Nanophotonic Computational Design

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Introduction

- As information grows, optical networks needed
  - across continents
  - within a datacenter
  - between chips and on-chip

- On-chip optical components are currently designed by tuning a small number of design parameters

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- What happens when we use the *full* parameter space for nanophotonic design?

- The full parameter space is *vast*

- Include/exclude per pixel gives us $2^{(15^2)} = 2^{225}$ possibilities
  - A virtually uncountable number
  - Can only be leveraged computationally

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- Many of these devices are
  - Completely novel (no previously known designs)
  - Extremely compact (footprints of a few vacuum wavelengths)
  - High efficiency ($> 80\%$ transmission)

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- If possible, we can design *any* nanophotonic/optical component!

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\omega^2 E \epsilon &= \nabla \times \mu_0^{-1} \nabla \times E + i\omega J \\
\epsilon &= (\nabla \times \mu_0^{-1} \nabla \times E + i\omega J)/\omega^2 E
\end{aligned}$$

- Solving for ϵ actually way faster than simulation (solving for E)!

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$$\begin{aligned} E &\rightarrow x \\ \epsilon &\rightarrow z \\ \nabla \times \mu_0^{-1} \nabla \times -\omega^2 \epsilon &\rightarrow A(z) \\ -i\omega J &\rightarrow b \end{aligned}$$

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- Key: If $A(z)$ is linear in z then $A(z)x = b$ is as well!

Direct design of nanophotonic devices

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  - Choose x (field)
  - Solve for z (structure) by minimizing the *physics residual*, $A(z)x - b$

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$$\underset{z}{\text{minimize}} \quad \|A(z)x - b\|^2$$

- Global minimum where $A(z)x - b = 0$ can be computed in one step

$$\epsilon = (\nabla \times \mu_0^{-1} \nabla \times E + i\omega J)/\omega^2 E$$

where $\epsilon \rightarrow z$

- Choose canonical 1D cavity field for x
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- Result
  - Perfect performance
  - But unmanufacturable structure (z not well-behaved)

Direct design with regularization

- Direct design "works" but not practical

$$\underset{z}{\text{minimize}} \quad \|A(z)x - b\|^2$$

- So, let's add a *regularization* term to z and solve the following instead

$$\underset{z}{\text{minimize}} \quad \|A(z)x - b\|^2 + \eta\|z - z_0\|^2$$

  - $\|z - z_0\|^2$ term keeps z close to z_0
  - η controls the strength of the regularization

- Solution can still be computed in one step

- Unfortunately, regularization on z decreases performance

$$\underset{z}{\text{minimize}} \quad \|A(z)x - b\|^2 + \eta\|z - z_0\|^2$$

- Decreased performance a result of non-zero physics residual at optimum

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- Realized that there do exist some x (fields) which result from manufacturable z (structures)
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  - However, it's not useful to ask the user to choose such x

- Therefore, a *useful* tool would optimize for *both* x and z

Iterative design of nanophotonic devices

- New algorithm: Iteratively solve for x (field) and z (structure)

$$\begin{aligned} \underset{z}{\text{minimize}} \quad & \|A(z)x - b\|^2 + \eta_0 \|z - z_{\text{prev}}\|^2 \\ \underset{x}{\text{minimize}} \quad & \|A(z)x - b\|^2 + \eta_1 \|x - x_{\text{prev}}\|^2 \end{aligned}$$

- Takes advantage of the *bi-linearity* of the physics residual
  - Jointly solving for x and z is a non-convex problem

- More concisely, we iteratively solve the following

$$\underset{\text{alternately } x \text{ then } z}{\text{minimize}} \quad \|A(z)x - b\|^2 + \eta_0 \|z - z_{\text{prev}}\|^2 + \eta_1 \|x - x_{\text{prev}}\|^2$$

- Design process now consists of *multiple* computational steps
  - η_0, η_1 gradually decreased to bring physics residual toward 0

- Iterative strategy produces z (structure) that
  - is better behaved
  - more accurately produces x

Iterative design with hard constraints on z

- We can also put hard limits on z (structure)

$$\begin{array}{rl} \text{minimize} & \|A(z)x - b\|^2 + \eta_1 \|x - x_{\text{prev}}\|^2 \\ \text{subject to} & z_{\text{min}} \leq z \leq z_{\text{max}} \end{array}$$

- $z_{\text{min}} \leq z \leq z_{\text{max}}$ constraint better represents manufacturability constraint
  - Corresponds to a minimum and maximum allowable permittivity (ϵ)

- Well-behaved, manufacturable z (structure)
- Final x (field) accurately reproduced
- Majority of elements of z are fortuitously at one limit or the other!

- Can be used to create 2D resonators

- 3D resonators can be designed using a "2.5D" approximation

Objective-first design of linear devices

- Next realization: for linear components, only certain elements of x (field) matter
  - Specifically, the elements of x at the input/output ports

$$\begin{aligned} \text{minimize} \quad & \|A(z)x - b\|^2 \\ \text{subject to} \quad & x_{\text{boundary}} - \hat{x}_{\text{boundary}} = 0 \\ & z_{\text{min}} \leq z \leq z_{\text{max}} \end{aligned}$$

- Instead of regularization term, we force the elements of x at the boundary to be equal to the ideal case ($\hat{x}$)

- Called *objective-first* design because the design objective is prioritized above the physics residual

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- Applied to the design of 2D waveguide mode couplers

- Produced designs which exhibited
  - High efficiency ($\sim 98\%$)
  - Small device footprints ($1.5 - 4$ square vacuum wavelengths)

- Coupler to wide, low-index waveguide

- Coupler from fundamental to second-order waveguide mode

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- Goal: Software to design *all* linear nanophotonic devices
  - Fully three-dimensional (no approximations)
  - Multi-mode
  - Discrete, planar, manufacturable structure

- Problem: Did not know how to solve $A(z)x - b = 0$ (simulation) in 3D
  - Millions of variables
  - Famously ill-conditioned
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- Fortunately, Wonseok had already solved this problem

Maxwell: Light-simulation supercomputer

- Partnered with Wonseok to develop a cloud-based electromagnetic solver using Amazon Web Services
  - GPU-accelerated implementation of Wonseok's algorithm
  - Cluster scales automatically to tens of nodes

- Scalable
  - Far outstrips computing clusters such as Teragrid
  - Can perform multiple solves in parallel, on a single Matlab instance
  - All computation is performed externally (in the cloud)
- Easy to use
  - Installs with a single Matlab command
  - Solves completed with a single Matlab command: `maxwell(...);`
- The key technological enabler in achieving 3D design

3D design: problem statement

$$\begin{aligned} \text{minimize} \quad & \sum_{i}^{M} \|A_i(z)x_i - b_i\|^2 \\ \text{subject to} \quad & \alpha_{ij} \leq |c_{ij}^{\dagger} x_i| \leq \beta_{ij}, \quad \text{for } i = 1, \ldots, M \text{ and } j = 1, \ldots, N_i \\ & z_{\text{min}} \leq z \leq z_{\text{max}} \end{aligned}$$

- M modes with N_i monitored output modes each
  - b_i is the input excitation for each mode
  - $|c_{ij}^{\dagger} x_i|$ is the field overlap with output mode c_{ij}
  - α_{ij} and β_{ij} is the design range for the overlap

- Show input and output modes here as explanation of problem statement
- Use 3D model of wgc te as example.

- TE mode converter

- Efficiency: 86.4%
- Power in rejection mode (transmitted fundamental): 0.7%
- 250 nm silicon slab surrounded by silica

- TM mode converter

- Efficiency: 76.9%

- Power in rejection mode (transmitted fundamental): 1.0%

- Spatial mode splitter
  - Efficiency: 88.7%, 77.4% (0.27%, 0.20%)

- TE/TM splitter
  - Efficiency: 87.6%, 88.8% (1.06%, 0.58%)

- Wavelength splitter
  - Efficiency: 83.2%, 78.7% (0.49%, 1.66%)

- 3x3 hub (88.6%, 90.6%, 87.3% efficiency)

- 4x4 hub

- Efficiency: 85.9%, 88.1%, 85.4%, 84.3%

- 2x2x2 hub (77.6%, 73.7%, 75.7%, 75.2% efficiency)

- fiber coupler (51.5%)

- fiber coupler mode splitter (32.6%, 22.7%)

- fiber coupler wdm (31.6%, 28.6%)