Simulations in integrated optics, brief general remarks Semianalytical treatment of rectangular 2D Helmholtz problems



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Photonic devices: Examples from the CIPS application





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Abstract scattering problem



Typical parameters:

- Vacuum wavelength $\lambda \in [400, 700] \text{ nm (visible light)},$ $\lambda \approx 1.3 \,\mu\text{m}, 1.55 \,\mu\text{m}$ (optical fibers, attenuation min.).
- Refractive indices n ∈ [1, 3.4], small attenuation (transparent dielectrica).
- Interesting domain: $(10 \lambda 100 \lambda)^d$, d = 2, 3 (2D, 3D).
- Details: $\approx \lambda/10$, $\approx \lambda/100$.
- Influx and outflux: Guided & nonguided waves ---- Boundary conditions.

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 - Macroscopic Maxwell equations
 - Stationary and time-domain problems
 - 2D problems
 - Modes of dielectric waveguides
- Semianalytical treatment of rectangular 2D Helmholtz problems
 - Problem setting
 - Eigenmode expansion
 - Algebraic procedure
 - Numerical results

... for electromagnetic fields

$$\mathcal{E}(x, y, z, t) = \frac{1}{2} \left(\tilde{E}(x, y, z) e^{i\omega t} + \tilde{E}^*(x, y, z) e^{-i\omega t} \right),$$

$$\hat{=} \mathcal{B}, \tilde{B}, \mathcal{D}, \tilde{D}, \mathcal{H}, \tilde{H}, \mathcal{P}, \tilde{P}, \mathcal{M}, \tilde{M}, \omega = kc = 2\pi c/\lambda,$$

in frequency domain form (SI):

$$\operatorname{curl} \tilde{\boldsymbol{E}} = -\mathrm{i}\omega\tilde{\boldsymbol{B}}, \quad \operatorname{curl} \tilde{\boldsymbol{H}} = \mathrm{i}\omega\tilde{\boldsymbol{D}}, \quad \operatorname{div} \tilde{\boldsymbol{D}} = 0, \quad \operatorname{div} \tilde{\boldsymbol{B}} = 0,$$

 $\tilde{\boldsymbol{B}} = \mu_0(\tilde{\boldsymbol{H}} + \tilde{\boldsymbol{M}}), \quad \tilde{\boldsymbol{D}} = \epsilon_0\tilde{\boldsymbol{E}} + \tilde{\boldsymbol{P}}.$

... for electromagnetic fields

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Typical media:

- uncharged, no free currents and charges,
- nonmagnetic at optical frequencies, $\tilde{M} = 0$,
- dielectrica, susceptibilities $\hat{\chi}^{(j)}(x, y, z; \omega)$:

$$\tilde{P}_j = \epsilon_0 \Big(\sum_k \chi_{j,k}^{(1)} \tilde{E}_k + \sum_{k,l} \chi_{j,k,l}^{(2)} \tilde{E}_k \tilde{E}_l + \sum_{k,l,m} \chi_{j,k,l,m}^{(3)} \tilde{E}_k \tilde{E}_l \tilde{E}_m \dots \Big).$$

Convention: Eliminate \tilde{D} and \tilde{B} \sim Formulation in \tilde{E} and \tilde{H} .

$$\tilde{\boldsymbol{P}} = \epsilon_0 \hat{\chi}^{(1)} \tilde{\boldsymbol{E}}, \quad \tilde{\boldsymbol{D}} = \epsilon_0 (1 + \hat{\chi}^{(1)}) \tilde{\boldsymbol{E}} = \epsilon_0 \hat{\epsilon} \tilde{\boldsymbol{E}};$$

 $\hat{\epsilon} = 1 + \hat{\chi}^{(1)}$: Relative permittivity.

Simplest case: Isotropic, lossless dielectrica; refractive index n:

$$\hat{\epsilon} = \epsilon \mathbf{1}, \quad \epsilon = n^2, \quad n(x, y, z; \omega) \in \mathbb{R}.$$

Frequently *n* is piecewise constant \checkmark Interface conditions for \tilde{E} , \tilde{H} .

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Complications:

- Anisotropic media, $\hat{\epsilon} \not\sim 1$ (crystals, ordered materials),
- Attenuation, $\hat{\epsilon}^{\dagger} \neq \hat{\epsilon}$, $n \notin \mathbb{R}$,
- Nonlinear problems, $\hat{\chi}^{(2)}$, $\hat{\chi}^{(3)}$...

Continuous wave excitation, ω a given parameter:

$$\begin{array}{ll} \operatorname{curl} \tilde{\boldsymbol{E}} = -\mathrm{i}\omega\mu_{0}\tilde{\boldsymbol{H}}, & \operatorname{curl} \tilde{\boldsymbol{H}} = \mathrm{i}\omega\epsilon_{0}\hat{\epsilon}\tilde{\boldsymbol{E}}, & \operatorname{div}\hat{\epsilon}\tilde{\boldsymbol{E}} = 0, & \operatorname{div}\tilde{\boldsymbol{H}} = 0, \\ \text{or} & \operatorname{curl}\operatorname{curl}\tilde{\boldsymbol{E}} = k^{2}\hat{\epsilon}\tilde{\boldsymbol{E}}, & \operatorname{curl}\hat{\epsilon}^{-1}\operatorname{curl}\tilde{\boldsymbol{H}} = k^{2}\tilde{\boldsymbol{H}}, \\ \tilde{\boldsymbol{E}}(x, y, z) \in \mathbb{C}^{3}, & \tilde{\boldsymbol{H}}(x, y, z) \in \mathbb{C}^{3}. \end{array}$$

Helmholtz solver:

Given $\hat{\epsilon}$ and an optical "influx", find \tilde{E} , \tilde{H} on a computational domain, subject to suitable boundary conditions.

Scans over $\omega \longrightarrow$ Spectral data.

Propagation of time dependent signals, pulsed excitation:

$$\begin{aligned} & \operatorname{curl} \boldsymbol{\mathcal{E}} = -\mu_0 \partial_t \boldsymbol{\mathcal{H}}, \quad \operatorname{curl} \boldsymbol{\mathcal{H}} = \epsilon_0 \hat{\epsilon} \partial_t \boldsymbol{\mathcal{E}}, \quad \operatorname{div} \hat{\epsilon} \boldsymbol{\mathcal{E}} = 0, \quad \operatorname{div} \boldsymbol{\mathcal{H}} = 0, \\ & \operatorname{or} \\ & \operatorname{curl} \operatorname{curl} \boldsymbol{\mathcal{E}} = -\frac{1}{c^2} \hat{\epsilon} \partial_t^2 \boldsymbol{\mathcal{E}}, \quad \operatorname{curl} \hat{\epsilon}^{-1} \operatorname{curl} \boldsymbol{\mathcal{H}} = -\frac{1}{c^2} \partial_t^2 \boldsymbol{\mathcal{H}}, \\ & \boldsymbol{\mathcal{E}}(x, y, z, t) \in \mathbb{R}^3, \ \boldsymbol{\mathcal{H}}(x, y, z, t) \in \mathbb{R}^3. \end{aligned}$$

Time domain solver:

Given $\hat{\epsilon}$ and an optical "influx" signal, find \mathcal{E} , \mathcal{H} on a computational domain within a certain time interval, subject to suitable boundary conditions.

Fourier transform with respect to time *~~* Spectral data.

 $\partial_y \hat{\epsilon} = 0, \ \partial_y \tilde{E} = 0, \ \partial_y \tilde{H} = 0;$ equations split into two subsets:

TE,
$$\tilde{E}_y$$
, \tilde{H}_x , and \tilde{H}_z , principal component \tilde{E}_y :
 $i\omega\mu_0\tilde{H}_x = \partial_z\tilde{E}_y$, $i\omega\mu_0\tilde{H}_z = -\partial_x\tilde{E}_y$, $i\omega\epsilon_0\epsilon\tilde{E}_y = \partial_z\tilde{H}_x - \partial_x\tilde{H}_z$, or
 $\partial_x^2\tilde{E}_y$, $+\partial_z^2\tilde{E}_y + k^2\epsilon\tilde{E}_y = 0$.

TM,
$$\tilde{H}_y$$
, \tilde{E}_x , and \tilde{E}_z , principal component \tilde{H}_y :
 $i\omega\epsilon_0\epsilon\tilde{E}_x = -\partial_z\tilde{H}_y$, $i\omega\epsilon_0\epsilon\tilde{E}_z = \partial_x\tilde{H}_y$, $-i\omega\mu_0\tilde{H}_y = \partial_z\tilde{E}_x - \partial_x\tilde{E}_z$, or
 $e^{-1}e^{-\tilde{\mu}}e^{-1}e^{-\tilde{\mu}}e^{-2\tilde{\mu}}e^$

$$\partial_x \frac{1}{\epsilon} \partial_x \tilde{H}_y, + \partial_z \frac{1}{\epsilon} \partial_z \tilde{H}_y + k^2 \tilde{H}_y = 0.$$

$$\partial_z \hat{\epsilon} = 0, \ \partial_z n = 0,$$

modal solutions with profile E, H, and propagation constant β :



$$\mathcal{E}(x, y, z, t) = \operatorname{Re} \mathbf{E}(x, y) \operatorname{e}^{\operatorname{i} \omega t - \operatorname{i} \beta z}, \quad \mathcal{H}(x, y, z, t) = \operatorname{Re} \mathbf{H}(x, y) \operatorname{e}^{\operatorname{i} \omega t - \operatorname{i} \beta z}.$$

Guided modes:
$$\iint |\mathbf{E}|^2 \mathrm{d} x \, \mathrm{d} y < \infty, \quad \iint |\mathbf{H}|^2 \mathrm{d} x \, \mathrm{d} y < \infty.$$

Mode solver: Eigenvalue problem for E, H, and β .

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modal solutions with profile E, H, and propagation constant β :

$$\begin{array}{c|c} & x, y \\ \hline & \\ & \\ \hline & \\ n(x) \\ n(x, y) \end{array} \end{array} \begin{array}{c} \\ z \end{array}$$

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Mode solver: Eigenvalue problem for E, H, and β .

- Basis for all kinds of design considerations,
- Basis fields for various types of perturbational simulations,
- Input / output fields for Helmholtz & time domain solvers.

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Semianalytical treatment of 2D rectangular Helmholtz problems

TE:
$$\tilde{E}_y, \tilde{H}_x, \tilde{H}_z; \quad \partial_x^2 \tilde{E}_y, + \partial_z^2 \tilde{E}_y + k^2 \epsilon \tilde{E}_y = 0.$$

TM: $\tilde{H}_y, \tilde{E}_x, \tilde{E}_z; \quad \partial_x \frac{1}{\epsilon} \partial_x \tilde{H}_y, + \partial_z \frac{1}{\epsilon} \partial_z \tilde{H}_y + k^2 \tilde{H}_y = 0.$
 $\left| \begin{array}{c} \omega, \lambda \end{array} \right|_{\omega, \lambda}$



• Piecewise constant, rectangular refractive index distribution; linear, lossless materials.

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- Piecewise constant, rectangular refractive index distribution; linear, lossless materials.
- Rectangular interior computational domain, influx & outflux across all four boundaries, external regions are homogeneous along x or z.

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TM: $\tilde{H}_y, \tilde{E}_x, \tilde{E}_z; \quad \partial_x \frac{1}{\epsilon} \partial_x \tilde{H}_y, + \partial_z \frac{1}{\epsilon} \partial_z \tilde{H}_y + k^2 \tilde{H}_y = 0.$
 $\left| \begin{array}{c} \omega, \lambda \end{array} \right|_{\omega, \lambda}$



- Piecewise constant, rectangular refractive index distribution; linear, lossless materials.
- Rectangular interior computational domain, influx & outflux across all four boundaries, external regions are homogeneous along x or z.
- Assumption $E_y = 0$, $H_y = 0$ on the corner points and on the external border lines is reasonable for the problems under investigation.

Basis fields, defined by Dirichlet boundary conditions $E_y = 0$ (TE) or $H_y = 0$ (TM):



Horizontally traveling eigenmodes:

 M_z profiles $\boldsymbol{\psi}_{s,m}^d(x)$ and propagation constants $\pm \beta_{s,m}$

of order m, on slice s, for propagation directions d = f, b, Basis fields, defined by Dirichlet boundary conditions $E_y = 0$ (TE) or $H_y = 0$ (TM):



... and vertically traveling fields:

 M_x profiles $\boldsymbol{\phi}_{l,m}^d(z)$ and propagation constants $\pm \gamma_{l,m}$

of order m, on layer l, for propagation directions d = u, d.

Ansatz for the optical field, ÷ for $z_{s-1} \le z \le z_s$, $s = 1, ..., N_z$, and $x_{l-1} \le x \le x_l, l = 1, ..., N_x$: x_0 2 $\binom{\boldsymbol{\mathcal{E}}}{\boldsymbol{\mathcal{H}}}(x,z,t) = \operatorname{Re}\left\{\sum_{n=1}^{M_{z}-1} F_{s,m}\boldsymbol{\psi}_{s,m}^{\mathrm{f}}(x) \,\mathrm{e}^{-\mathrm{i}\beta_{s,m}(z-z_{s-1})}\right\}$ z_1 $M_z - 1$ + $\sum B_{s,m} \psi^{\mathrm{b}}_{s,m}(x) \mathrm{e}^{+\mathrm{i}\beta_{s,m}(z-z_s)}$ m = 0 $M_r - 1$ + $\sum U_{l,m} \phi^{\rm u}_{l,m}(z) e^{-i \gamma_{l,m}(x-x_{l-1})}$ m=0 $M_x - 1$ $+\sum_{n=1}^{\infty} D_{l,m}\phi_{l,m}^{d}(z) e^{+i\gamma_{l,m}(x-x_l)} \bigg\} e^{i\omega t}.$ m=015



Mode products \leftrightarrow normalization, projection:

$$(\boldsymbol{E}_{1}, \boldsymbol{H}_{1}; \boldsymbol{E}_{2}, \boldsymbol{H}_{2})_{x} = \frac{1}{4} \int (E_{1,x}^{*} H_{2,y} - E_{1,y}^{*} H_{2,x} + H_{1,y}^{*} E_{2,x} - H_{1,x}^{*} E_{2,y}) dx,$$

$$(\boldsymbol{E}_{1}, \boldsymbol{H}_{1}; \boldsymbol{E}_{2}, \boldsymbol{H}_{2})_{z} = \frac{1}{4} \int (E_{1,y}^{*} H_{2,z} - E_{1,z}^{*} H_{2,y} + H_{1,z}^{*} E_{2,y} - H_{1,y}^{*} E_{2,z}) dz.$$

Algebraic procedure



- Consistent bidirectional projection at all interfaces \longrightarrow linear system of equations in $\{F_{s,m}, B_{s,m}, U_{l,m}, D_{l,m}\}$.
- Influx: F_0 , B_{N_x+1} , U_0 , $D_{N_z+1} \longrightarrow \text{RHS}$.
- Outflux: B_0 , F_{N_x+1} , D_0 , U_{N_z+1} .

Algebraic procedure

• "Exact" mode profiles —> interior problems decouple:



Solve for F_2, \ldots, F_{N_z} and B_1, \ldots, B_{N_z-1} in terms of F_1 and B_{N_z} \longrightarrow BEP.

Solve for U_2, \ldots, U_{N_x} and D_1, \ldots, D_{N_x-1} in terms of U_1 and $D_{N_x} \longrightarrow$ BEP.

• Continuity of *E* and *H* on outer interfaces:



Interior BEP solutions + equations at $z = z_0, z_{N_z}, x = x_0, x_{N_x}$ $\longrightarrow B_0, F_{N_x+1}, D_0, U_{N_z+1}.$

"QUadridirectional Eigenmode Propagation method" (QUEP).

Gaussian beams in free space



Gaussian beams in free space



Gaussian beams in free space

 $M_x = M_z = 150.$



Top: $4 \,\mu\text{m}$ beam width, 10° tilt angle, $2 \,\mu\text{m}$ offset bottom: 45° tilt angle, initially centered beams.

Bragg grating: COST268 benchmark problem



 $x \in [-4, 2] \mu m$, 60 modes (QUEP, BEP $E_y = 0$ b.c.), $z \in [-1.8, 10.185] \mu m$, 120 modes (QUEP). *J. Čtyroký et. al., Optical and Quantum Electronics **34**, 455–470, 2002; reference: BEP2 (PML b.c.).

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Waveguide crossings



 $n_{\rm g} = 3.4, \ n_{\rm b} = 1.45, \ \lambda = 1.55 \,\mu\text{m}, \ h = 0.2 \,\mu\text{m}, \ \text{TE}, \ x, z \in [-3, 3] \,\mu\text{m}, \ M_x = M_z = 120.$ Power conservation: error $< 10^{-3}$.

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Waveguide crossings



Square resonator with perpendicular ports



 $n_{\rm g} = 3.4, \ n_{\rm b} = 1.0, \ W = 1.786 \ \mu\text{m}, \ w = 0.1 \ \mu\text{m}, \ g_{\rm h} = 0.355 \ \mu\text{m}, \ g_{\rm v} = 0.385 \ \mu\text{m}, \ q = 0.355 \ \mu\text{m}, \ T\text{E}, \ x, z \in [-4, 4] \ \mu\text{m}, \ M_x = M_z = 100.$

Square resonator with perpendicular ports



Photonic crystal bend



 $n_{\rm r} = 3.4, \ n_{\rm b} = 1.0, \ r = 0.15 \,\mu{\rm m}, \ p = 0.6 \,\mu{\rm m}, \ n_{\rm g} = 1.8, \ w = 0.5 \,\mu{\rm m}, \ N_{\rm r} = 4,^*$ TE, $x, z \in [-1, 5.95] \,\mu{\rm m}, \ M_x = M_z = 120.$

* R. Stoffer et. al., Optical and Quantum Electronics 32, 947–961, 2000
J. D. Joannopoulos et. al., *Photonic crystals: Molding the Flow of Light*, Princeton UP, New Jersey, 1995.

Photonic crystal bend



$$\begin{split} n_{\rm r} &= 3.4, \ n_{\rm b} = 1.0, \ r = 0.15\,\mu{\rm m}, \ p = 0.6\,\mu{\rm m}, \ n_{\rm g} = 1.8, \ w = 0.5\,\mu{\rm m}, \ N_{\rm r} = 4,^* \\ {\rm TE}, \ x, z \in [-1, 5.95]\,\mu{\rm m}, \ M_x = M_z = 120. \end{split}$$

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QUEP scheme:

- Eigenmode expansion technique, 2D Helmholtz problems with piecewise constant, rectangular permittivity.
- Equivalent treatment of the propagation along the two relevant axes.
- Way to realize transparent boundaries for the interior region on a cross-shaped computational domain.
- Basis modes can be restricted to simple Dirichlet boundary conditions.
- Examples, C++-sources: http://www.math.utwente.nl/~hammerm/Metric/



