Automated Design of Nanophotonic Waveguide Couplers

Jesse Lu and Jelena Vučković
Stanford University, Stanford, California, USA.
jesselu@stanford.edu

Abstract: We introduce an "objective-first" approach to the design of nanophotonic waveguide couplers. We show that our method is computationally fast (20 minutes), requires no trial-and-error, does not require 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).

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 [], 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 [], but other waveguides, such as photonic crystal waveguides or slot waveguides, may be better suited for slow-light [] or energy-focusing devices [].
3. Coupling between different materials such as passive, active [], and non-linear [] materials.

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 to-date 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 [] and waveguide-waveguide [] couplers, even if the resulting devices require large footprints. However, adiabatic approaches cannot be used in many important cases where the mode structure is more complex, such as coupling from ridge to some photonic crystal waveguides [], or where the geometry of the problem is non-trivial, 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 [] 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 in a very small footprint.

We outline the general design strategy, as well as how it is applied to nanophotonic 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. 1, we attempt to decrease the design objective (Eq. 1a), while in Eq. 2, the design objective is kept at zero (Eq. 2b);
2. in Eq. 1, we always satisfy the underlying physics (Eq. 1b), while in Eq. 2, physics is not satisfied, since the physics residual is generally non-zero (Eq. 2a).

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 breaking the physics which govern 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. In Eq. 1, the constraint that physics must be satisfied, $g(x,p) = 0$, essentially forces x to be a dependentent 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 the 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 so quickly (as shown below) that future implementations may even produce designs in the same amount of time as required to simulate them!

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, methods based on Eq. 2 perform just as well when started from a completely non-functional design (e.g. a coupler which transfers no power into the desired output mode).

In conclusion, an objective-first approach results in a method that is computationally fast (since it does not require simulation), and that can be applied to non-intuitive problems where a functional starting design is not readily available.

2.3. *Objective-first approach to waveguide coupler design*

We now apply an 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, and ε^{-1} (inverse of the permittivity) as the structure variable. This results in the following representation of the physics residual, based on the time-harmonic electromagnetic wave equation without sources;

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

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

For the design objective, we choose a boundary element 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, repectively, and of zero-amplitude fields at the unused ports. The actual 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, in any objective-first approach, the physics residual is never 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

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

$$\text{subject to} \quad H_z - H_z^{\text{perfect}} \Big|_{\text{boundary}} = 0 \tag{5b}$$

$$\frac{\partial H_z}{\partial n} - \frac{\partial H_z^{\text{perfect}}}{\partial n} \Bigg|_{\text{boundary}} = 0. \tag{5c}$$

This problem contains many local minima (it is non-convex []); 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 []. 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 require any tuning. 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

The method described above is applied to the design of three different waveguide couplers as shown in Figs. 1, 2 and 3. 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%).

Lastly, note that the couplers in Figs. 2 and 3 must convert between modes of opposing symmetry, in which case adiabatic approaches cannot be applied. Note also that the output waveguide in Fig. 3 even operates on a completely different principle (distributed reflection instead of index-guiding).

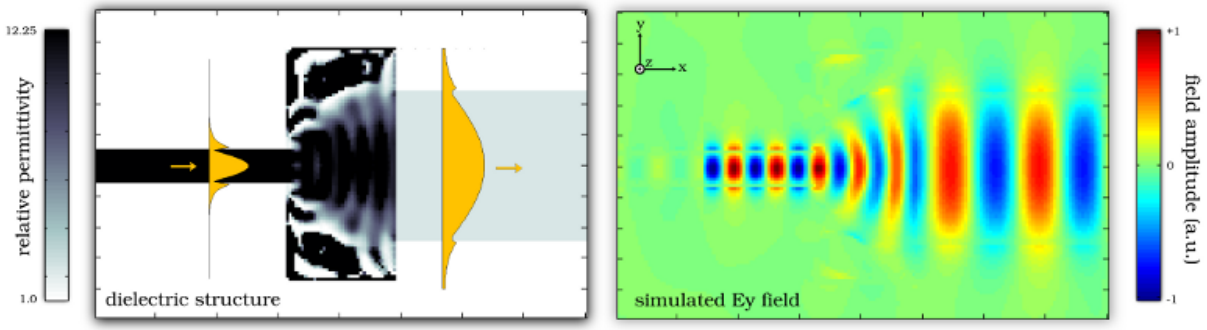

Fig. 1. Waveguide coupler for a wide, low-index ($\varepsilon = 2.25$) waveguide. The dielectric structure of the coupler and surrounding input and output waveguides is shown on the left, while the simulation validating our results is shown on the right. The coupler converts 96.3% of the input power to the designated output mode. The device is 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.

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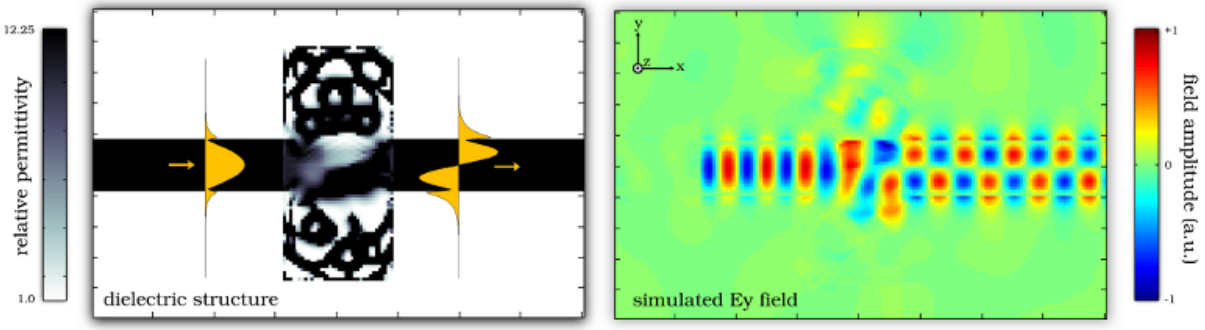

Fig. 2. Coupler that converts the fundamental waveguide mode to the second-order waveguide mode. This problem is quite difficult since the two modes are of opposite symmetry. For example, adiabatic approaches cannot be applied to this case. However, our method produces a device (which has the same dimensions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

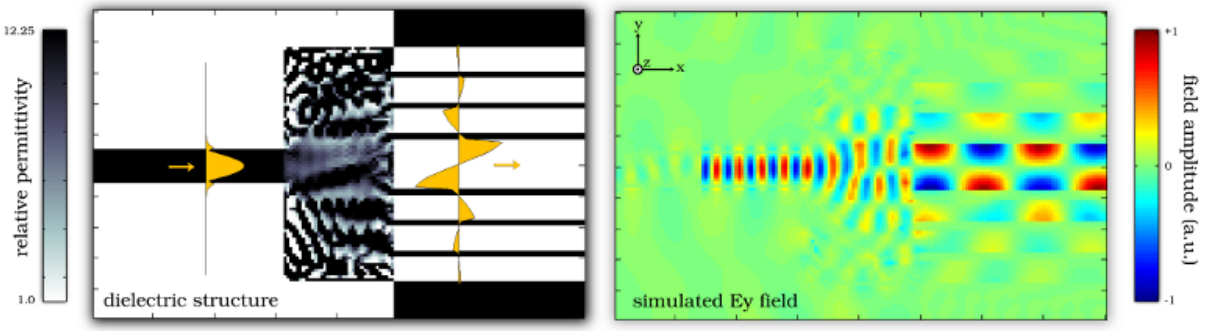

Fig. 3. Coupler to an air-core mode. Here, not only are the modes of opposite symmetry, but the output waveguide operates on a fundamentally different principle (guided by Bragg reflection) than the input waveguide (index guided). The device still achieves an efficiency of 83.3%, demonstrating the versatility 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.