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
Abstract scattering problem

Typical parameters:
- Vacuum wavelength \( \lambda \in [400, 700] \text{ nm} \) (visible light), \( \lambda \approx 1.3 \text{ \( \mu \text{m} \)}, 1.55 \text{ \( \mu \text{m} \)} \) (optical fibers, attenuation min.).
- Refractive indices \( n \in [1, 3.4] \), small attenuation (transparent dielectrics).

- 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 \( \leftrightarrow \) Boundary conditions.
Simulations in integrated optics, brief general remarks
  - 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
Macroscopic Maxwell equations

... for electromagnetic fields

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

\( \tilde{B}, \tilde{B}, \tilde{D}, \tilde{D}, \tilde{H}, \tilde{H}, \tilde{P}, \tilde{P}, \tilde{M}, \tilde{M}, \omega = kc = 2\pi c / \lambda, \)

in frequency domain form (SI):

\[ \text{curl} \, \tilde{E} = -i\omega \tilde{B}, \quad \text{curl} \, \tilde{H} = i\omega \tilde{D}, \quad \text{div} \, \tilde{D} = 0, \quad \text{div} \, \tilde{B} = 0, \]

\[ \tilde{B} = \mu_0 (\tilde{H} + \tilde{M}), \quad \tilde{D} = \epsilon_0 \tilde{E} + \tilde{P}. \]
Macrosopic Maxwell equations

... for electromagnetic fields

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

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

in frequency domain form (SI):

\[
\begin{align*}
\text{curl } \tilde{\mathcal{E}} &= -i\omega \tilde{\mathcal{B}}, \\
\text{curl } \tilde{\mathcal{H}} &= i\omega \tilde{\mathcal{D}}, \\
\text{div } \tilde{\mathcal{D}} &= 0, \\
\text{div } \tilde{\mathcal{B}} &= 0,
\end{align*}
\]

\[ \tilde{\mathcal{B}} = \mu_0(\tilde{\mathcal{H}} + \tilde{\mathcal{M}}), \quad \tilde{\mathcal{D}} = \epsilon_0 \tilde{\mathcal{E}} + \tilde{\mathcal{P}}. \]

Typical media:

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

\[ \tilde{P}_j = \epsilon_0 \left( \sum_k \chi^{(1)}_{j,k} \tilde{E}_k + \sum_{k,l} \chi^{(2)}_{j,k,l} \tilde{E}_k \tilde{E}_l + \sum_{k,l,m} \chi^{(3)}_{j,k,l,m} \tilde{E}_k \tilde{E}_l \tilde{E}_m \ldots \right). \]

Convention: Eliminate \( \tilde{\mathcal{D}} \) and \( \tilde{\mathcal{B}} \) Formulation in \( \tilde{\mathcal{E}} \) and \( \tilde{\mathcal{H}}. \)
**Linear problems**

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

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

Simplest case: Isotropic, lossless dielectrics; refractive index \(n\):

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

Frequently \(n\) is piecewise constant \(\Longleftrightarrow\) Interface conditions for \(\tilde{E}, \tilde{H}\).
**Linear problems**

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

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Simplest case: Isotropic, lossless dielectrics; refractive index \( n : \)

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

Frequently \( n \) is piecewise constant \( \iff \) Interface conditions for \( \tilde{E}, \tilde{H} \).

Complications:

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

Continuous wave excitation, $\omega$ a given parameter:

$$\begin{align*}
curl \tilde{E} &= -i\omega\mu_0\tilde{H}, \\
curl \tilde{H} &= i\omega\varepsilon_0\hat{\varepsilon}\tilde{E}, \\
\text{div } \hat{\varepsilon}\tilde{E} &= 0, \\
\text{div } \tilde{H} &= 0,
\end{align*}$$
or

$$\begin{align*}
curl \text{curl } \tilde{E} &= k^2\hat{\varepsilon}\tilde{E}, \\
\text{curl } \hat{\varepsilon}^{-1}\text{curl } \tilde{H} &= k^2\tilde{H},
\end{align*}$$

\(\tilde{E}(x, y, z) \in \mathbb{C}^3, \quad \tilde{H}(x, y, z) \in \mathbb{C}^3.\)

Helmholtz solver:

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

Scans over $\omega \quad \leadsto$ Spectral data.


**Time dependent modeling**

Propagation of time dependent signals, pulsed excitation:

\[
\text{curl } \mathbf{E} = -\mu_0 \partial_t \mathbf{H}, \quad \text{curl } \mathbf{H} = \epsilon_0 \hat{\epsilon} \partial_t \mathbf{E}, \quad \text{div } \hat{\epsilon} \mathbf{E} = 0, \quad \text{div } \mathbf{H} = 0,
\]

or

\[
\text{curl curl } \mathbf{E} = -\frac{1}{c^2} \hat{\epsilon} \partial_t^2 \mathbf{E}, \quad \text{curl } \hat{\epsilon}^{-1} \text{curl } \mathbf{H} = -\frac{1}{c^2} \partial_t^2 \mathbf{H},
\]

\(\mathbf{E}(x, y, z, t) \in \mathbb{R}^3, \quad \mathbf{H}(x, y, z, t) \in \mathbb{R}^3.\)

**Time domain solver:**

Given \(\hat{\epsilon}\) and an optical “influx” signal, find \(\mathbf{E}, \mathbf{H}\) on a computational domain within a certain time interval, subject to suitable boundary conditions.

Fourier transform with respect to time \(\sim\) Spectral data.
2D problems

\[ \partial_y \hat{e} = 0, \ \partial_y \tilde{E} = 0, \ \partial_y \tilde{H} = 0; \] equations split into two subsets:

**TE, \ \tilde{E}_y, \ \tilde{H}_x, \ and \ \tilde{H}_z, \ principal \ component \ \tilde{E}_y:**

\[ i \omega \mu_0 \tilde{H}_x = \partial_z \tilde{E}_y, \quad i \omega \mu_0 \tilde{H}_z = -\partial_x \tilde{E}_y, \quad i \omega \epsilon_0 \epsilon \tilde{E}_y = \partial_z \tilde{H}_x - \partial_x \tilde{H}_z, \]

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:**

\[ i \omega \epsilon_0 \epsilon \tilde{E}_x = -\partial_z \tilde{H}_y, \quad i \omega \epsilon_0 \epsilon \tilde{E}_z = \partial_x \tilde{H}_y, \quad -i \omega \mu_0 \tilde{H}_y = \partial_z \tilde{E}_x - \partial_x \tilde{E}_z, \]

or

\[ \partial_x \frac{1}{\epsilon} \partial_x \tilde{H}_y + \partial_z \frac{1}{\epsilon} \partial_z \tilde{H}_y + k^2 \tilde{H}_y = 0. \]
Dielectric waveguides

\[ \partial_z \hat{\epsilon} = 0, \quad \partial_z n = 0, \]

modal solutions with profile \( E, H \), and propagation constant \( \beta \):

\[ E(x, y, z, t) = \text{Re} E(x, y) e^{i \omega t - i \beta z}, \quad H(x, y, z, t) = \text{Re} H(x, y) e^{i \omega t - i \beta z}. \]

Guided modes: \( \iint |E|^2 \, dx \, dy < \infty, \quad \iint |H|^2 \, dx \, dy < \infty. \)

Mode solver: Eigenvalue problem for \( E, H \), and \( \beta \).
**Dielectric waveguides**

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profile \( E, H \), and propagation constant \( \beta \):

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**Mode solver:** Eigenvalue problem for \( E, H, \) and \( \beta \).

- 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: \[ \vec{E}_y, \vec{H}_x, \vec{H}_z; \quad \partial_x^2 \vec{E}_y, + \partial_z^2 \vec{E}_y + k^2 \epsilon \vec{E}_y = 0. \]

TM: \[ \vec{H}_y, \vec{E}_x, \vec{E}_z; \quad \partial_x \frac{1}{\epsilon} \partial_x \vec{H}_y, + \partial_z \frac{1}{\epsilon} \partial_z \vec{H}_y + k^2 \vec{H}_y = 0. \]

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

\[ \omega, \lambda \]
Semianalytical treatment of 2D rectangular Helmholtz problems

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

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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 \( z \).
Semianalytical treatment of 2D rectangular Helmholtz problems

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

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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 \(z\).
- Assumption \(E_y = 0, H_y = 0\) on the corner points and on the external border lines is reasonable for the problems under investigation.
**Modal basis fields**

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

Horizontally traveling eigenmodes:

- $M_z$ profiles
- and propagation constants $\pm \beta_{s,m}$

of order $m$, on slice $s$, for propagation directions $d = f, b,$
**Modal basis fields**

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

... and vertically traveling fields:

<table>
<thead>
<tr>
<th>$M_x$ profiles</th>
<th>$\phi_{l,m}^d(z)$</th>
</tr>
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<tbody>
<tr>
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<td>$\pm \gamma_{l,m}$</td>
</tr>
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</table>

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


Eigenmode expansion

Ansatz for the optical field,
for $z_{s-1} \leq z \leq z_s$, $s = 1, \ldots, N_z$,
and $x_{l-1} \leq x \leq x_l$, $l = 1, \ldots, N_x$:

$$
\left( \mathcal{E} \right)(x, z, t) = \text{Re} \left\{ \sum_{m=0}^{M_z-1} F_{s,m} \psi_{s,m}^f(x) e^{-i\beta_{s,m}(z-z_{s-1})} \\
+ \sum_{m=0}^{M_z-1} B_{s,m} \psi_{s,m}^b(x) e^{i\beta_{s,m}(z-z_{s})} \\
+ \sum_{m=0}^{M_x-1} U_{l,m} \phi_{l,m}^u(z) e^{-i\gamma_{l,m}(x-x_{l-1})} \\
+ \sum_{m=0}^{M_x-1} D_{l,m} \phi_{l,m}^d(z) e^{i\gamma_{l,m}(x-x_{l})} \right\} e^{i\omega t}. 
$$
Mode products $\leftrightarrow$ normalization, projection:

$$(E_1, H_1; E_2, H_2)_x = \frac{1}{4} \int (E^*_1, x H_2, y - E^*_1, y H_2, x + H^*_1, y E_2, x - H^*_1, x E_2, y) \, dx,$$

$$(E_1, H_1; E_2, H_2)_z = \frac{1}{4} \int (E^*_1, y H_2, z - E^*_1, z H_2, y + H^*_1, z E_2, y - H^*_1, y E_2, z) \, dz.$$
Algebraic procedure

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

- “Exact” mode profiles $\rightarrow$ 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 $B_{N_z} \rightarrow$ BEP.

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

- Continuity of $E$ and $H$ on outer interfaces:

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

“QUadridirectional Eigenmode Propagation method” (QUEP).
Gaussian beams in free space

\[ E_y(x, z) : \]

\( n = 1.0, \ \lambda = 1.0 \mu m, \)

TE polarization,

\( x, z \in [0, 15.1] \mu m, \)

\( M_x = M_z = 150. \)

Top: 4 \( \mu m \) beam width, 10° tilt angle, 2 \( \mu m \) offset;
**Gaussian beams in free space**

$E_y(x, z)$:

$n = 1.0$, $\lambda = 1.0 \, \mu m$, TE polarization, $x, z \in [0, 15.1] \, \mu m$, $M_x = M_z = 150$. 

Top: 4 $\mu m$ beam width, $10^\circ$ tilt angle, 2 $\mu m$ offset;
**Gaussian beams in free space**

\[ n = 1.0, \quad \lambda = 1.0 \, \mu m, \]

TE polarization,

\[ x, z \in [0, 15.1] \, \mu m, \]

\[ M_x = M_z = 150. \]

\[ E_y(x, z): \]

Top: 4 \, \mu m beam width, 10° tilt angle, 2 \, \mu m offset;

bottom: 45° tilt angle, initially centered beams.
Bragg grating: COST268 benchmark problem

\[ \begin{align*}
\text{BEP, b.c. } E_y &= 0 \\
\lambda &= [0.8, 1.8] \text{ [\mu m]} \\
P_{R,T} &\quad \text{100 modes (QUEP, BEP)}
\end{align*} \]

\( x \in [-4, 2] \text{ [\mu m]}, \) 60 modes (QUEP, BEP \( E_y = 0 \) b.c.), \( z \in [-1.8, 10.185] \text{ [\mu m]}, \) 120 modes (QUEP).

\(^*\) J. Čtyroký et. al., Optical and Quantum Electronics 34, 455–470, 2002; reference: BEP2 (PML b.c.).
Bragg grating: COST268 benchmark problem

$(\star)$

$d_g = 0.500 \mu m,$
$d_e = 0.125 \mu m,$
$n_s \approx 1.45 (\text{SiO}_2),$
$n_g \approx 1.99 (\text{Si}_3\text{N}_4),$
$n_a = 1.0,$
$\Lambda = 0.430 \mu m,$
$g = \frac{\Lambda}{2}, \quad N_g = 20.$

$x \in [-4, 2] \mu m,$ 60 modes (QUEP, BEP $E_y = 0$ b.c.), $z \in [-1.8, 10.185] \mu m,$ 120 modes (QUEP).

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Bragg grating: COST268 benchmark problem

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\( n_g \approx 1.99 \) (Si\(_3\)N\(_4\)),

\( n_a = 1.0 \),

\( \Lambda = 0.430 \, \mu m \),

\( g = \Lambda / 2 \), \( N_g = 20 \).

\( x \in [-4, 2] \, \mu m \), 60 modes (QUEP, BEP \( E_y = 0 \) b.c.),

\( z \in [-1.8, 10.185] \, \mu m \), 120 modes (QUEP).

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Waveguide crossings

\[ n_g = 3.4, \ n_b = 1.45, \ \lambda = 1.55 \mu m, \ h = 0.2 \mu m, \ TE, \ x, z \in [-3, 3] \mu m, \ M_x = M_z = 120. \]

Power conservation: error < $10^{-3}$. 
Waveguide crossings

\[ n_g = 3.4, \ n_b = 1.45, \ \lambda = 1.55 \, \mu m, \ h = 0.2 \, \mu m, \ TE, \ x, z \in [-3, 3] \, \mu m, \ M_x = M_z = 120. \]

Power conservation: error < 10^{-3}.  

Waveguide crossings
**Square resonator with perpendicular ports**

\[ n_g = 3.4, \quad n_b = 1.0, \quad W = 1.786 \, \mu\text{m}, \quad w = 0.1 \, \mu\text{m}, \quad g_h = 0.355 \, \mu\text{m}, \quad g_v = 0.385 \, \mu\text{m}, \quad q = 0.355 \, \mu\text{m}, \]

TE, \( x, z \in [-4, 4] \, \mu\text{m}, \quad M_x = M_z = 100. \]
Square resonator with perpendicular ports

\[ n_g = 3.4, \quad n_b = 1.0, \quad W = 1.786 \, \mu m, \quad w = 0.1 \, \mu m, \]
\[ g_h = 0.355 \, \mu m, \quad g_v = 0.385 \, \mu m, \quad q = 0.355 \, \mu m, \]
TE, \( x, z \in [-4, 4] \, \mu m, \quad M_x = M_z = 100. \]
\[ \lambda = 1.55 \, \mu m, \quad T = 5.17 \, \text{fs}, \quad E_y(x, z, t): \]
Photonic crystal bend

\[ n_r = 3.4, \quad n_b = 1.0, \quad r = 0.15 \, \mu m, \quad p = 0.6 \, \mu m, \quad n_g = 1.8, \quad w = 0.5 \, \mu m, \quad N_r = 4, * \]

TE, \( x, z \in [-1, 5.95] \, \mu m, \quad M_x = M_z = 120. \)

* R. Stoffer et. al., Optical and Quantum Electronics 32, 947–961, 2000

Photonic crystal bend

\[ n_T = 3.4, \; n_b = 1.0, \; r = 0.15 \, \mu m, \; p = 0.6 \, \mu m, \; n_g = 1.8, \; w = 0.5 \, \mu m, \; N_r = 4,^* \]

TE, \( x, z \in [-1, 5.95] \, \mu m, \; M_x = M_z = 120. \)

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Photonic crystal bend

\[ \lambda = 1.461 \, \mu m \]

\[ \lambda = 1.551 \, \mu m \]
Quadridirectional mode expansion

**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/](http://www.math.utwente.nl/~hammerm/Metric/)