Computational photonics

— scattering problems in guided wave optics



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"Photonics is the science and technology of generating, controlling, and detecting photons, particularly in the visible light and near infra-red spectrum.

... quantum optics, ... optoelectronics ...

... the overlap between all these fields and optics is unclear, and different definitions are used in different parts of the world and in different industries.

... goal of establishing an electronics of photons instead of electrons.

... strong interest in optical communication ... usually based on laser light."

http://www.wikipedia.org

Outline

• Simulations in guided wave optics

- Macroscopic Maxwell equations
- Stationary and time-domain problems
- 2-D problems
- Modes of dielectric waveguides
- Quadridirectional eigenmode propagation
 - Problem setting
 - Eigenmode expansion
 - Algebraic procedure
- 2-D PSTM model
 - Probing evanescent fields
 - Hole defect in a slab waveguide
 - Waveguide Bragg grating: experiment & 2-D model
 - Resonant defect cavity
- Optical switching by NEMS-actuated resonator arrays

Abstract scattering problem



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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 (2-D, 3-D).
- Details: $\approx \lambda/10$, $\approx \lambda/100$.
- Influx and outflux: guided & nonguided waves ---- boundary conditions.

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- Details: $\approx \lambda/10$, $\approx \lambda/100$.
- Influx and outflux: guided & nonguided waves ---- boundary conditions.
- Emphasis: device concepts, design.

... for the electromagnetic fields

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

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

in frequency domain form, SI (source-free):

curl
$$E = -i\omega B$$
, curl $H = i\omega D$, div $D = 0$, div $B = 0$,
 $B = \mu_0 (H + M)$, $D = \epsilon_0 E + P$.

... for the electromagnetic fields

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, curl $\boldsymbol{H} = i\omega\boldsymbol{D}$, div $\boldsymbol{D} = 0$, div $\boldsymbol{B} = 0$,
 $\boldsymbol{B} = \mu_0(\boldsymbol{H} + \boldsymbol{M})$, $\boldsymbol{D} = \epsilon_0\boldsymbol{E} + \boldsymbol{P}$.

Typical media:

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

$$P_{j} = \epsilon_{0} \Big(\sum_{k} \chi_{j,k}^{(1)} E_{k} + \sum_{k,l} \chi_{j,k,l}^{(2)} E_{k} E_{l} + \sum_{k,l,m} \chi_{j,k,l,m}^{(3)} E_{k} E_{l} E_{m} \dots \Big).$$

Convention: eliminate D and $B \longrightarrow$ formulation in E and H.

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

 $\hat{\epsilon} = 1 + \hat{\chi}^{(1)}$: 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 \frown interface conditions for *E*, *H*.

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Frequently n is piecewise constant \triangleleft interface conditions for E, 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, $\hat{\chi}^{(2)}$, $\hat{\chi}^{(3)}$...

Continuous wave excitation, ω a given parameter:

 $\operatorname{curl} \boldsymbol{E} = -\mathrm{i}\omega\mu_0 \boldsymbol{H}, \quad \operatorname{curl} \boldsymbol{H} = \mathrm{i}\omega\epsilon_0 \hat{\epsilon} \boldsymbol{E}, \quad \operatorname{div} \hat{\epsilon} \boldsymbol{E} = 0, \quad \operatorname{div} \boldsymbol{H} = 0,$ or $\operatorname{curl} \operatorname{curl} \boldsymbol{E} = k^2 \hat{\epsilon} \boldsymbol{E}, \quad \operatorname{curl} \hat{\epsilon}^{-1} \operatorname{curl} \boldsymbol{H} = k^2 \boldsymbol{H},$ $\boldsymbol{E}(x, y, z) \in \mathbb{C}^3, \ \boldsymbol{H}(x, y, z) \in \mathbb{C}^3.$

Helmholtz solver:

Given $\hat{\epsilon}$ and an optical "influx", find E, 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 \longrightarrow spectral data.

 $\partial_y \epsilon = 0, \ \epsilon(x, z) = n^2(x, z),$ $\partial_y \mathbf{E} = 0, \ \partial_y \mathbf{H} = 0;$ equations split into two subsets:



TE, E_y , H_x , and H_z , principal component E_y : $i\omega\mu_0H_x = \partial_z E_y$, $i\omega\mu_0H_z = -\partial_x E_y$, $i\omega\epsilon_0\epsilon E_y = \partial_z H_x - \partial_x H_z$, or $\partial_x^2 E_y$, $+\partial_z^2 E_y + k^2\epsilon E_y = 0$.

TM, H_y , E_x , and E_z , principal component H_y : $i\omega\epsilon_0\epsilon E_x = -\partial_z H_y$, $i\omega\epsilon_0\epsilon E_z = \partial_x H_y$, $-i\omega\mu_0 H_y = \partial_z E_x - \partial_x E_z$, or

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

 $\partial_z \epsilon = 0, \ \partial_z n = 0, \text{ modal solutions with}$ profile \tilde{E}, \tilde{H} , and propagation constant β ; $E(x, y, z) = \tilde{E}(x, y) e^{-i\beta z},$ $H(x, y, z) = \tilde{H}(x, y) e^{-i\beta z}$:

$$\begin{array}{c|c} & & & \\ & & \\ \hline & & \\$$

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

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

Mode solver: Eigenvalue problem for \tilde{E} , \tilde{H} , and β .

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Mode solver: Eigenvalue problem for \tilde{E} , \tilde{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.

$$\begin{split} \left(\partial_x^2 + k^2 n^2(x)\right) \tilde{E}_y &= \beta^2 \tilde{E}_y \,, \quad \int |\tilde{E}_y|^2 \mathrm{d}x < \infty \,, \quad \tilde{H}_x = \frac{-\beta}{\omega\mu_0} \tilde{E}_y \,, \quad \tilde{H}_z = \frac{\mathrm{i}}{\omega\mu_0} \partial_x \tilde{E}_y \,, \\ \mathcal{E}(x, z, t) &= \mathrm{Re} \begin{pmatrix} 0\\ \tilde{E}_y\\ 0 \end{pmatrix} (x) \, \mathrm{e}^{\mathrm{i}\,\omega t \, - \, \mathrm{i}\,\beta z} \,, \quad \mathcal{H}(x, z, t) = \mathrm{Re} \begin{pmatrix} \tilde{H}_x\\ 0\\ \tilde{H}_z \end{pmatrix} (x) \, \mathrm{e}^{\mathrm{i}\,\omega t \, - \, \mathrm{i}\,\beta z} \,, \end{split}$$

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 $\beta_0/k = 1.923, \beta_1/k = 1.697.$

- Mode propagation
- "Coupling" of modes





$$\left(\partial_x^2 + k^2 n^2(x)\right) \tilde{E}_y = \beta^2 \tilde{E}_y, \qquad \int |\tilde{E}_y|^2 \mathrm{d}x < \infty.$$



$$\left(\partial_x^2 + k^2 n^2(x)\right) \tilde{E}_y = \beta^2 \tilde{E}_y, \quad \int_{x_0}^{x_1} |\tilde{E}_y|^2 \mathrm{d}x = 1, \quad \tilde{E}_y(x_0) = \tilde{E}_y(x_1) = 0.$$



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 $\{\beta_i, E_{y,i}\}$: complete discrete set of eigenmodes, expansion basis.

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- 2-D TE/TM Helmholtz problem, vacuum wavelength $\lambda = 2\pi/k$.
- Piecewise constant, rectangular refractive index distribution; linear, lossless materials.
- Rectangular interior computational domain, influx & outflux across all four boundaries, outwards homogeneous external regions.
- 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_x profiles	$\boldsymbol{\psi}^{d}_{s,m}(x)$
and propagation constants	$\pm eta_{s,m}$

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_z profiles	$\hat{oldsymbol{\psi}}^{d}_{l,m}(z)$
and propagation constants	$\pm \hat{eta}_{l,m}$

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





Mode products \leftrightarrow normalization, projection:

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

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

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 , $D_{N_z+1} \longrightarrow$ RHS, given.
- Outflux: B_0 , F_{N_x+1} , D_0 , $U_{N_z+1} \longrightarrow$ primary unknowns.

Algebraic procedure

• "Exact" mode profiles \longrightarrow 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 I.

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 II.

• 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).

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Photon scanning tunneling microscopy (PSTM) of photonic devices







$$P_{in} = 1. \quad S(p) = ?$$
$$R(p), T(p) = ?$$
$$S(p) \stackrel{?}{\longleftrightarrow} (optical field)|_p$$



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Fixed optical frequency, rectangular piecewise constant refractive index, horizontal & vertical guided wave in- and outflux

 \rightarrow **QUEP** simulations



$$\begin{split} n_{\rm s} &= 1.45, n_{\rm f} = 2.0, n_{\rm c} = 1.0, t = 0.2\,\mu{\rm m}, w = 100\,{\rm nm}, n_{\rm p} = 1.5, \\ \lambda &= 0.633\,\mu{\rm m}, (x,z) \in [-3.0,3.0] \times [-3.0,3.0]\,\mu{\rm m}^2, M_x = M_z = 80. \end{split}$$



TE, g = 10 nm

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- Sample: Rib waveguide with a series of deep, rectangular slits, $n_{\rm s} = 3.4, n_{\rm b} = 1.45, n_{\rm f} = 2.01, n_{\rm c} = 1.0, t = 55 \text{ nm}, h = 11 \text{ nm}, w = 1.5 \,\mu\text{m},$ $W = 2.5 \,\mu\text{m}, b = 3.2 \,\mu\text{m}, \Lambda = 220 \text{ nm}, s = 110 \text{ nm}, d = 70 \text{ nm}, N_{\rm g} = 15.$
- **Probe:** Tapered cylindrical fiber tip with aluminium coating, $a \approx 80 \text{ nm}, c \approx 100 \text{ nm}, g = 10 \text{ nm}, n_{p} = 1.5;$ TE polarized light, vacuum wavelength $\lambda = 0.6328 \,\mu\text{m}.$
- * E. Flück, M. Hammer, A. M. Otter, J. P. Korterijk, L. Kuipers, N. F. van Hulst, *Amplitude and phase evolution of optical fields inside periodic photonic structures*, Journal of Lightwave Technology **21**(5), 1384-1393 (2003)



Waveguide Bragg grating



$$\begin{split} n_{\rm s} &= 3.4, n_{\rm b} = 1.45, n_{\rm f} = 2.01, n_{\rm c} = 1.0, t = 55 \, {\rm nm}, b = 3.2 \, \mu {\rm m}, d = 70 \, {\rm nm}, \\ \Lambda &= 220 \, {\rm nm}, s = 110 \, {\rm nm}, N_{\rm g} = 15, g = 10 \, {\rm nm}, w = 100 \, {\rm nm}, n_{\rm p} = 1.5, \\ {\rm TE}, \lambda &= 0.6328 \, \mu {\rm m}, (x,z) \in [-3.5, 1.5] \times [-2.0, 5.2] \, \mu {\rm m}^2, M_x = 80, M_z = 100. \end{split}$$

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$$\begin{split} n_{\rm s} &= 3.4, n_{\rm b} = 1.45, n_{\rm f} = 2.01, n_{\rm c} = 1.0, t = 55 \, {\rm nm}, b = 3.2 \, \mu {\rm m}, d = 70 \, {\rm nm}, \\ \Lambda &= 220 \, {\rm nm}, s = 110 \, {\rm nm}, N_{\rm g} = 15, g = 10 \, {\rm nm}, w = 100 \, {\rm nm}, n_{\rm p} = 1.5, \\ {\rm TE}, \lambda &= 0.6328 \, \mu {\rm m}, (x,z) \in [-3.5, 1.5] \times [-2.0, 5.2] \, \mu {\rm m}^2, M_x = 80, M_z = 100. \end{split}$$









$$\begin{split} n_{\rm s} &= 1.45, n_{\rm f} = 2.0, n_{\rm c} = 1.0, t = 0.2 \,\mu\text{m}, d = 0.6 \,\mu\text{m}, \\ \Lambda &= 0.21 \,\mu\text{m}, s = 0.11 \,\mu\text{m}, L = 0.2275 \,\mu\text{m}, g = 10 \,\text{nm}, w = 100 \,\text{nm}, n_{\rm p} = 1.5, \\ \text{TE}, \lambda &= 0.633 \,\mu\text{m}, (x, z) \in [-3.0, 3.0] \times [-3.0, 4.7075] \,\mu\text{m}^2, M_x = 100, M_z = 120. \end{split}$$



 $n_{\rm s} = 1.45, n_{\rm f} = 2.0, n_{\rm c} = 1.0, t = 0.2 \,\mu{\rm m}, d = 0.6 \,\mu{\rm m},$ $\Lambda = 0.21 \,\mu{\rm m}, s = 0.11 \,\mu{\rm m}, L = 0.2275 \,\mu{\rm m}, g = 10 \,{\rm nm}, w = 100 \,{\rm nm}, n_{\rm p} = 1.5,$ TE, $\lambda = 0.633 \,\mu{\rm m}, (x, z) \in [-3.0, 3.0] \times [-3.0, 4.7075] \,\mu{\rm m}^2, M_x = 100, M_z = 120.$



$$\begin{split} n_{\rm s} &= 1.45, n_{\rm f} = 2.0, n_{\rm c} = 1.0, t = 0.2 \,\mu\text{m}, d = 0.6 \,\mu\text{m}, \\ \Lambda &= 0.21 \,\mu\text{m}, s = 0.11 \,\mu\text{m}, L = 0.2275 \,\mu\text{m}, g = 10 \,\text{nm}, w = 100 \,\text{nm}, n_{\rm p} = 1.5, \\ \text{TE}, \lambda &= 0.633 \,\mu\text{m}, (x, z) \in [-3.0, 3.0] \times [-3.0, 4.7075] \,\mu\text{m}^2, M_x = 100, M_z = 120. \end{split}$$



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T(p), R(p): the probe switches the transmission.

Outline

- Simulations in guided wave optics
 - Macroscopic Maxwell equations
 - Stationary and time-domain problems
 - 2-D problems
 - Modes of dielectric waveguides
- Quadridirectional eigenmode propagation
 - Problem setting
 - Eigenmode expansion
 - Algebraic procedure
- 2-D PSTM model
 - Probing evanescent fields
 - Hole defect in a slab waveguide
 - Waveguide Bragg grating: experiment & 2-D model
 - Resonant defect cavity

• Optical switching by NEMS-actuated resonator arrays



Olena Ivanova

Projection techniques for dimensionality reduction 3-D \rightarrow 2-D



NanoPhotonics Flagship, project TOE.7143

Optical switching by NEMS actuated resonator arrays — modeling & simulation tools



Milan Maksimovic

Time domain characterization of resonances & perturbations



NanoPhotonics Flagship, project TOE.7143 Optical switching by NEMS actuated resonator arrays — modeling & simulation tools


Remco Stoffer

Numerical simulation tools & interaction with projects TOE.7144, NEMS, group TST (EEMCS, EL), TOE.7145, Optics, group IOMS (EEMCS, EL).



NanoPhotonics Flagship, project TOE.7143 Optical switching by NEMS actuated resonator arrays — modeling & simulation tools



http://www.math.utwente.nl/aamp/

http://www.math.utwente.nl/aamp/research.html#MATHOPT