A variational formulation of guided wave scattering problems
— hybrid analytic / numerical coupled mode modeling of guided wave devices —

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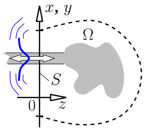
1 Guided wave scattering problems

A functional of the six electromagnetic field components is proposed for 2-D / 3-D frequency domain problems in integrated optics. Stationarity implies that the Maxwell equations in the interior of the domain of interest and transparent influx conditions for incoming waveguides on its boundary port planes are satisfied. This constitutes a variational basis for rigorous numerical treatments of the scattering problems, but also for more approximate modeling: A generalized version of coupled mode theory can be derived by restricting the functional to suitable field templates [8].



Abstract scattering problem

The boundary $\partial\Omega$ of the domain of interest Ω includes an exemplary port plane S. Axes x and y of a local coordinate system span S, the z-axis is oriented towards the interior of Ω. Incoming waveguides are parallel to the z-axis, i.e. the exterior is z-homogeneous. Within Ω, the source-free frequency domain Maxwell equations for the optical electric field $\boldsymbol{E}$ and magnetic field $\boldsymbol{H}$ are to be solved:

$$\nabla\times\boldsymbol{H} - \mathrm{i}\omega\epsilon_0\epsilon\boldsymbol{E} = 0\,, \qquad -\nabla\times\boldsymbol{E} - \mathrm{i}\omega\mu_0\boldsymbol{H} = 0\,; \tag{1}$$

ω: given real angular frequency; ϵ_0, μ_0: vacuum permittivity and permeability; the relative permittivity $\epsilon(x,y,z) = n^2(x,y,z)$ includes the geometry and material properties.

Transparent boundary conditions [3, 4, 5, 8] have to be specified on the port plane S that permit guided and nonguided waves from inside Ω to pass through S towards the exterior, and that allow to prescribe optical influx on S, e.g. in the form of modal amplitudes of inward traveling waves.

2 Transparent influx boundary conditions

. . . for inhomogeneous exterior: incoming waveguides. Preliminaries:

- Complete set of normal modes on S, profiles $(\tilde{\boldsymbol{E}}_m, \pm\tilde{\boldsymbol{H}}_m)(x,y)$ ⟷ propagation along $\pm z$, toward the interior/exterior of Ω.
- Bilinear product on S:

$$\langle\boldsymbol{A},\boldsymbol{B}\rangle = \iint_S (\boldsymbol{A}\times\boldsymbol{B})\cdot\boldsymbol{e}_z\,\mathrm{d}x\,\mathrm{d}y\,. \tag{2}$$

- Modal orthogonality properties

$$\langle\tilde{\boldsymbol{E}}_l,\tilde{\boldsymbol{H}}_k\rangle = \delta_{lk}N_k\,, \quad \text{with nonzero} \quad N_k = \langle\tilde{\boldsymbol{E}}_k,\tilde{\boldsymbol{H}}_k\rangle\,. \tag{3}$$

- "Any" electric field $\boldsymbol{E}$ and magnetic field $\boldsymbol{H}$ on S can be expanded as

$$\boldsymbol{E} = \sum_m e_m\tilde{\boldsymbol{E}}_m \quad \text{and} \quad \boldsymbol{H} = \sum_m h_m\tilde{\boldsymbol{H}}_m \tag{4}$$

with coefficients $e_m = \langle\boldsymbol{E},\tilde{\boldsymbol{H}}_m\rangle/N_m$, $h_m = \langle\tilde{\boldsymbol{E}}_m,\boldsymbol{H}\rangle/N_m$, alternatively as

$$\begin{pmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{pmatrix} = \sum_m f_m\begin{pmatrix}\tilde{\boldsymbol{E}}_m\\ \tilde{\boldsymbol{H}}_m\end{pmatrix} + \sum_m b_m\begin{pmatrix}\tilde{\boldsymbol{E}}_m\\ -\tilde{\boldsymbol{H}}_m\end{pmatrix}. \tag{5}$$

with $f_m = (e_m + h_m)/2$, $b_m = (e_m - h_m)/2$ (transverse components only).

Transparent influx boundary conditions (TIBCs) [8] on S:

$$\begin{aligned}\boldsymbol{E} &= \sum_m 2F_m\tilde{\boldsymbol{E}}_m - \sum_m\frac{1}{N_m}\langle\tilde{\boldsymbol{E}}_m,\boldsymbol{H}\rangle\tilde{\boldsymbol{E}}_m\,,\\ \boldsymbol{H} &= \sum_m 2F_m\tilde{\boldsymbol{H}}_m - \sum_m\frac{1}{N_m}\langle\boldsymbol{E},\tilde{\boldsymbol{H}}_m\rangle\tilde{\boldsymbol{H}}_m\,;\end{aligned} \tag{6}$$

F_m: influx, given coefficients of incoming waves.

↪ For a general field (5), Eqs. (6) require $f_m = F_m$, while b_m can be arbitrary.

3 Variational form of the scattering problem

. . . based on a functional [8] of the six electromagnetic field components:

$$\begin{aligned}\mathcal{F}(\boldsymbol{E},\boldsymbol{H}) = &\iiint_\Omega\{\boldsymbol{E}\cdot(\nabla\times\boldsymbol{H}) + \boldsymbol{H}\cdot(\nabla\times\boldsymbol{E})\\ &\quad - \mathrm{i}\omega\epsilon_0\epsilon\boldsymbol{E}^2 + \mathrm{i}\omega\mu_0\boldsymbol{H}^2\}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\\ &- \sum_m 2F_m\{\langle\tilde{\boldsymbol{E}}_m,\boldsymbol{H}\rangle - \langle\boldsymbol{E},\tilde{\boldsymbol{H}}_m\rangle\}\\ &+ \sum_m\frac{1}{2N_m}\{\langle\tilde{\boldsymbol{E}}_m,\boldsymbol{H}\rangle^2 - \langle\boldsymbol{E},\tilde{\boldsymbol{H}}_m\rangle^2\}\end{aligned} \tag{7}$$

(cf. [1, 4, 5], generalized to 3-D with inhomogeneous exterior).

First variation:

$$\begin{aligned}\delta\mathcal{F}(\delta\boldsymbol{E},\delta\boldsymbol{H};\boldsymbol{E},\boldsymbol{H}) = &\iiint_\Omega\{2\delta\boldsymbol{E}\cdot(\nabla\times\boldsymbol{H} - \mathrm{i}\omega\epsilon_0\epsilon\boldsymbol{E})\\ &\quad + 2\delta\boldsymbol{H}\cdot(\nabla\times\boldsymbol{E} + \mathrm{i}\omega\mu_0\boldsymbol{H})\}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\\ &+ \langle\boldsymbol{E} - \sum_m 2F_m\tilde{\boldsymbol{E}}_m + \sum_m\frac{1}{N_m}\langle\tilde{\boldsymbol{E}}_m,\boldsymbol{H}\rangle\tilde{\boldsymbol{E}}_m,\,\delta\boldsymbol{H}\rangle\\ &- \langle\delta\boldsymbol{E},\,\boldsymbol{H} - \sum_m 2F_m\tilde{\boldsymbol{H}}_m + \sum_m\frac{1}{N_m}\langle\boldsymbol{E},\tilde{\boldsymbol{H}}_m\rangle\tilde{\boldsymbol{H}}_m\rangle\\ &- \iint_{\partial\Omega\setminus S}\{(\boldsymbol{n}\times\boldsymbol{E})\cdot\delta\boldsymbol{H} + (\boldsymbol{n}\times\boldsymbol{H})\cdot\delta\boldsymbol{E}\}\,\mathrm{d}A\,.\end{aligned} \tag{8}$$

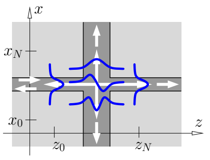
Stationarity $\delta\mathcal{F}(\delta\boldsymbol{E},\delta\boldsymbol{H};\boldsymbol{E},\boldsymbol{H}) = 0$ for arbitrary $\delta\boldsymbol{E}$, $\delta\boldsymbol{H}$ implies

- that $\boldsymbol{E}$, $\boldsymbol{H}$ satisfy the Maxwell equations (1) in Ω,
- that $\boldsymbol{E}$, $\boldsymbol{H}$ satisfy TIBCs (6) on S,
- and that transverse components of $\boldsymbol{E}$ and $\boldsymbol{H}$ vanish on $\partial\Omega\setminus S$.

4 Hybrid analytic/numerical coupled mode theory

Starting point: a plausible and convenient template [2] for the electromagnetic fields in the form of a reasonable superposition of known fields (typically modes of optical channels) with amplitudes that are functions of suitable propagation coordinate(s).

HCMT field template



Waveguide crossing, basis elements:

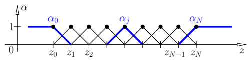
- guided modes of the horizontal WG $\boldsymbol{\psi}_m^{\mathrm{f,b}}(x,z) = \begin{pmatrix}\tilde{\boldsymbol{E}}\\ \tilde{\boldsymbol{H}}\end{pmatrix}_m^{\mathrm{f,b}}(x)\,\mathrm{e}^{\mp\mathrm{i}\beta_m^{\mathrm{f,b}}z}$,
- guided modes of the vertical WG $\boldsymbol{\psi}_m^{\mathrm{u,d}}(x,z) = \begin{pmatrix}\tilde{\boldsymbol{E}}\\ \tilde{\boldsymbol{H}}\end{pmatrix}_m^{\mathrm{u,d}}(z)\,\mathrm{e}^{\mp\mathrm{i}\beta_m^{\mathrm{u,d}}x}$
- (and further terms).

$$\begin{aligned}\begin{pmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{pmatrix}(x,z) = &\sum_m f_m(z)\boldsymbol{\psi}_m^{\mathrm{f}}(x,z) + \sum_m b_m(z)\boldsymbol{\psi}_m^{\mathrm{b}}(x,z)\\ &+ \sum_m u_m(x)\boldsymbol{\psi}_m^{\mathrm{u}}(x,z) + \sum_m d_m(x)\boldsymbol{\psi}_m^{\mathrm{d}}(x,z)\end{aligned} \tag{9}$$

f_m, b_m, u_m, d_m: ?

Amplitude functions, discretization

. . . by 1-D linear finite elements



$$f_m(z) = \sum_{j=0}^{N} f_{m,j}\,\alpha_j(z)\,, \qquad b_m(z),\ u_m(x),\ d_m(x) \text{ analogous.}$$

$$↪\quad \begin{pmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{pmatrix}(x,z) = \sum_k a_k\Big(\alpha_\cdot(\cdot)\boldsymbol{\psi}_\cdot^\cdot(x,z)\Big) =: \sum_k a_k\begin{pmatrix}\boldsymbol{E}_k\\ \boldsymbol{H}_k\end{pmatrix}(x,z), \tag{10}$$

$k\in\{\text{waveguides, modes, elements}\}$, $a_k\in\{f_{m,j}, b_{m,j}, u_{m,j}, d_{m,j}\}$.

5 Variational HCMT scheme

$$\mathcal{F}(\boldsymbol{E},\boldsymbol{H}) \xrightarrow{\ (\boldsymbol{E},\boldsymbol{H}) = \sum_k a_k(\boldsymbol{E}_k,\boldsymbol{H}_k)\ } \mathcal{F}_{\mathrm{r}}(\boldsymbol{a})$$

Restricted functional:

$$\mathcal{F}_{\mathrm{r}}(\boldsymbol{a}) = \sum_{l,k} a_l a_k F_{lk} + \sum_l a_l R_l + \sum_{l,k} a_l a_k B_{lk} = \boldsymbol{a}\cdot\mathsf{F}\boldsymbol{a} + \boldsymbol{R}\cdot\boldsymbol{a} + \boldsymbol{a}\cdot\mathsf{B}\boldsymbol{a} \tag{11}$$

$$\begin{aligned}F_{lk} = &\iiint_\Omega\{\boldsymbol{E}_l\cdot(\nabla\times\boldsymbol{H}_k) + \boldsymbol{H}_l\cdot(\nabla\times\boldsymbol{E}_k)\\ &\quad - \mathrm{i}\omega\epsilon_0\epsilon\boldsymbol{E}_l\cdot\boldsymbol{E}_k + \mathrm{i}\omega\mu_0\boldsymbol{H}_l\cdot\boldsymbol{H}_k\}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\end{aligned}$$

$$R_l = -\sum_m 2F_m\{\langle\tilde{\boldsymbol{E}}_m,\boldsymbol{H}_l\rangle - \langle\boldsymbol{E}_l,\tilde{\boldsymbol{H}}_m\rangle\}$$

$$B_{lk} = \sum_m\frac{1}{2N_m}\{\langle\tilde{\boldsymbol{E}}_m,\boldsymbol{H}_l\rangle\langle\tilde{\boldsymbol{E}}_m,\boldsymbol{H}_k\rangle - \langle\boldsymbol{E}_l,\tilde{\boldsymbol{H}}_m\rangle\langle\boldsymbol{E}_k,\tilde{\boldsymbol{H}}_m\rangle\}$$

+ contributions from port planes at $z = z_N$ and at $x = x_0, x_N$.

↪ Require $\delta\mathcal{F}_{\mathrm{r}} = \delta\boldsymbol{a}\cdot\big(((\mathsf{F}+\mathsf{B}) + (\mathsf{F}+\mathsf{B})^{\mathsf{T}})\,\boldsymbol{a} + \boldsymbol{R}\big) = 0$ for all $\delta\boldsymbol{a}$

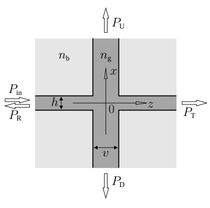
$$\mathsf{M}\boldsymbol{a} + \boldsymbol{R} = 0\,, \quad \text{with} \quad \mathsf{M} = \big((\mathsf{F}+\mathsf{B}) + (\mathsf{F}+\mathsf{B})^{\mathsf{T}}\big)\,. \tag{12}$$

Split $\boldsymbol{a} = (\boldsymbol{u},\boldsymbol{g})$ into given values and unknowns, divide M, $\boldsymbol{R}$ accordingly:

$$\mathsf{M}_{\mathrm{u}}\boldsymbol{u} = -\boldsymbol{h} \quad \text{with} \quad \mathsf{M}_{\mathrm{u}} = \begin{pmatrix}\mathsf{M}_{\mathrm{uu}}\\ \mathsf{M}_{\mathrm{gu}}\end{pmatrix}, \quad \boldsymbol{h} = \begin{pmatrix}\boldsymbol{R}_{\mathrm{u}}\\ \boldsymbol{R}_{\mathrm{g}}\end{pmatrix} + \begin{pmatrix}\mathsf{M}_{\mathrm{ug}}\\ \mathsf{M}_{\mathrm{gg}}\end{pmatrix}\boldsymbol{g} \quad \text{(overdetermined).}$$

Unknown coefficients $\boldsymbol{u}$ are found as solutions of $\mathsf{M}_{\mathrm{u}}^\dagger\mathsf{M}_{\mathrm{u}}\boldsymbol{u} = \mathsf{M}_{\mathrm{u}}^\dagger\boldsymbol{h}$. (V)

6 Waveguide crossing, results I

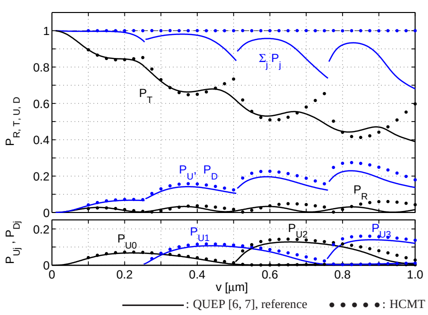


$n_{\mathrm{g}} = 3.4$, $n_{\mathrm{b}} = 1.45$, $\lambda = 1.55\,\mu$m, $h = 0.2\,\mu$m, variable v, TE polarization.

FEM discretization: $z\in[v/2 - 1.5\,\mu\mathrm{m}, v/2 + 1.5\,\mu\mathrm{m}]$, $x\in[w/2 - 1.5\,\mu\mathrm{m}, w/2 + 1.5\,\mu\mathrm{m}]$, $\Delta x = \Delta z = 0.025\,\mu$m.

Computational window: $z\in[-4\,\mu\mathrm{m}, 4\,\mu\mathrm{m}]$, $x\in[-4\,\mu\mathrm{m}, 4\,\mu\mathrm{m}]$.

Power transfer

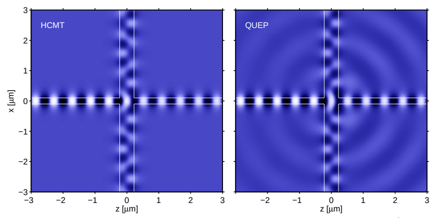


———: QUEP [6, 7], reference • • • • •: HCMT

7 Waveguide crossing, results II

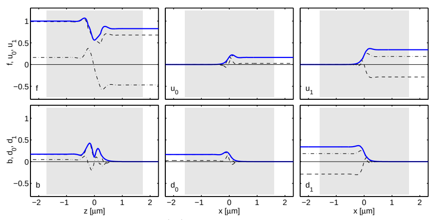
$v = 0.45\,\mu$m

Field snapshots



TE, E_y; QUEP: [6, 7], reference

Amplitude functions



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8 Alternative: Galerkin projection procedure

$$\begin{aligned}\nabla\times\boldsymbol{H} - \mathrm{i}\omega\epsilon_0\epsilon\boldsymbol{E} &= 0\\ -\nabla\times\boldsymbol{E} - \mathrm{i}\omega\mu_0\boldsymbol{H} &= 0\end{aligned} \quad \Big| \quad \cdot\begin{pmatrix}\boldsymbol{E}'\\ \boldsymbol{H}'\end{pmatrix}^*, \quad \iiint_\Omega \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

$$⟷\quad \iiint_\Omega \mathcal{K}(\boldsymbol{E}',\boldsymbol{H}';\boldsymbol{E},\boldsymbol{H})\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = 0 \quad \text{for all } \boldsymbol{E}',\ \boldsymbol{H}', \tag{13}$$

$$\begin{aligned}\mathcal{K}(\boldsymbol{E}',\boldsymbol{H}';\boldsymbol{E},\boldsymbol{H}) = &(\boldsymbol{E}')^*\cdot(\nabla\times\boldsymbol{H}) - (\boldsymbol{H}')^*\cdot(\nabla\times\boldsymbol{E})\\ &- \mathrm{i}\omega\epsilon_0\epsilon(\boldsymbol{E}')^*\cdot\boldsymbol{E} - \mathrm{i}\omega\mu_0(\boldsymbol{H}')^*\cdot\boldsymbol{H}\,.\end{aligned}$$

- Insert the HCMT template $\begin{pmatrix}\boldsymbol{E}\\ \boldsymbol{H}\end{pmatrix} = \sum_k a_k\begin{pmatrix}\boldsymbol{E}_k\\ \boldsymbol{H}_k\end{pmatrix}$,
- require $\iiint_\Omega \mathcal{K}(\boldsymbol{E}_l,\boldsymbol{H}_l;\boldsymbol{E},\boldsymbol{H})\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = 0$ for all modal elements l,
- compute $K_{lk} = \iiint_\Omega \mathcal{K}(\boldsymbol{E}_l,\boldsymbol{H}_l;\boldsymbol{E}_k,\boldsymbol{H}_k)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$,
- select $\boldsymbol{u}$: unknown coefficients, $\boldsymbol{g}$: given values related to prescribed influx,

$$↪\quad \begin{pmatrix}\mathsf{K}_{\mathrm{uu}} & \mathsf{K}_{\mathrm{ug}}\\ \mathsf{K}_{\mathrm{gu}} & \mathsf{K}_{\mathrm{gg}}\end{pmatrix}\begin{pmatrix}\boldsymbol{u}\\ \boldsymbol{g}\end{pmatrix} = 0\,, \quad \text{or} \quad \mathsf{K}_{\mathrm{u}}\boldsymbol{u} = -\mathsf{K}_{\mathrm{g}}\boldsymbol{g} \quad \text{with} \quad \mathsf{K}_{\mathrm{u}} = \begin{pmatrix}\mathsf{K}_{\mathrm{uu}}\\ \mathsf{K}_{\mathrm{gu}}\end{pmatrix}, \quad \mathsf{K}_{\mathrm{g}} = \begin{pmatrix}\mathsf{K}_{\mathrm{ug}}\\ \mathsf{K}_{\mathrm{gg}}\end{pmatrix}.$$

Least squares; unknowns $\boldsymbol{u}$ are solutions of $\mathsf{K}_{\mathrm{u}}^\dagger\mathsf{K}_{\mathrm{u}}\boldsymbol{u} = -\mathsf{K}_{\mathrm{u}}^\dagger\mathsf{K}_{\mathrm{g}}\boldsymbol{g}$. (G)

9 Comments

. . . concerning a comparison of the variational (V) and Galerkin scheme (G):

- Waveguide crossing: identical results of (V) and (G) on the scale of the figures.
- (V): TIBCs explicitly included, full mode expansions required in specific cases (not for the present HCMT example).
  (G): No boundary constraints, template with corresponding properties required.
- (V): Bidirectional versions of modal elements must be included in the template.
  (G): Where reasonable, unidirectional modal fields are sufficient (complex conjugates).
- The weak form (13) appears to be related to the functional [1]

$$\begin{aligned}\mathcal{C}(\boldsymbol{E},\boldsymbol{H}) = &\iiint_\Omega\{\boldsymbol{E}^*\cdot(\nabla\times\boldsymbol{H}) - \boldsymbol{H}^*\cdot(\nabla\times\boldsymbol{E})\\ &\quad - \mathrm{i}\omega\epsilon_0\epsilon\boldsymbol{E}^*\cdot\boldsymbol{E} + \mathrm{i}\omega\mu_0\boldsymbol{H}^*\cdot\boldsymbol{H}\}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\end{aligned} \tag{14}$$

up to boundary terms $-\iint_{\partial\Omega}\{(\boldsymbol{n}\times\boldsymbol{E}^*)\cdot\delta\boldsymbol{H} - (\boldsymbol{n}\times\boldsymbol{H}^*)\cdot\delta\boldsymbol{E}\}\,\mathrm{d}A$ in $\delta\mathcal{C}$.

?

- Extend $\mathcal{C}$ by boundary integrals such that the boundary terms in $\delta\mathcal{C}$ cancel ⟷ (G) could be viewed as a variational restriction of $\mathcal{C}$.
- Extend $\mathcal{C}$ by boundary integrals such that TIBCs are satisfied as natural boundary conditions if $\mathcal{C}$ becomes stationary ⟷ variational scheme with complex conjugate fields.

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