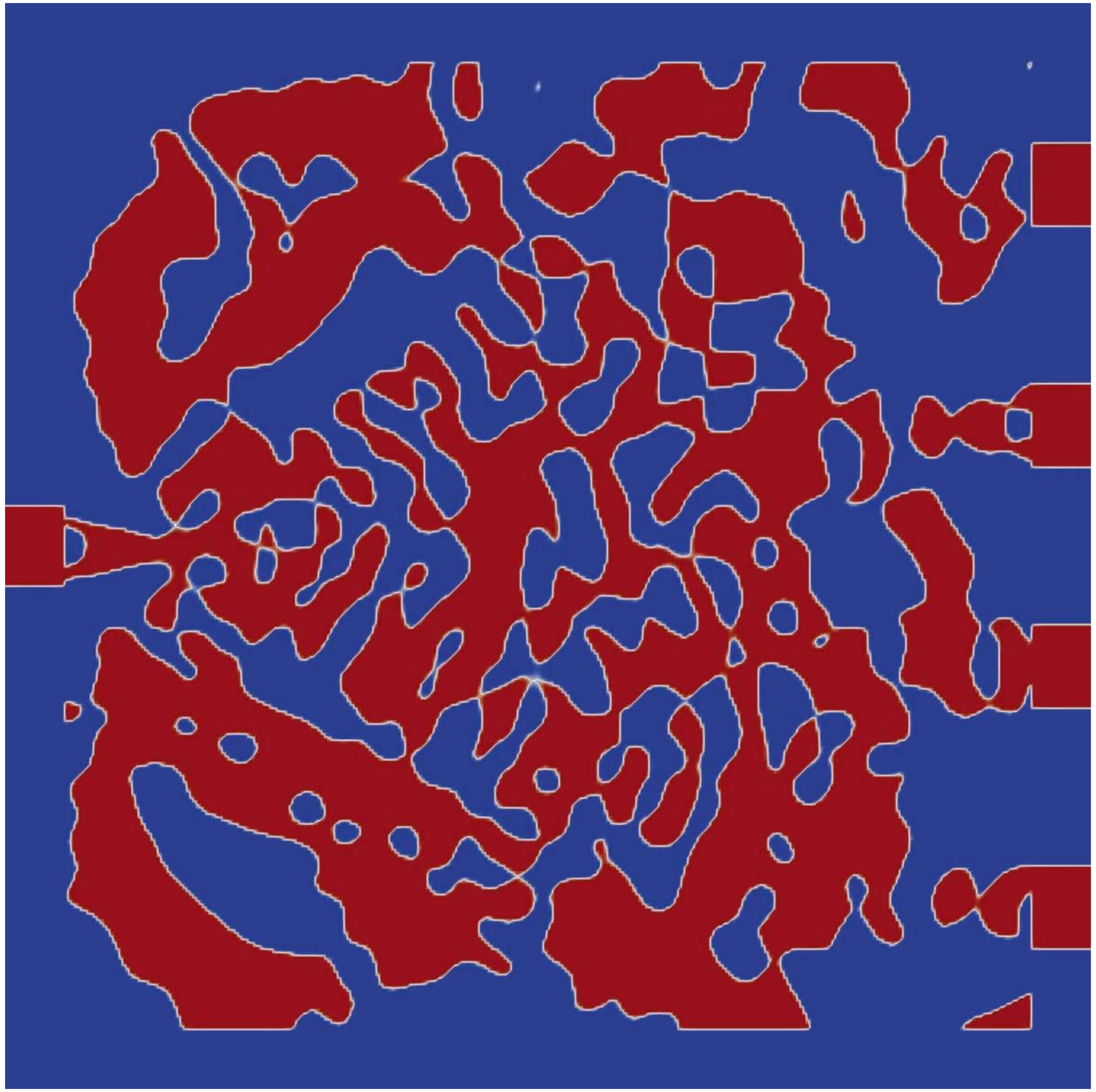
Example: 4-Channel Wavelength Demultiplexer in the O-band

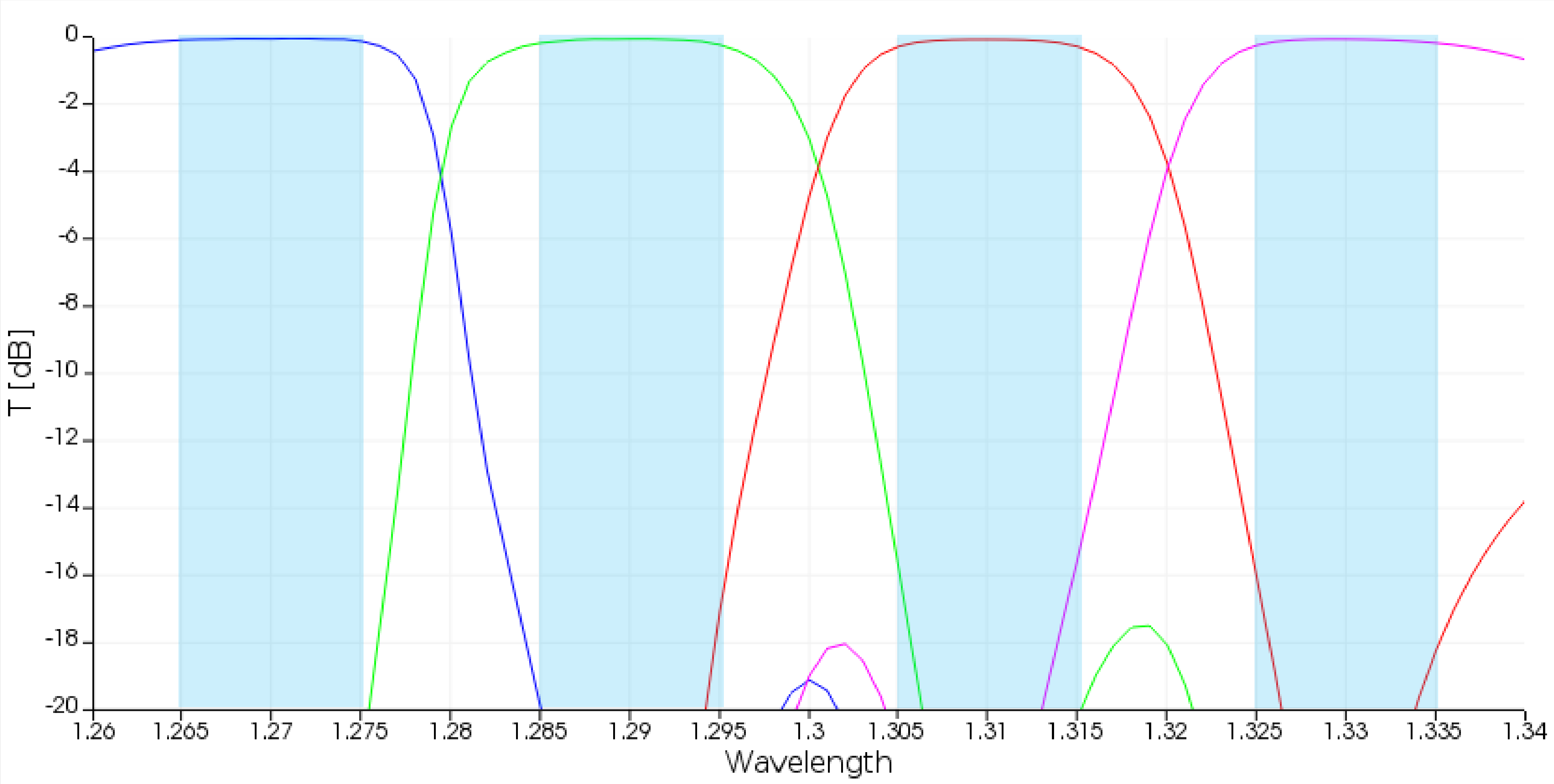
- Use topology optimization to design a 4-channel CWDM demultiplexer



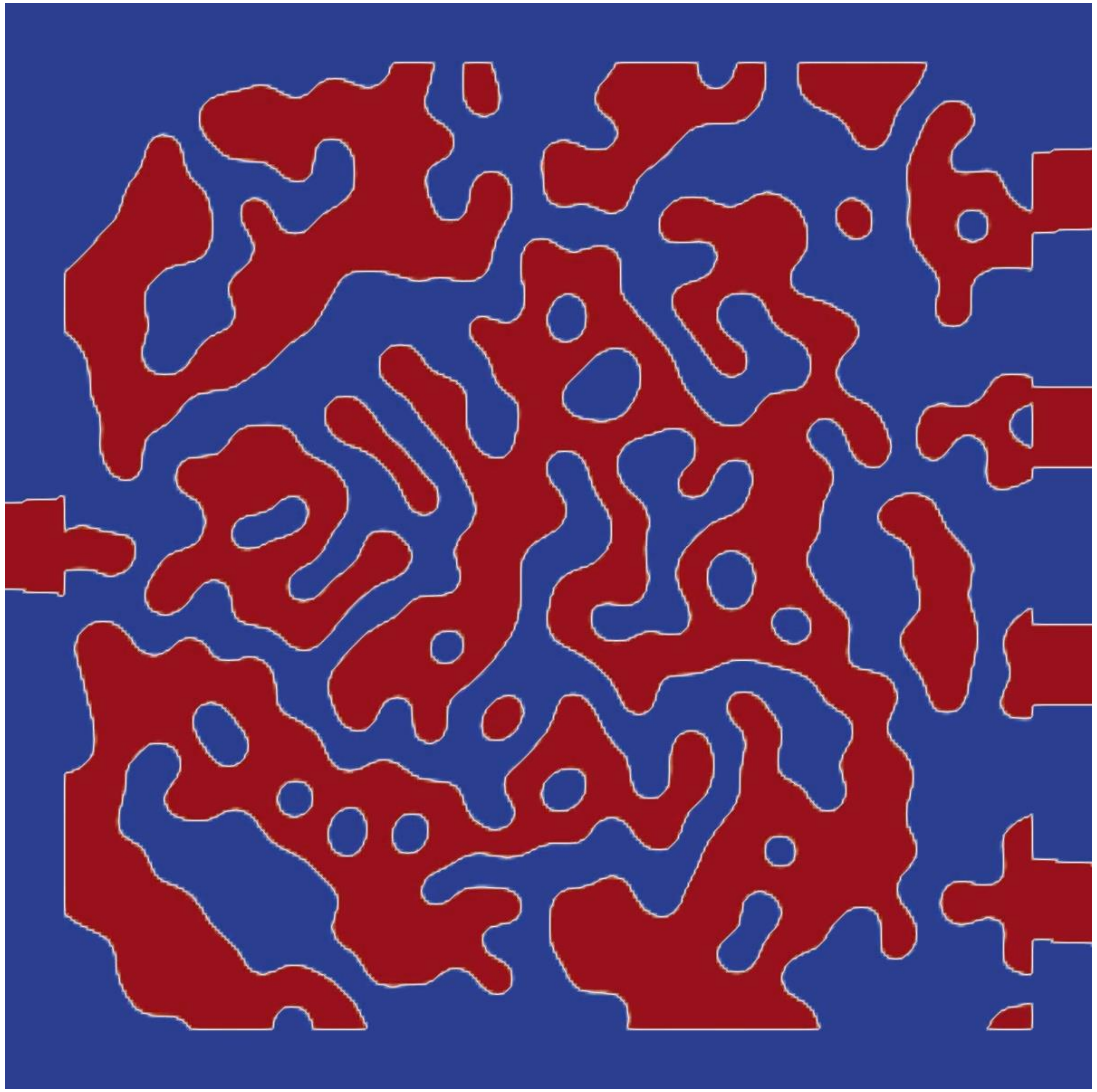
- Best known theoretical proposals have a footprint of over $1\mathrm{mm}^2$, here we aim for $36\mu\mathrm{m}^2$, a reduction of around 5×10^4!

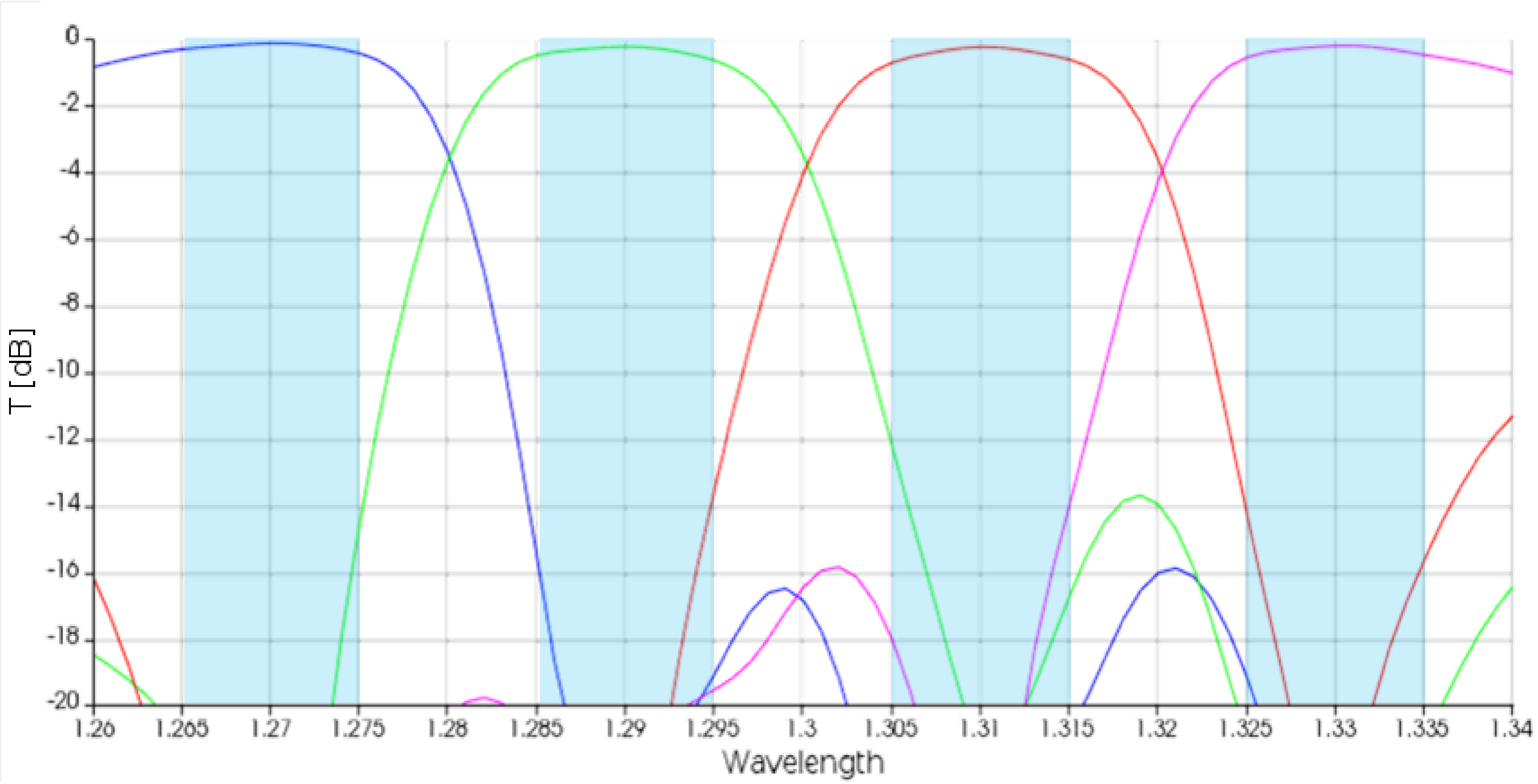
4-Channel Wavelength Demultiplexer in the O-band





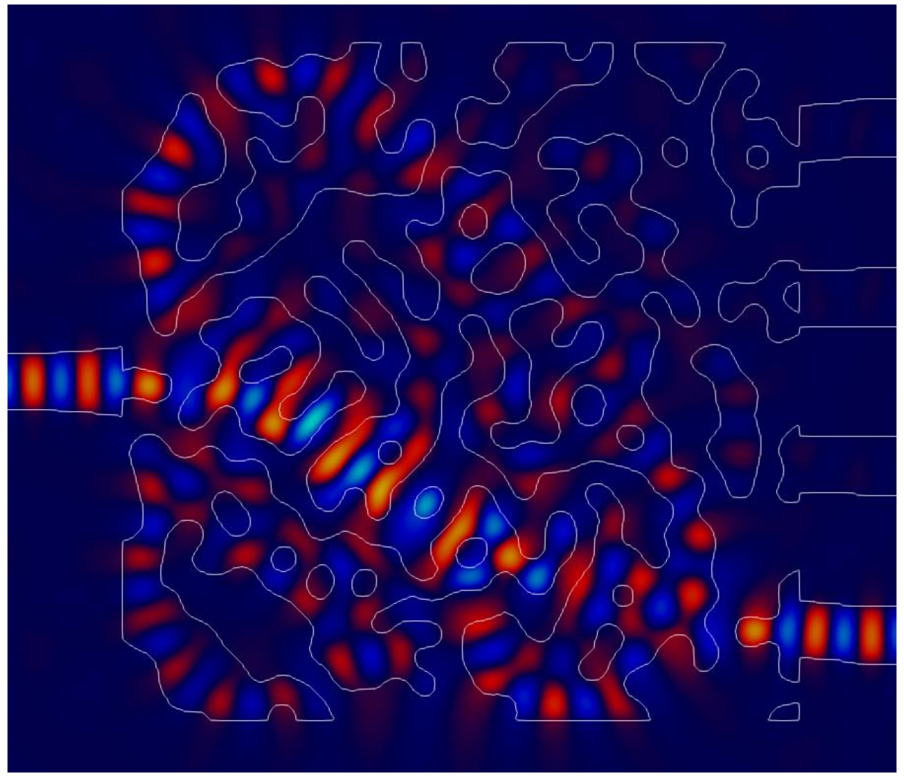
With constraints (150nm min feature size)



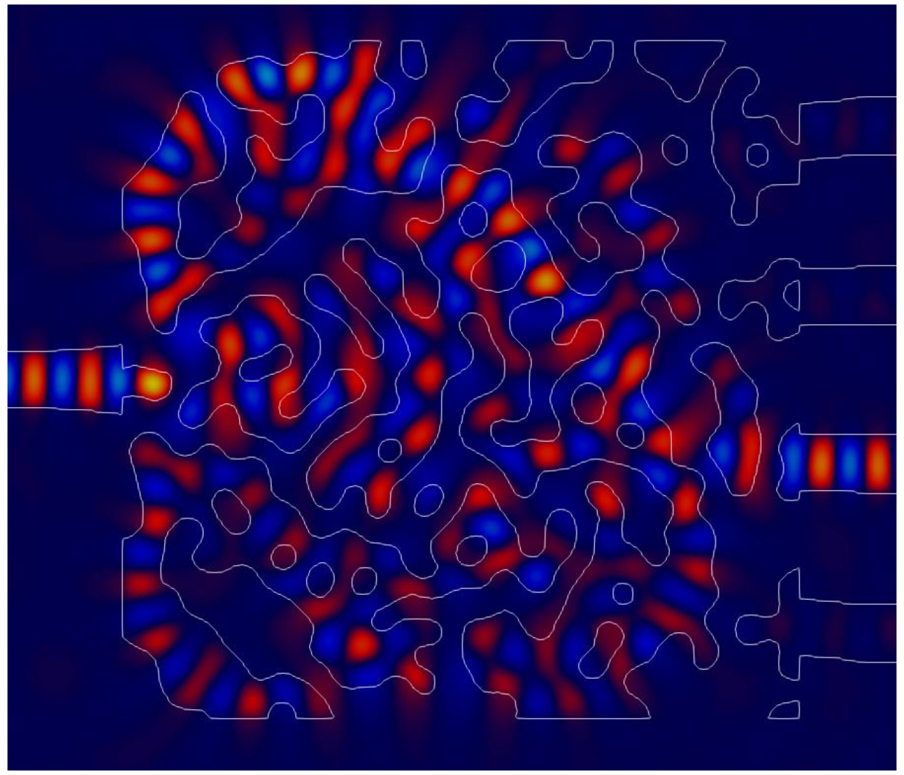


Field distribution

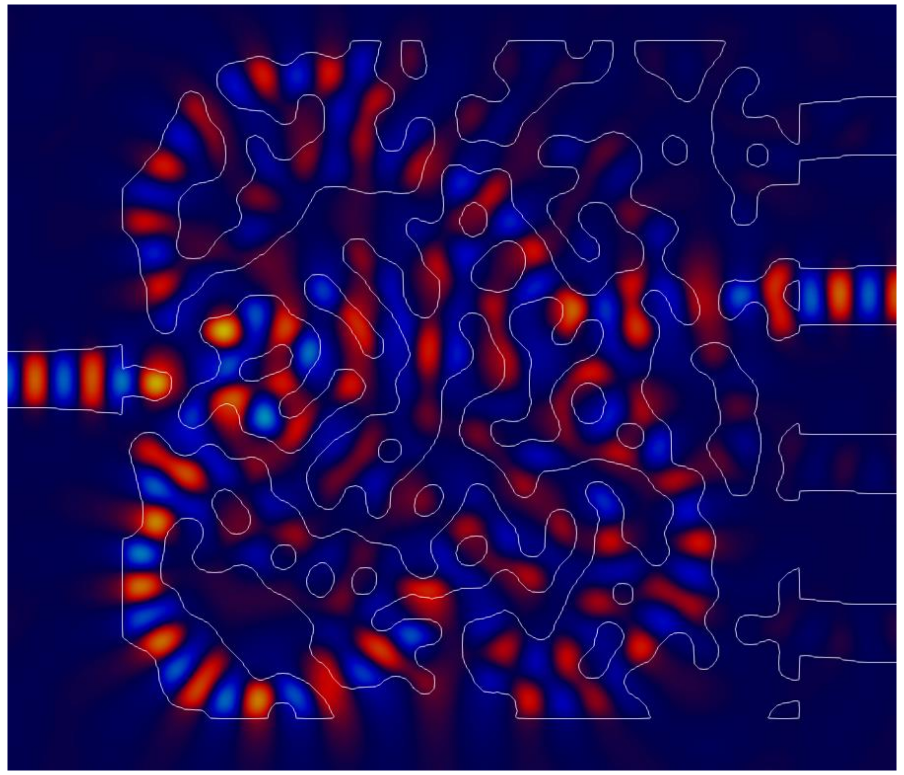
- Plotting the real part of H_z component



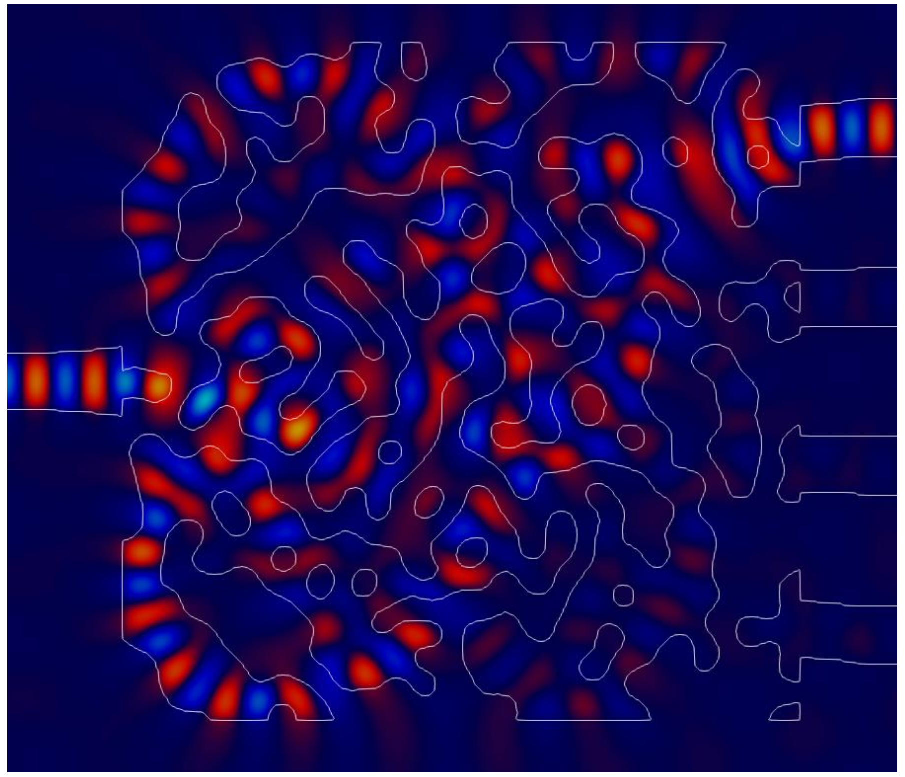
$\lambda = 1270\text{nm}$



$\lambda = 1290\text{nm}$



$\lambda = 1310\text{nm}$



$\lambda = 1330\text{nm}$

- Scale of colorbar is identical in all plots
- No extreme hotspots

Summary

- Photonic Inverse Design has transitioned from a research topic to a design method
- Parametric shape optimization can quickly improve existing designs
- Topology optimization can yield large improvements in both performance and footprint
- Strict enforcement of minimum feature sizes is possible and necessary to generate manufacturable designs

Q&A