# Objective-first optimization for nanophotonics

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- example
- ongoing and future work

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# Adjoint method

Typical formulation of a structural optimization problem:

$$\text{decrease} \quad f(x) \tag{1}$$

$$\text{subject to} \quad g(x, p) = 0 \tag{2}$$

- $f(x) : \mathbf{C}^n \to \mathbf{R}$ is the *design objective*
- $g(x, p) : \mathbf{C}^n \times \mathbf{R}^n \to \mathbf{C}^n$ is the *governing physics*
- $x \in \mathbf{C}^n$ is the field
- $p \in \mathbf{R}^n$ is the structure
- $x$ is the dependent variable, $p$ is the independent variable

- problem is generally non-convex, so we optimize using only the first-order approximations,

$$f(x_0 + dx) \approx f(x_0) + \frac{\partial f}{\partial x} dx \tag{3}$$

$$g(x_0 + dx, p_0 + dp) \approx g(x_0, p_0) + \frac{\partial g}{\partial x} dx + \frac{\partial g}{\partial p} dp \tag{4}$$

- assuming that $g(x_0, p_0) = 0$, the equality constraint is satisfied via

$$dx = -\left(\frac{\partial g}{\partial x}\right)^{-1} \frac{\partial g}{\partial p} dp \tag{5}$$

- now we can decrease $f(x_0 + dx)$,

$$f(x_0 + dx) \approx f(x_0) + \frac{\partial f}{\partial x} dx \tag{6}$$

$$\approx f(x_0) - \frac{\partial f}{\partial x} \left( \frac{\partial g}{\partial x} \right)^{-1} \frac{\partial g}{\partial p} dp \tag{7}$$

$$\approx f(x_0) + \frac{\partial f}{\partial p} dp \tag{8}$$

  by choosing $dp$ in the direction of $dp \propto -\frac{\partial f}{\partial p}$

- computing $\frac{\partial f}{\partial p}$ can be reduced to a single field solve ($i.e.$ solving $g(x, p)$ for $x$, given $p$)

Characteristics of the adjoint method:

- can use existing field solvers
- each iteration requires two solves, one to calculate $\frac{\partial f}{\partial p}$, and the other to calculate the new $x$
- need good initial guess, since this heavily influences what the final structure will be
- optimization generally "stalls" on local minima

# Objective-first approach

ob-1 means that we prioritize the design objective over satisfying physics

$$\begin{aligned} \text{decrease} \quad & \|g(x,p)\|^2 && (9) \\ \text{subject to} \quad & f(x) = 0 && (10) \end{aligned}$$

- $r(x,p) = \|g(x,p)\|^2$ is the *physics residual*

- $x$ always satisfies our design objective, we change $x$ and $p$ only to increasingly satisfy physics

- $x$ and $p$ are both independent variables

- this problem is still non-convex, use linear approximation

$$r(x_0 + dx, p_0 + dp) \approx r(x_0, p_0) + \frac{\partial r}{\partial x} dx + \frac{\partial r}{\partial p} dp \tag{11}$$

$$f(x_0 + dx) \approx f(x_0) + \frac{\partial f}{\partial x} dx \tag{12}$$

- decrease $r$ by choosing $dp \propto -\frac{\partial r}{\partial p}$

- decrease $r$ by choosing $dx \propto -(I - P_{f_x})\frac{\partial r}{\partial x}$

- $P_{f_x}$ is the projector onto the vector space defined by $\frac{\partial f}{\partial x}$, used to satisfy equality constraint

- computing $P_{f_x}$ requires solving for $\left(\frac{\partial f}{\partial x}^T \frac{\partial f}{\partial x}\right)^{-1}$, but this is often *trivial* ob-1 requires only matrix multiplication (and trivial matrix solve)

- For 3D structures, most field solvers are based on (often $> 10,000$) matrix multiplies

- this means that is may be possible to solve larger design problems in the same amount of time needed for a field solve

ob-1 should be less dependent on starting guess

- some previous problems (using a similar approach) did not depend at all on initial structure

- such a formulation may result in fewer local minima to stall on

# Field constraint: boundary-value problem

- our problem is

$$\begin{aligned} \text{decrease} \quad & \|g(x,p)\|^2 && (13) \\ \text{subject to} \quad & f(x) = 0 && (14) \end{aligned}$$

- physics residual is the error in Maxwell's sourceless, time-harmonic equations

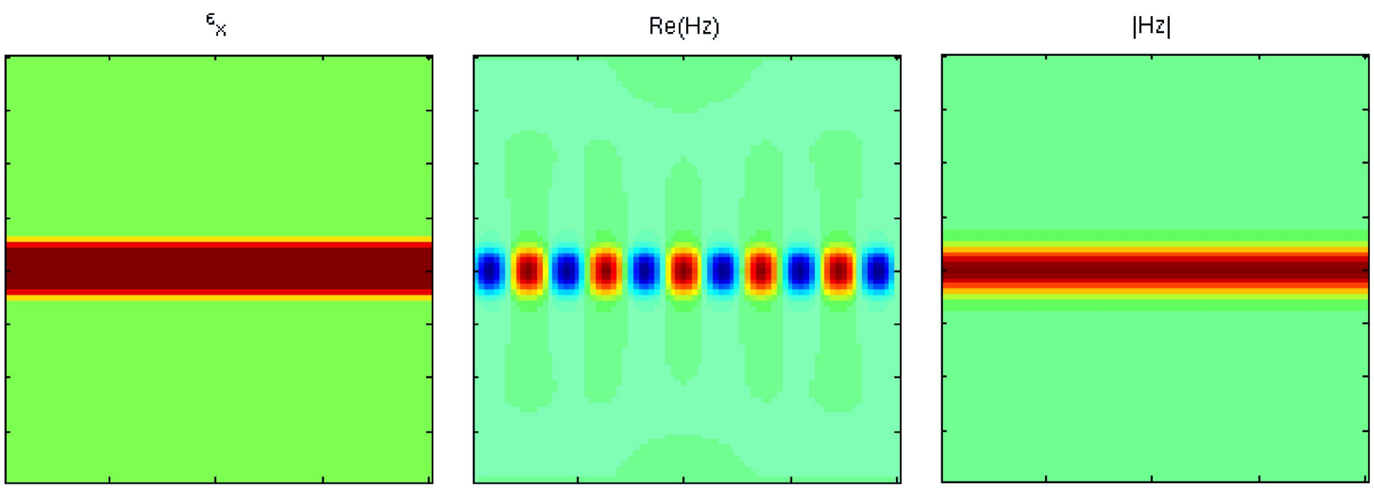
$$\|g(x,p)\|^2 = \|A(p)x\|^2 = \left\| \begin{bmatrix} \nabla\times & i\mu\omega \\ -ip\omega & \nabla\times \end{bmatrix} \begin{bmatrix} x_E \\ x_H \end{bmatrix} \right\|^2 \tag{15}$$

- here $p$ determines the values of $\epsilon$

- key issue: formulation of the constraint

- a sufficient constraint for most devices is to match field values along the border

$$f(x) = \|x^{\text{border}} - x_0^{\text{border}}\|^2 = 0 \tag{16}$$



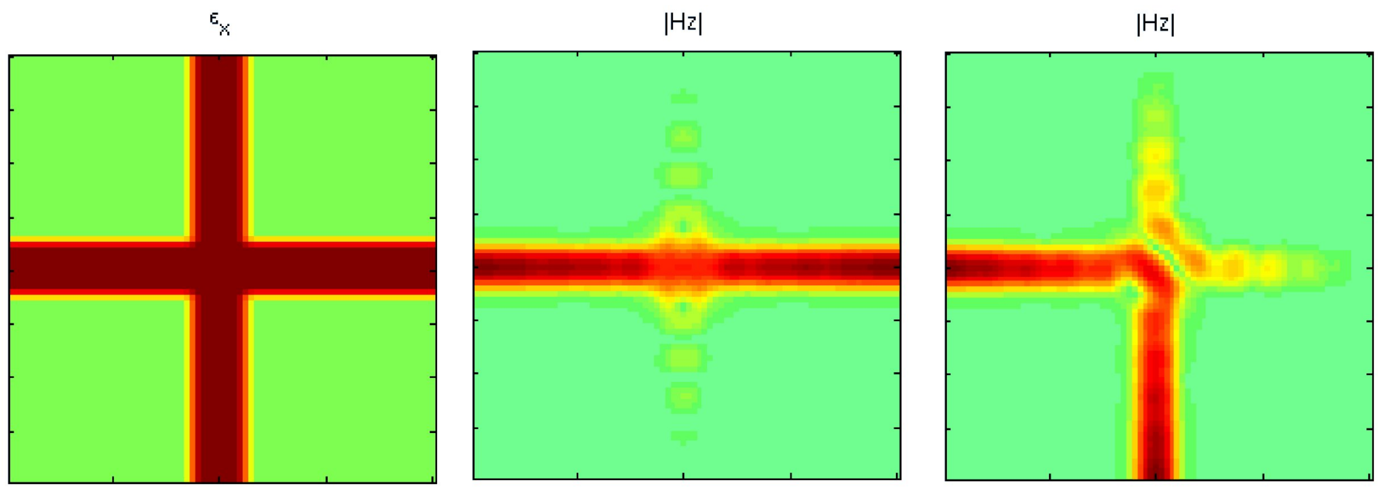

- here, $p$ is a waveguide structure, and the design objective is a perfect waveguide mode at input and output

- to experiment, we fix $p = p_0$, which convexifies the ob-1 formulation

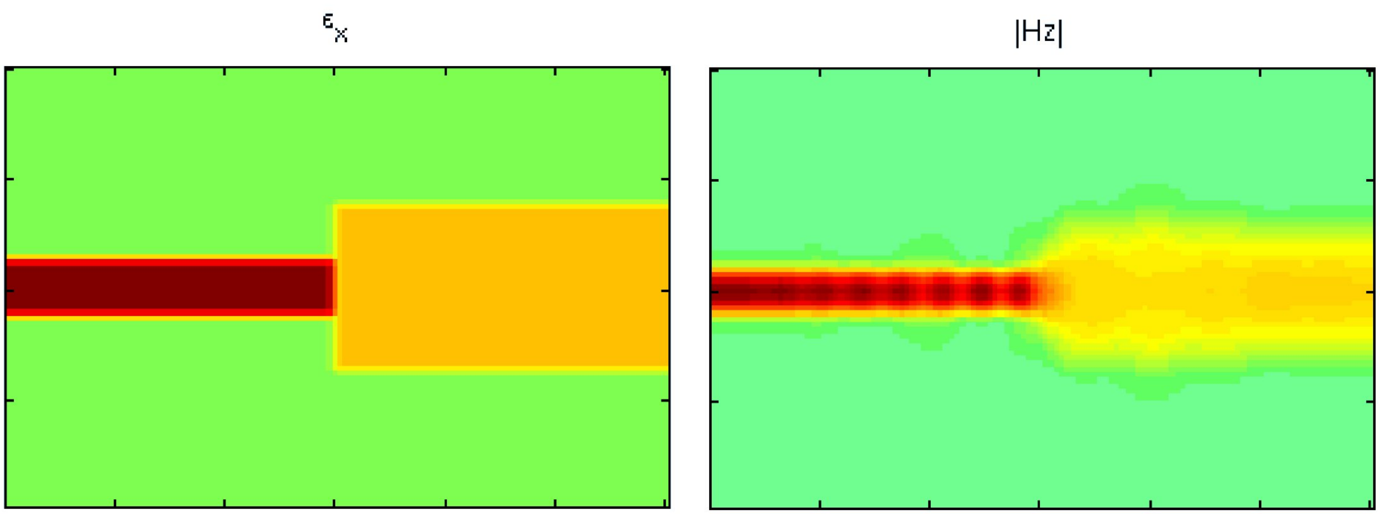
$$\text{minimize} \quad \|A(p_0)x\|^2 \tag{17}$$

$$\text{subject to} \quad x^{\text{border}} = x_0^{\text{border}} \tag{18}$$

- for general structures and design objectives, this results in a "soft physics" field solve



- prioritizing the design objective means we allow physics to be “bent”
- here, reflected waves from the junction magically disappear as they approach the border




- matlab files available at `https://github.com/JesseLu/wave-tools`, look for `em_bval_2dte/demo.m`

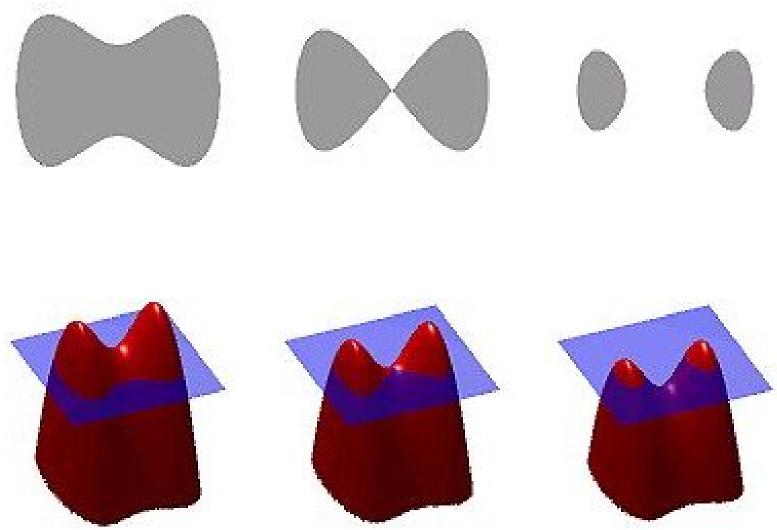
## Structure constraint: level-set method

- a more detailed statement of our problem is

$$
\begin{aligned}
\text{decrease} \quad & \|g(x,p)\|^2 && (19)\\
\text{subject to} \quad & f(x) = 0 && (20)\\
& p \in \{p_{\text{manufacturable}}\} && (21)
\end{aligned}
$$

- need to constrain possible $p$ to what can be fabricated
- for nanophotonics this means two distinct materials only
- however, using $p \in \{\epsilon_1, \epsilon_2\}$ defeats the purpose of using linear approximations

- need ability to *incrementally* update the topology of the structure
- describe $p$ using the *interface* between the two materials
- implicitly describe boundary using the *level-set* of a higher-dimensional function



source: `http://en.wikipedia.org/wiki/Level_set_method`

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