Objective-First Design of Nanophotonic Waveguide Couplers

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Abstract: We introduce an "objective-first" approach to the design of nanophotonic waveguide couplers. Our method is computationally fast (20 minutes on a single-core personal computer), requires no trial-and-error, does not require guessing a good starting design, can be applied to arbitrary waveguide modes, and generates devices with high coupling efficiencies (typically 95%) and small footprints (1-4 square vacuum wavelengths).

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1. Motivation

1.1. The importance of waveguide mode conversion

Optical mode conversion, the efficient transfer of photons from one guided mode to another, is a fundamental requirement in nanophotonics. Efficient conversion between waveguides modes is critical in the many cases, including:

1. Coupling to and from optical fiber [1], to communicate with the outside world.

2. Coupling between various nanophotonic waveguides, since different waveguides are best suited for different applications. For example, ridge waveguides seem ideal for low-loss transport [2], but other waveguides, such as photonic crystal waveguides or slot waveguides, may be better suited for slow-light [3] or nonlinear optical devices based on localized field intensities [4].

3. Coupling between different materials systems such as passive, active [5], and metallic [6] devices.

Although efficient waveguide coupling is essential in any nanophotonic system, practical methods to design couplers have not yet been developed.

1.2. Approaches to designing waveguide couplers

Of the design strategies currently available, brute-force parameter search is the most often employed because of its sheer simplicity. Although it may be suitable for tuning existing designs, the parameter space for most practical devices is simply too large for such a strategy to be tractable.

Adiabatic mode conversion strategies have been succesful for certain fiber-waveguide [7] and waveguide-waveguide [8] couplers, even if the resulting devices often require large footprints. However, adiabatic approaches cannot be used in many important cases such as coupling in the out-of-plane direction, or coupling between modes of opposite symmetry.

On the other hand, optimization methods based on local topological derivatives seem very promising [9] in that they are both much faster than brute-force methods and more adaptable than adiabatic strategies. However, these methods still carry a significant computational burden in that every updated design must be simulated at least once. Also, there is a significant burden for the user from whom a good initial design is usually required.

In contrast, our method

- does not employ brute-force parameter searches,
- does not require a good initial design,
- is computationally fast (no simulations required),
- generates couplers between seemingly arbitrary waveguide modes, and
- can generate these couplers within a very small footprint.

We outline the general design strategy, as well as how it is applied to coupler design, in the section below.

2. Methods

2.1. Objective-first optimization

The typical approach to designing physical structures can be formulated in the following way, where x is the field variable and p is the structure variable,

$$\begin{aligned} \text{decrease} \quad & f(x) && \text{(1a)} \\ \text{subject to} \quad & g(x,p) = 0. && \text{(1b)} \end{aligned}$$

Here, $f(x)$, the *design objective*, calculates the performance of the device (e.g. amount of power not coupled to output mode); while $g(x,p)$ is the underlying physical equation for the system (e.g. the electromagnetic wave equation).

In contrast, the objective-first formulation is

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

where $\|g(x,p)\|^2$ is the *physics residual*. We term this formulation "objective-first" because the design objective is prioritized even above satisfying physics; specifically, we force our design to always exhibit the desired performance ($f(x) = 0$).

The differences between Eqs. 1 and 2 are:

1. in Eq. 1a, we attempt to decrease the design objective, while in Eq. 2b, the design objective is kept at zero (i.e. we force the optimization to satisfy the design objective);

2. in Eq. 1b, we always satisfy the underlying physics, while in Eq. 2a, physics is not necessarily satisfied, since the physics residual is generally non-zero (although the optimization is directed at minimizing this residual).

Thus, the fundamental innovation in the objective-first approach is simply this: we forcibly impose the desired performance on the device at the expense of not perfectly satisfying the physical equation which governs its operation.

2.2. Numerical implications of the objective-first approach

While the differences between the design strategies presented in Eqs. 1 and 2 are straightforward, the numerical implications are more subtle.

The first practical implication of the objective-first approach is that the number of independent variables is increased to include both x and p. This occurs because in Eq. 1, the constraint that physics must be satisfied, $g(x,p)=0$, essentially forces x to be a dependent variable, since the choice of p implicitly determines the value of x (there is generally a one-to-one mapping from p to x). In contrast, Eq. 2 allows both x and p to vary independently, because the constraint, $f(x)=0$, is only a function of x.

Secondly, the amount of computation needed to enforce the constraint is drastically reduced in our objective-first approach. This is because Eq. 1 requires a full solution of $g(x,p)=0$ (i.e. a full simulation of the structure, p) to compute x. In contrast, the constraint $f(x)=0$ in Eq. 2 can often be enforced with a trivial amount of computation (as shown below).

Lastly, the objective-first approach eliminates the need for even a reasonable initial design. Generally, methods based on Eq. 1 require an initial design which already provides some limited functionality (e.g. a coupler which already transfers a non-zero amount of power to the desired output mode). In constrast, out method, based on Eq. 2, performs just as well when started from a completely non-functional design (e.g. a coupler which transfers no power into the desired output mode).

2.3. Objective-first approach to waveguide coupler design

We now apply the objective-first approach to the problem of designing two-dimensional nanophotonic waveguide couplers.

We choose to work in the two-dimensional transverse electric mode, which only couples E_x, E_y, and H_z ($E_z, H_x, H_y = 0$), since it is most relevant for on-chip devices. We choose to use H_z as the field variable (x in Eq. 2), and ε^{-1} (inverse of the permittivity) as the structure variable p. This results in the following representation of the physics residual, based on the time-harmonic electromagnetic wave equation without sources;

$$\|g(H_z,\varepsilon^{-1})\|^2 = \|\nabla\times\varepsilon^{-1}\nabla\times H_z - \mu_0\omega^2 H_z\|^2, \tag{3}$$

where ω is the angular frequency, and μ_0 is the permeability of free-space.

For the design objective, we choose a boundary-value formulation based on H_z^{perfect}, where H_z^{perfect} is constructed of the exact input and output waveguide modes at the input and output ports of the optimization region (where the coupler will be placed), repectively, and of zero-amplitude fields at the unused ports.

The mathematical form of the design objective is simply,

$$f(H_z) = \left[\begin{array}{c} H_z - H_z^{\text{perfect}} \\ \frac{\partial H_z}{\partial n} - \frac{\partial H_z^{\text{perfect}}}{\partial n} \end{array}\right]_{\text{boundary}} = 0. \tag{4}$$

That is to say, the values of H_z and $\partial H_z/\partial n$ (spatial derivative along normal direction) along the device boundary are forced to be those of a device with perfect performance (100% coupling efficiency).

Such a design objective is both extremely simple and widely adaptable to the design of nearly every kind of nanophotonic device. Most importantly, it is trivial to enforce, requiring only that we overwrite boundary field values. Although there is ambiguity in the relative phases of the input and output boundary fields, our experience suggests that successful designs are possible for arbitrary choice of relative phase.

Finally, as in any method based on an objective-first approach, the physics residual is not guaranteed to decrease to zero. Thus, it is entirely possible to never achieve a physically realizable field, H_z. In such cases, which are the norm rather than the exception, we find that a relatively small residual usually leads to fairly good, although imperfect, device performance.

2.4. *Numerical methods used to solve the objective-first design problem*

The design problem is now

$$\text{decrease} \quad \|\nabla \times \varepsilon^{-1} \nabla \times H_z - \mu_0 \omega^2 H_z\|^2 \tag{5a}$$

$$\text{subject to} \quad \begin{bmatrix} H_z - H_z^{\text{perfect}} \\ \frac{\partial H_z}{\partial n} - \frac{\partial H_z^{\text{perfect}}}{\partial n} \end{bmatrix}_{\text{boundary}} = 0. \tag{5b}$$

This problem contains many local minima (it is non-convex [10]); however, when either the field (H_z) or the structure (ε^{-1}) variable is considered separately, Eq. 5 has only one minimum (it is convex), and can be easily solved using standard methods such as employed in our previous work [11]. We employ such an alternating directions strategy, where both H_z and ε^{-1} are solved independently. This process is extremely inefficient, but is employed because the underlying numerical methods do not need to be tuned by the user. We expect considerable improvements in computational efficiency when more sophisticated algorithms are applied, especially those which can update H_z and ε^{-1} independently.

Lastly, we limit the allowable values of ε to be between the permittivity of vacuum and of silicon,

$$\varepsilon_0 \leq \varepsilon \leq \varepsilon_{\text{silicon}}. \tag{6}$$

A completely binary structure would be preferred, $\varepsilon = \{\varepsilon_0, \varepsilon_{\text{silicon}}\}$, and will be pursued in a future work. That said, the final designs presented here all have significant portions which are already binary.

3. Results

We apply our method to three practically interesting problems that are hard to solve using other available methods:

1. a coupler between waveguides of different refractive index and width,
2. a coupler between waveguide modes of different order and symmetry, and
3. a coupler between waveguides that confine light using different principles (index guided vs. distributed Bragg reflection guided), i.e., between a slab waveguide and a photonic crystal fiber.

The corresponding designs as well as the boundary values which make up the respective design objectives (H_z^{perfect}) are shown in Figs. 1, 2 and 3. As initial designs, we uniformly choose $\varepsilon = 9$ throughout the whole computational region. These results demonstrate that our method

- is computationally fast, requiring only 20 minutes on a single-core personal computer;
- generates compact devices with footprints of only 1-4 square vacuum wavelengths;
- generates highly efficient devices with typical coupling efficiencies of 95%;
- can be applied to arbitrary input and output modes, as seen from the diverse selection of desired output waveguide modes;
- does not require a good initial design. The initial design was simply $\varepsilon = 9$ everywhere (a somewhat arbitrary guess, other values work as well), which in the case of Figs. 2 and 3 produces an initially non-functional device (coupling efficiency of 0%).

4. Conclusion

We develop a fundamentally new approach to designing physical structures, which we term “objective-first”, in that we choose to satisfy the design objective even above satisfying the physical equation which governs its operation. We show that such an approach drastically reduces the amount of computation required per iteration, and performs well even with a non-functional initial design.

We then apply an objective-first approach to the design of three practical nanophotonic waveguide couplers which are difficult, at best, to solve with existing methods. We show that our method produces high-efficiency designs

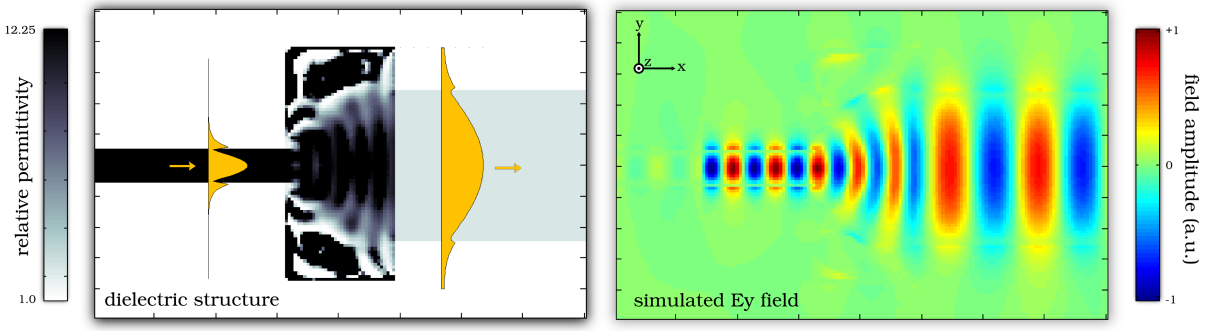

Fig. 1. Coupler from a narrow, high-index ($\varepsilon = 12.25$) waveguide to a wide, low-index ($\varepsilon = 2.25$) waveguide. On the left, the dielectric structure of the coupler and surrounding input and output waveguides are shown. The H_z^{perfect} boundary values used as the design objective are plotted on the left as well (top and bottom boundary values were set to zero). On the right, we show the simulation results used to compute the performance of the device. The coupler converts 96.3% of the input power to the designated output mode. The device is also extremely compact, convering only 36×66 grid points, where the vacuum wavelength is 42 grid points. Computation time was 20 minutes on a personal computer.

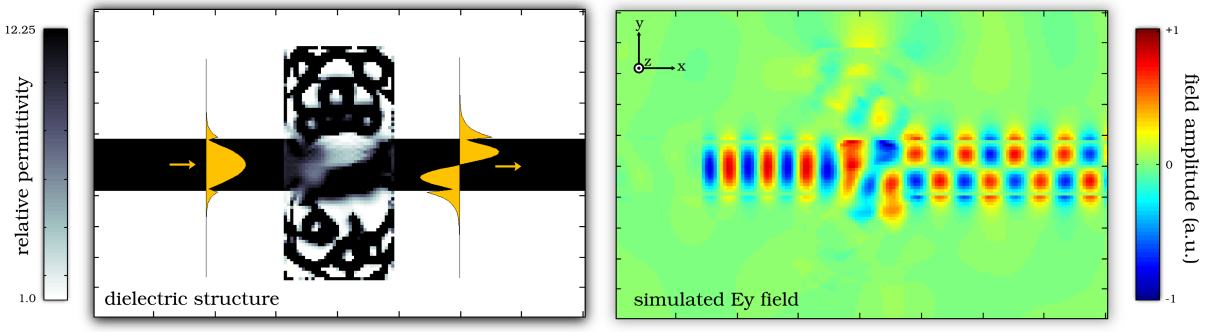

Fig. 2. Coupler that converts the fundamental waveguide mode to the second-order waveguide mode (a movie of the design progress is included as a supplementary material). This problem is quite difficult since the two modes are of opposite symmetry. For example, adiabatic approaches cannot be applied to this case. However, our method produces a device (which has the same dimensions and vacuum wavelength as Fig. 1) with a coupling efficiency of 95.5%. Computation time was 20 minutes on a personal computer.

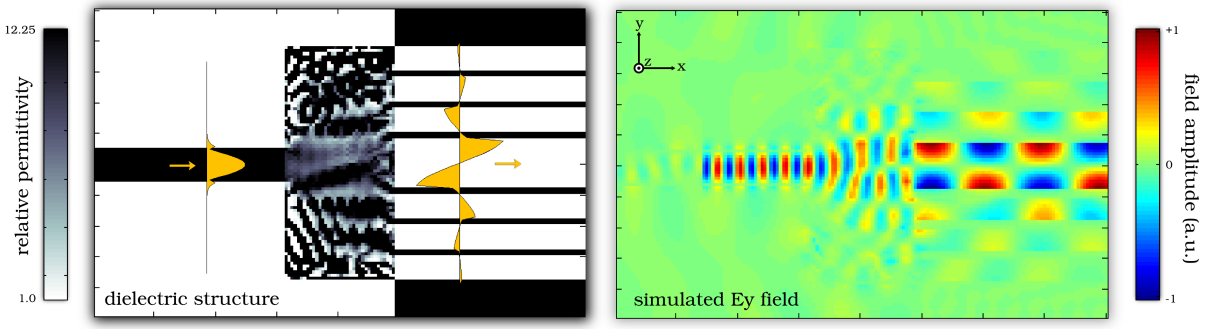

Fig. 3. Coupler between a dielectric slab waveguide to an air-core waveguide. Here, not only are the modes of opposite symmetry, but the output waveguide operates on a fundamentally different principle (distributed reflection) than the input waveguide (index guided). The device still achieves an efficiency of 83.3%, demonstrating the versatility of our method. The vacuum wavelength is 25 grid points, while the device footprint is still 36×66 grid points. Computation time was 20 minutes on a personal computer.

($\sim$ 95% efficiency) in small footprints ($\sim$ 1 square vacuum wavelength), is computationally fast (20 minutes on a single-core personal computer), and does not require trial-and-error, or even a good starting design.

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