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Chapter 1
Objective-First Nanophotonic Design

Abstract The abstract for the book.
In this chapter, we introduce an "objective-first" strategy for designing nanophotonic devices.
General description:

- Only uses desired fields.
- Can attempt to design any linear device.
- Allows for non-physical fields.

This strategy is unique in that it asks the user only for what electromagnetic field the device should produce, and then attempts to generate the design without further user intervention.

1.1 The electromagnetic wave equation

We start by understanding the underlying physical equation. We extend it beyond its usual use in simulation, and use it for design.

1.1.1 Physics formulation

First, let's derive our wave equation, starting with the differential form of Maxwell's equations,

$$\nabla \times E = -\mu_0 \frac{\partial H}{\partial t} \tag{1.1}$$

$$\nabla \times H = J + \varepsilon \frac{\partial E}{\partial t}, \tag{1.2}$$

where E, H, and J are the electric, magnetic and electric current vector fields, respectively, ε is the permittivity and μ_0 is the permeability, which we assume to be that of vacuum everywhere.

For time dependence $\exp(-i\omega t)$, where ω is the angular frequency, these become

$$\nabla \times E = -i\mu_0 \omega H \tag{1.3}$$

$$\nabla \times H = J + i\varepsilon\omega E, \tag{1.4}$$

which we can combine to form our wave equation,

$$\nabla \times \varepsilon^{-1} \nabla \times H - \mu_0 \omega^2 H = \nabla \times \varepsilon^{-1} J. \tag{1.5}$$

For further information, as well as simplifications to the wave equation in reduced dimensions, please see the Appendix.

1.1.2 Numerical formulation

Now, on top of the analytical formulation of the wave equation (1.5) we will now add a numerical, or discretized, formulation. This will be needed in order to solve for arbitrary structures.

First, we discretize our computational space according to the Yee grid, which allows us to easily define the curl $(\nabla\times)$ operators in (1.5) as described in the Appendix. This allows us, with a change of variables to formulate (1.5) as

$$A(p)x = b(p), \tag{1.6}$$

where $H \to x$, $\varepsilon^{-1} \to p$; and where

$$A(p) = \nabla \times \varepsilon^{-1} \nabla \times -\mu_0 \omega^2 \tag{1.7}$$

and

$$b(p) = \nabla \times \varepsilon^{-1} J. \tag{1.8}$$

Note that our use of $A(p)$ and $b(p)$ instead of A and b simply serves to clarify the dependence of both A and b to p.

Additionally, we use periodic boundary conditions with stretched-coordinate perfectly matched layers where necessary for our examples.

1.1.3 Solving for H

With our numerical formulation, we can now solve for the H-field (the E-field can be computed from the H-field using (1.4)) by using general linear algebra solvers.

Doing so is also simply known as a time-harmonic or a finite-difference frequency-domain (FDFD) simulation.

Now, while a full three-dimensional problem is computationally quite taxing; in one- and two-dimensions, (1.6) is easily solved using the standard sparse solver included in Matlab, and this technique is regularly employed in the examples which follow.

1.1.4 Solving for ε^{-1}

The next step, after having built a field-solver or simulator (finds x given p) for our wave equation, is to build a structure-solver for it. In other words, we need to be able to solve for p given x.

To do so, we return to (1.5) and remark that $\varepsilon^{-1}(\nabla \times H) = (\nabla \times H)\varepsilon^{-1}$ and $\varepsilon^{-1}J = J\varepsilon^{-1}$ since scalar multiplication is communicative. This allows us to rearrange (1.5) as

$$\nabla \times (\nabla \times H)\varepsilon^{-1} - \nabla \times J\varepsilon^{-1} = \mu_0\omega^2 H \tag{1.9}$$

which we now write as

$$B(x)p = d(x), \tag{1.10}$$

where

$$B(x) = \nabla \times (\nabla \times H) - \nabla \times J \tag{1.11}$$

and

$$d(x) = \mu_0\omega^2 H. \tag{1.12}$$

Solving this system would now seem to allow us to choose an electromagnetic field and then find the structure to produce it; which strongly suggests that it will be useful in the design of nanophotonic devices.

In terms of computational complexity, as with (1.6), (1.10) in its current form can be solved using standard tools.

1.1.5 Bi-linearity of the wave equation

Although additional mathematical machinery must still be added in order to get a useful design tool, we have really shown so far is that the wave equation is separately linear or *bi-linear* in x and p. Namely that,

$$A(p)x - b(p) = B(x)p - d(x). \tag{1.13}$$

In other words, fixing p makes solving the wave equation for x a linear problem, and vice versa. Note that the joint problem, where both x and p are allowed to vary, is not linear.

The bi-linearity of the wave equation is fundamental in our objective-first strategy which relies on the fact that we already know how to solve linear systems well, and is the reason why we chose $\varepsilon^{-1} \rightarrow p$ instead of the more natual $\varepsilon \rightarrow p$. Indeed, this property forms a natural division of labor in the objective-first scheme, which we outline below.

1.2 The objective-first design problem

We now build off of the field-solver and the structure-solver, as previously outlined, by formulating the design problem and outlining the objective-first strategy.

1.2.1 Design objectives

A design objective, $f(x)$, is simply defined as a function we wish to be minimal for the design to be produced.

For instance, in the design of a device which must transmit efficiently into a particular mode, we could choose $f(x)$ to be the negative power into that mode. Or, if the device was to be a low-loss resonator, we could choose $f(x)$ to be the amount of power leaking out of the device.

1.2.2 Convexity

Convex optimization quick intro.

1.2.3 Typical design formulation

Typically,

$$\underset{x,p}{\text{minimize}} \quad f(x) \tag{1.14}$$

$$\text{subject to} \quad g(x,p) = 0 \tag{1.15}$$

$$p \in 0,1 \tag{1.16}$$

1.2.4 Objective-first design formulation

Objective-first does

$$\underset{x,p}{\text{minimize}} \quad \|g(x,p)\|^2 \tag{1.17}$$

$$\text{subject to} \quad f(x) = f_{\text{ideal}} \tag{1.18}$$

$$0 \leq p \leq 1 \tag{1.19}$$

This is a bi-convex problem, which we solve using an alternating directions method.

1.2.5 Field sub-problem

$$\underset{x}{\text{minimize}} \quad \|A(p)x - b(p)\|^2 \tag{1.20}$$

$$\text{subject to} \quad f(x) = f_{\text{ideal}} \tag{1.21}$$

1.2.6 Structure sub-problem

$$\underset{p}{\text{minimize}} \quad \|B(x)p - d(x)\|^2 \tag{1.22}$$

$$\text{subject to} \quad 0 \leq p \leq 1 \tag{1.23}$$

1.3 Metamaterials design

1.3.1 Modification of the design objective

1.3.2 Cloak devices

1.3.3 Mimic devices

1.4 Extending the method

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1.5 Appendix

1.5.1 Full 3D curl

1.5.2 1D

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