

Robust shape optimization for nano-photonics

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Silicon photonic

Nanophotonic components are devices allowing to manipulate light (see as an electromagnetic wave) at the nano/micro-metric scale.



Fig. Examples of nanophotonics devices.

By connecting several components it is possible to complete circuit with complex optical properties.

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Silicon photonic + topology optimization

Shape-optimization applied to nanophotonic: complex geometries.



(a) B. Shen et al., Nature photonics (2015)

(b) *A. Y. Piggot et al., Nature photonics (2015)*

(c) L. F. Frellsen et al., Optics Express (2016)

Fig. MEB images of manufactured nanophotonic devices



 $\mathcal{C} \setminus \Omega = \text{air.}$

optimization of a shape in order to maximize a physical objective

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Nanophotonic: description & modelization

- Silicon photonic
- PDE, Maxwell's equations
- Waveguide modes

Shape optimization problem

- Objective function
- Algorithm
- Results

3 Multi-objectives & robustness

- Multi objectives
- Worst-case robustness
- Wavelength robustness

Geometrical robustness

- Lithography and etching
- Shape derivative for dilated/eroded shape
- Application with lithography-etching

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Maxwell's equations

(linear) Maxwell's equations allows to describe the electric field $E : \mathbb{R}^3 \to \mathbb{C}^3$ propagation at a given wavelength λ :

$$\nabla \times \nabla \times \mathbf{E} - k^2 n^2_{\downarrow} \mathbf{E} = 0$$

where $k = 2\pi c/\lambda$ is the wavenumber, *n* the **the material's optical index** and *c* the speed of light.



Optical indices:

- silicon in red ($n_{\rm silicon} \simeq 3.5$),
- silica in **blue** $(n_{\text{silica}} \simeq 1.45)$,
- air in green $(n_{air} = 1)$,
- optimizable domain in yellow (C),

$$n_{
m component} = \left\{ egin{array}{cc} n_{
m silicon} & {
m in} & \Omega \ n_{
m air} & {
m in} & \mathcal{C} igar \Omega \end{array}
ight. .$$

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Waveguide modes 1/2

Components are linked through **waveguides**. Studying them shows that there exist several **propagation modes** (eigenvectors associated with the operator $\nabla \times \nabla \times -k^2 n^2 ld$ such that $\mathbf{E}(x, y, z) = \mathbf{E}(x, y)e^{i\beta z}$).



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Waveguide modes 2/2

• Every electric field on a waveguide may be decomposed on the \mathcal{E}_j :



• Orthogonality for all $i \neq j$:

$$\int_{\Gamma} \left[\boldsymbol{\mathcal{E}}_i \times \boldsymbol{\mathcal{H}}_j^* + \boldsymbol{\mathcal{H}}_i \times \boldsymbol{\mathcal{E}}_j^* \right] \cdot \mathbf{n} \, ds = 0.$$

• Injection of the *n*-th mode $(\mathbf{E} = \mathcal{E}_n + \sum_{j=1} \alpha_{-j} \mathcal{E}_{-j})$:



$$\mathbf{n} imes
abla imes \mathbf{E} + rac{1}{2} i \omega \mu_0 \sum_{j=1}^N \mathbf{n} imes \mathcal{H}_j \int_{\Gamma} \left[\mathbf{E} imes \mathcal{H}_j^*
ight] \cdot \mathbf{n} \ ds = 2 i \omega \mu_0 \ \mathbf{n} imes \mathcal{H}_n.$$

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Perfectly Matched Layer

To ensure the unicity of a solution in $\mathbb{R}^3,$ the electric field must verify at infinity the Silver-Müller radiation condition

$$\lim_{|\mathbf{x}|\to\infty} |\mathbf{x}| \left(\nabla \times \mathbf{E} \times \frac{\mathbf{x}}{|\mathbf{x}|} - i\omega \mathbf{E} \right) = 0.$$

Numerically we use Perfectly Matched Layers (PML); areas around the component which **fully absorb electromagnetic waves** without causing **any reflections**.



where Λ is a complex anisotrope matrix.

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E Full PDE

Variational formulation: $\mathbf{E} \in H(\mathbf{rot}, \mathcal{D})$ solution for all $\phi \in H(\mathbf{rot}, \mathcal{D})$ to

$$\int_{\mathcal{D}} \Lambda^{-1} \nabla \times \mathbf{E} \cdot \nabla \times \phi^* - k^2 n^2 \Lambda \mathbf{E} \cdot \phi^* \, d\mathbf{x} + i\omega\mu_0 \int_{\Gamma} \mathbf{n} \times \left(2 \,\mathcal{H}_n - \frac{1}{2} \sum_{j=1}^N \mathcal{H}_j \int_{\Gamma} \left[\mathbf{E} \times \mathcal{H}_j^* \right] \cdot \mathbf{n} \, dt \right) \cdot (\mathbf{n} \times \phi^* \times \mathbf{n}) \, ds = 0.$$

(a) Typical mesh ($\approx 5 \times 10^5$ tetras.) (b) FEM simulation (Nédélec el., order 2)

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Objective function

We consider a nanophotonic component with N input waveguides and M output waveguides. For j = 1, ..., N, we launch a mode $\mathcal{E}_{\text{in},j}$ into the *j*-th waveguide. We want to obtain other modes $\mathcal{E}_{\text{out},j}$ in the output waveguides.



The **power** through a surface Γ is physically defined as:

$$P^{\Gamma} = \frac{1}{2} \int_{\Gamma} \mathcal{R}e\left[\mathbf{E} \times \mathbf{H}^*\right] \cdot \mathbf{n} \, ds$$

We deduce the **power carried by a** waveguide mode \mathcal{E}_n along Γ as:

$$P_n^{\Gamma} = \left| \frac{1}{4} \int_{\Gamma} \left[\mathbf{E} \times \mathcal{H}_n^* + \mathbf{H} \times \mathcal{E}_n^* \right] \cdot \mathbf{n} \, ds \right|^2$$

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Shape optimization methods

Shape optimization (a.k.a. inverse design) is a set of methods allowing to find an unparameterized structure which maximizes a given figure of merit.



(a) Genetic algorithm, B. Shen et al., Nature photonics (2015)

(b) Density-based, A. Y. Piggot et al., Nature C. M. Lalau-Keraly et al., photonics (2015)

(c) Geometric (level-set), Optics express (2013)

Fig. Different shape optimization methods.

Shape optim. (Hadamard's method) 1/2

Goal: for an objective function $\mathcal{J}(\Omega)$, implement a gradient-based algorithm using the **shape derivative** of $\mathcal{J}(\Omega)$.

Difficulty: how to define what we meant by "small variation" of a shape ?





Let $\theta : \mathbb{R}^3 \to \mathbb{R}^3$ a vector field such that Ω is modified into $(\mathsf{Id} + \theta)(\Omega) = \{\mathbf{x} + \theta(\mathbf{x}), \mathbf{x} \in \Omega\}.$

The following first order expansion holds

$$\mathcal{J}((\mathsf{Id}+ heta)(\Omega)) = \mathcal{J}(\Omega) + \mathcal{J}'(\Omega)(heta) + o(heta).$$

Shape optim. (Hadamard's method) 2/2

Maximization of the power carried by a mode on a waveguide Γ_{out} , that is:

$$\mathcal{J}(\Omega) \hspace{2mm} = \hspace{2mm} \left| rac{1}{4\omega\mu_0} \int_{\Gamma_{\mathrm{out}}} [\mathsf{E}_\Omega imes (
abla imes \mathcal{E}_j^*) + (
abla imes \mathsf{E}_\Omega) imes \mathcal{E}_j^*] \cdot \mathbf{n} \hspace{0.5mm} ds
ight|^2,$$

where \mathbf{E}_{Ω} is solution of the PDE with $n_{\text{component}} = n_{\text{air}} + (n_{\text{silicon}} - n_{\text{air}})\chi_{\Omega}$.

Using an adjoint-based method we find that:

$$\mathcal{J}'(\Omega)(oldsymbol{ heta}) = \int_{\partial\Omega} oldsymbol{ heta} \cdot \mathbf{n} \; V(s) \; ds$$

where
$$V(s) = k^2 \int_0^l \mathcal{R}e\left[\frac{\mathbf{n} \times \mathbf{E} \times \mathbf{n} \cdot \mathbf{n} \times \mathbf{A}^* \times \mathbf{n}}{(n_{silicon}^2 - n_{air}^2)^{-1}} - \frac{(n^2 \mathbf{E}) \cdot \mathbf{n} (n^2 \mathbf{A}^*) \cdot \mathbf{n}}{(n_{silicon}^{-2} - n_{air}^{-2})^{-1}}\right] dl,$$

with **A** solution of a PDE close to the one of **E**.

 $\theta_{\text{opt}} = tV(s) \mathbf{n} \text{ and } t \text{ small} \quad \Rightarrow \quad \mathcal{J}((\mathsf{Id} + \theta_{\text{opt}})(\Omega)) > \mathcal{J}(\Omega).$

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Discontinuity at interfaces and regularity

The shape derivative use $(n^2 \mathbf{E}) \cdot \mathbf{n}$. n^2 and $\mathbf{E} \cdot \mathbf{n}$ are discontinuous on an interface but numerically all the quantities are continuous on the same tetrahedron



(a) E_v , explicit **(b)** E_v , non-explicit

Fig. An explicit mesh forces all the field's components to be continuous.

Optical index regularization:

$$n_\eta^2 = n_{
m air}^2 + (n_{
m silicon}^2 - n_{
m air}^2) h_\eta(d_\Omega)$$

where h_n is a smooth approximation of the Heaviside function and d_{Ω} the signed distance to Ω .

let \mathbf{E}_n be solution to Maxwell equation using n_{η} . We have

$$\lim_{\eta\to 0} \|\mathbf{E}_{\eta} - \mathbf{E}\|_{\mathcal{H}(\mathbf{rot},\mathcal{D})} = 0.$$

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Numerical representation of shapes





(a) Level-set function



The shape Ω is represented by the 0 level set of the function $\phi : \mathbb{R}^2 \to \mathbb{R}$:

$$\Omega = \{\mathbf{x}, \phi(\mathbf{x}) < \mathbf{0}\}, \qquad \partial \Omega = \{\mathbf{x}, \phi(\mathbf{x}) = \mathbf{0}\}.$$

If Ω_0 is represented by $\phi_0 = \phi(\mathbf{x}, 0)$ then $\Omega_1 = (Id + Vn)(\Omega_0)$ is given by $\phi_1 = \phi(\mathbf{x}, 1)$ where ϕ is solution to the following Hamilton-Jacobi equation

$$\begin{cases} \partial_t \phi(\mathbf{x}, t) + V \| \nabla_{\mathbf{x}} \phi(\mathbf{x}, t) \| = 0 \\ \phi(\mathbf{x}, 0) = \phi_0 \end{cases}$$

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Algorithm in practice



(a) Computation of the electric field \mathbf{E}_{Ω} and the adjoint by FEM

(b) *Computation of the vector field using the shape derivative*

(c) Modification of the shape solving the Hamilton-Jacobi

Fig. One step of the shape optimization algorithm.

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Example 1/3: crossing



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Example 1/3: crossing, multiple initializations



Fig. Initial shape as 2×2 Fig. Initial shape as 5×5 Fig. Initial shape as 8×8
holes.holes.holes.

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Example 2/3: power divider



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Example 3/3: modes converters



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Multi-objectives: duplexer





Note: on this slide (only) simulations are done in 2D.

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Multi-objectives descent

We are interested in the case where all the objectives $\mathcal{J}_i(\Omega)$ are of equal importance, meaning that we maximize

 $\max_{\Omega} \min_{i=1,\ldots,N} \mathcal{J}_i(\Omega).$

At each iteration we search for $\boldsymbol{\theta}$ such that

$$\max_{\theta} \min_{i=1,...,N} \mathcal{J}_i(\Omega) + \mathcal{J}'_i(\Omega)(\theta).$$

We can find a **common** descent direction for each objectives by solving the following linear program:

$$\left\{\begin{array}{ll} \max\limits_{\alpha, r} r \\ \textbf{s.t.} \quad \alpha \in \left[0, 1\right]^{N}, \ r \in \mathbb{R}, \\ \sum\limits_{i=1}^{N} \alpha_{i} = 1, \mathcal{J}_{i}(\Omega) + \sum\limits_{j=1}^{N} \alpha_{j} \left\langle V_{i}, V_{j} \right\rangle < r, \ i = 1, ..., N \end{array}\right.$$

2 Worst-case robustness

Nanophotonic components are subject to **several uncertain parameters**: wavelength, temperature, height of the silicon plate, edges rugosity, etching process etc. ...

Let X be the set of possibe parameters. For instance if we only consider λ then $X = [\lambda_0 - \varepsilon_{\lambda}, \lambda_0 + \varepsilon_{\lambda}]$ (more generally X is an hypercube).

We are looking for a robust component (worst-case), that is

$$\max_{\Omega} \min_{\delta \in X} \mathcal{J}_{\delta}(\Omega) \simeq \max_{\Omega} \min_{\delta = \delta_1, ..., \delta_n} \mathcal{J}_{\delta}(\Omega).$$

For a $\pm 50 \text{ nm}$ robustness we could maximize:

$$\max_{\Omega} \min \left[\mathcal{J}_{-50 \text{ nm}}(\Omega), \mathcal{J}_{0 \text{ nm}}(\Omega), \mathcal{J}_{+50 \text{ nm}}(\Omega) \right].$$

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Wavelength robustness 1/2: power divider



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Wavelength robustness 2/2: duplexer



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22 Physical problem

Because of the manufacturing process the produced shapes are not exactly the same as the ones we are asking for.



If we try to produce Ω we will get $\Psi_{\delta}(\Omega)$ with δ an uncertain parameter.

Question: What is the shape derivative of $\mathcal{J}_{\delta}(\Omega) = \mathcal{J}(\Psi_{\delta}(\Omega))$?



Fig. Main steps of the lithography-etching process.





• Lithography: convolution-thresholding of the caracteristic function

$$\Omega_{\mathsf{lithography}} = \{ \mathsf{x}, (\chi_{\Omega} * G)(\mathsf{x}) > s \}$$

where G correspond to a centered gaussian with fixed variance and $s \in]0,1[$ the threshold to change the resin's state.

• Etching: dilation or erosion

$$\Omega_{\text{etching}} = (\mathsf{Id} + \delta \mathbf{n})(\Omega_{\text{lithography}})$$

where δ is a small uncertain parameter with values in the interval $[-\eta, \eta]$.

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Lithography approximation

Reminder:

$$\Omega_{\text{lithography}} = \{\mathbf{x}, (\chi_{\Omega} * G)(\mathbf{x}) > s\}$$

Hardly differentiable ...

We locally approximate the shape up to the second order (locally convolution between a parabola and a gaussian). As such

$$\widetilde{\Omega}_{\text{lithography}} = (\text{Id} + f(\kappa)\mathbf{n})(\Omega)$$

where f is an analytic function.



Fig. Optimized shape Ω , Ω after lithography, Ω after approximation.

In conclusion we have $\Omega_{\text{etching}} \simeq (\text{Id} + g_{\delta}(\mathbf{x})\mathbf{n})(\Omega).$

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Shape derivative for dilated/eroded shape

Theorem:

Let $\mathcal{J}_{\delta}(\Omega) = \mathcal{J}((\mathsf{Id} + \delta \mathbf{n})(\Omega))$ where \mathcal{J} is defined as previously. If δ is sufficiently small so that $(\mathsf{Id} + \delta \mathbf{n})$ is a diffeormorphism from Ω into the dilated shape $(\mathsf{Id} + \delta \mathbf{n})(\Omega)$ then we have the following shape derivative:

$$\mathcal{J}_{\delta}'(\Omega)(oldsymbol{ heta}) = \int_{\partial\Omega} oldsymbol{ heta} \cdot {\sf n} V_{(\mathsf{Id}+\delta\mathsf{n})(\Omega)} \circ (\mathsf{Id}+\delta\mathsf{n})(s) H \, ds$$

where $H = ((Id + \delta \nabla \mathbf{n})^{-1} \mathbf{n} \cdot \mathbf{n}) |det(Id + \delta \nabla \mathbf{n})|.$

 \rightarrow In other word, simulating Maxwell equations with $(Id + \delta \mathbf{n})(\Omega)$ gives us information on how to modify Ω to optimize $\mathcal{J}_{\delta}(\Omega)$.

Solving $\max_{\Omega} \min[\mathcal{J}_{\mathcal{G}_{-\eta}}(\Omega), \mathcal{J}(\Omega), \mathcal{J}_{\mathcal{G}_{+\eta}}(\Omega)]$ should give us a shape which is robust to the (simplified) lithography-etching process with $\delta \in [-\eta, \eta]$.

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Example 1/4: power divider



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Real part of H

Real part of H

Real part of H

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Example 2/4: mode converter $1 \rightarrow 3$



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Example 3/4: mode converter $1 \rightarrow 2$



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Example 4/4: duplexer





- **Nicolas Lebbe**, Charles Dapogny, Édouard Oudet, Karim Hassan and Alain Glière, *Robust shape and topology optimization of nanophotonic devices using the level set method*, in press, Journal of Computational physics (2018).
- **Nicolas Lebbe**, Alain Glière and Karim Hassan, *High-efficiency and broadband photonic polarization rotator based on multilevel shape optimization*, published in Optics Letters 44, no. 8, 1960–1963 (2019).