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# Finite element modeling of nanophotonic structures - Applications LAM Seminar

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### Foreword: Fresnel on the map





#### Foreword: Fresnel by themes

#### ELECTROMAGNÉTISME MÉTAMATÉRIAUX



 Modèles et fondamentaux en électromagnétisme (Analogie micro-onde, Nouvelles approches d'homogénéisation, Etude des effets de la dispersion, Non-linéarités spatiales)

 Méthodes numériques (Méthode intégrale de volume et forces optiques, Méthode des éléments finis, Méthode intégrale de surface, Méthode Monte Carlo et milieux diffusants)

 Réseaux de diffraction et fibres micro-structurées (Analyse d'effets physiques, Fitres à résonance de mode guide, Fibres optiques micro-structurées, Conception de composants optiques)

 Métamatériaux, invisibilité et protection (métamatériaux en optique et micro-ondes, métamatériaux en acoustique et mécanique, Protections hydrodynamique et sismique, Chaleur et mimétisme, Application des métamatériaux au bio-médical)

#### NANOPHOTONIQUE COMPOSANTS OPTIQUES



 Interactions lumière-matière aux échelles nanométriques (Aspects fondamentaux de la mécanique quantique, Emission exaltée par des nanoantennes, Contrôle nano-optique de la directivité d'émission)

 Thermoplasmonique et nano-résonateurs optiques (Absorption de lumière et thermoplasmonique, Théories multipolaires et modales, Nanophotonique sur particules diélectriques)

 Couches minces optiques (Filtres optiques interférentiels à hautes performances, Composants et concepts innovants, Métrologie extrême et diffusion lumineuse, nouveaux instruments et procédés)

 Interaction laser-matière aux forts flux (Etude des processus physiques de l'interaction laser-matière aux forts flux, Composants optiques pour lasers de puissance, Procédés laser)

#### TRAITEMENT DE L'INFORMATION ONDES ALÉATOIRES



 Polarisation et cohérence optique (Milieux désordonnés et aléatoires, Optique statistique, Instrumentation...)

 Télécommunications et traitement d'antenne (Réseaux de capteurs, Systèmes de communication optique sans fil, Cryptographie quantique...)

 Traitements et modèles pour la Télédétection (Interactions onde / surface océanique, Imagerie hyper-spectrale, Imagerie SAR polarimétrique et inter-férométrique, Imagerie sous-marine...)

• Eléments méthodologiques pour l'image et le signal

multi-dimensionnel (Segmentation et poursuite pour les images bruitées, Biométrie et reconnaissance de gestes, Imagerie médicale, Segmentation ultra-rapide...)

#### IMAGERIE AVANCÉE VIVANT



 Instrumentation (Techniques de microscopie optique, Fibres optiques pour la spectroscopie et l'endoscopie, Instrumentation et caractérisation en hyperfréquence, Autres développements en instrumentation...)

 Reconstruction numérique (Microscopie tomographique diffractive optique, Tomographie micro-ondes, Tomographie photo-acoustique quantitative, Microscopie de fluorescence à illumination structure, Imagerie X cohérente, Caractérisation multiéchelle)

 Etude du vivant (Imagerie des tissus, Imagerie des structures biologiques à l'échelle cellulaire, Imagerie quantitative de phase et de température en milieu cellulaire, Nouveles sondes moléculaires et inorganiques pour l'imagerie biologique)





1 Introductory example: Miniaturization of CMOS color sensors and spectral filtering

2 Finite element modeling

3 Demo!

4 Selected applications

5 If I have some time left...



# Drastic reduction of the pixel pitch in CMOS "cheap" sensors





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CMOS imagers: A complex diffraction gratings.

OPTICAL and technological issues

- Reduction of pixel pitch = transverse dimensions.
- Unchanged thickness:

Modeling issues



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  - absorbing color resins  $\approx$  50% of the stack thickness
  - Transmission spectral profile set by thickness

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  - Snell-Descartes lows no longer valid





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### SOLVING MAXWELL EQUATIONS

<sup>1</sup>Catrysse et al., J. Opt. Soc. Am. A 20(12), 2003



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## SOLVING MAXWELL EQUATIONS

Requires a very flexible and general method.



Subwavelength filtering in the visible range.

Independently from CMOS imagers domain

Some bibliographical leads on 0<sup>th</sup>-order diffractive spectral filtering independent from incident polarization, angle, in the visible frequency range:

 Crossed-gratings made of cylindrical holes<sup>1</sup> in a thin silver layer



<sup>1</sup>Barnes *et al.*, Nature, **424**, 2003 <sup>2</sup>Poujet *et al.*, Opt. Lett., **32**(20), 2007  Crossed-gratings made of cylindrical annular apertures<sup>2</sup> in a thin silver layer



Bandpass spectral profile with a 90% transmission at  $\lambda = 700 \, \text{nm}$ 



# Application to a CMOS pixel



- Looking for resonant phenomena inside a 3D complex structure
- Requires a model able to represent closely both the geometry and constitutive materials of the pixel pixel
- A 2D step is essential.





2 Finite element modeling

3 Demo!

4 Selected applications

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Find the unique (E, H) solution of:

$$\begin{cases} \operatorname{curl} \mathbf{E} = i \,\omega \,\mu_0 \,\mu \,\mathbf{H} \\ \\ \operatorname{curl} \mathbf{H} = -i \,\omega \,\varepsilon_0 \,\varepsilon \,\mathbf{E} \end{cases}$$















 $\operatorname{div}(\mu(x,y)\operatorname{grad} e) + k_0^2 \varepsilon(x,y) e = 0$ 

 $\operatorname{div}(\mu_1(y)\operatorname{grad} e_1) + k_0^2 \varepsilon_1(y) e_1 = 0$ 





 $\operatorname{div}(\mu(x,y)\operatorname{grad} e^d) + k_0^2 \, \mathcal{E}(x,y) \, e^d = 0 \quad (1) \quad \operatorname{div}(\mu_1(y) \operatorname{grad} e^d_1) + k_0^2 \, \mathcal{E}_1(y) \, e^d_1 = 0 \quad (2)$ 





 $div(\mu(x,y) \operatorname{grad} e^{d}) + k_0^2 \mathcal{E}(x,y) e^{d} = 0 \quad (1) \quad div(\mu_1(y) \operatorname{grad} e_1^{d}) + k_0^2 \mathcal{E}_1(y) e_1^{d} = 0 \quad (2)$  $e_2^{d} := e - e_1 = e^{d} - e_1^{d} \quad (3)$ 





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 $(1) - (2) \Longrightarrow \operatorname{div}(\mu(x, y) \operatorname{grad} e_2^d) + k_0^2 \varepsilon(x, y) e_2^d = \operatorname{S}(x, y)$ 




















<sup>1</sup>Demésy et al., Optics Express 15, 2007





■ Infinity of periods + quasi-periodicity of the incident plane wave → Quasi-periodic (or Bloch) conditions





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  - ightarrow Equivalence to a radiative
    - problem with localized sources





- Infinity of periods + quasi-periodicity of the incident plane wave → Quasi-periodic (or Bloch) conditions
- Infinite Substrate/Superstrate → Rectangular PML
- Plane wave sources at infinity
  - $\rightarrow$  Equivalence to a radiative
    - problem with localized sources
- Meshing of the structure: 2<sup>nd</sup> order nodal elements
- Weak form associated to equation (3)
- Solving thanks to a direct solver adapted to sparse matrix (MUMPS)

<sup>&</sup>lt;sup>1</sup>Demésy et al., Optics Express 15, 2007



### Weak formulation and discrete problem

- For example, let us consider nodal elements (first order = circus big top) built on a triangular mesh *m* with its set of nodes is denoted *N*.
- Projection of the field  $e_2^d$  on this (non-orthogonal) basis:

$$e_2^{d,m}(x,y) = \sum_{i\in N} \alpha_i \lambda_i(x,y)$$

"Weak form" of the problem:

$$\mathscr{R}_{\mu,\varepsilon}(e_{2}^{d},e') = -\int_{\Omega} \left( \mu \,\nabla e_{2}^{d} \right) \cdot \nabla \overline{e'} + k_{0}^{2} \varepsilon \, e_{2}^{d} \,\overline{e'} \, d\Omega + \int_{\partial \Omega} \overline{e'} \left( \mu \,\nabla e_{2}^{d} \right) \cdot \mathbf{n}_{|\partial \Omega} \, \mathrm{d}S \quad (1)$$

•  $e_2^d$ , solution of the radiation problem, is therefore the element of  $L^2(\operatorname{curl}, d, k)$  of quasiperiodic functions (i.e. such that  $u(x, y) = u_{\#}(x, y)e^{ikx}$  with  $u_{\#}(x, y) = u_{\#}(x + d, y)$ , a *d*-periodic function of  $H^1(\operatorname{div})$ ) on  $\Omega$  such that:  $\forall e' \in H^1(\operatorname{div}, d, k), \, \mathscr{R}_{\mu, \varepsilon}(e_2^d, e') = -\mathscr{R}_{\mu-\mu_1, \varepsilon-\varepsilon_1}(e_1, e').$  (2)

According to the Galerkin formulation, we choose the set of basis function λ<sub>i</sub> as set of weight function e', which leads to a final algebraic system of the form:

$$A\begin{bmatrix} \alpha_1\\ \vdots\\ \alpha_n \end{bmatrix} = b \text{ where } A \text{ is a sparse matrix.}$$



Diffraction Efficiencies - Losses - Energy Balance

Arbitrary geometry: an example of edge detection





Diffraction Efficiencies - Losses - Energy Balance

### Studied configuration: TM case, oblique incidence, strong losses





Diffraction Efficiencies - Losses - Energy Balance



$$e_0(x,y) = \exp(i(\alpha x + \beta^{sup} y))$$

 $\Re e[e_0]$ , Incident plane wave



Diffraction Efficiencies - Losses - Energy Balance



$$e_1(x,y) = e_0(x,y) + \exp(i\alpha x) \begin{cases} r \exp(-i\beta^{sup} y) & \text{for } y > 0 \\ t \exp(i\beta^{sub} y) & \text{for } y < 0 \end{cases}$$

 $\Re e[e_1]$ , Total field solution of the ancillary problem (plane diopter)



Diffraction Efficiencies - Losses - Energy Balance



$$e_1^d(x,y) = \exp(i\,\alpha\,x) \begin{cases} r\exp(-i\,\beta^{sup}\,y) & \text{for } y > 0\\ t\exp(i\,\beta^{sub}\,y) & \text{for } y < 0 \end{cases}$$

 $\left( \mathfrak{R} \boldsymbol{e} [ \boldsymbol{e}_1^d ] \right)$ , Field "diffracted" by the plane diopter





$$S(x, y) = k_0^2 \left( \varepsilon_{smurf} - \varepsilon_{air} \right) \exp(\alpha x + \beta^{sup} y) + k_0^2 \left( \varepsilon_{smurf} - \varepsilon_{air} \right) r \exp(\alpha x - \beta^{sup} y)$$

$$\operatorname{div}(\mu(x,y)\operatorname{grad} e_2^d) + k_0^2 \,\varepsilon(x,y) \, e_2^d = \boxed{\operatorname{S}(x,y)}$$



































• Losses : 
$$\frac{1}{2} \int_{smurf} \omega \varepsilon_0 \varepsilon'' |e(x, y)|^2 dx dy$$
  
• Losses (in fraction of incident energy) :  $Q = 0.5601$ 

$$\left(\frac{1}{2}\sigma|\mathbf{e}|^2\right)$$







"Quantum" efficiency in the case of a semi-conductor substrate A grating on a  $n^+/p$  junction



#### Studied configuration: semi-conductor substrate





Demo!

# https://gitlab.onelab.info/doc/models/tree/master/DiffractionGratings/



# Aluminum color filters



Let us map 
$$|H_z|^2(x,y,\lambda)$$
 vs  $\mathcal{T}_{0,0}(\lambda)$ 



# Aluminum color filters



# Aluminum color filters





Later...

Frequency selective reflective surface with silver nano-particles



Design - "optimization"



Fab



#### Carac



<sup>1</sup> Y. Brülé, G. Demésy, A-L. Fehrembach, B. Gralak, E. Popov, G. Tayeb, M. Grangier, D. Barat, H. Berlin, P. Gogol, and B. Dagens, "Design of metallic nanoparticle gratings for filtering properties in the visible spectrum". Appl. Opt. 54, 010359 (2015).























Sub-wavelength phase control



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Sub-wavelength phase control





B)







# Conclusion

Solving Maxwell's equations in small but open boxes.

Applications for filtering.

... We are also calculating mode...



#### The eigenvalue problem

2D p-polarization case:  $\mathbf{H} = H_z(x, y)\mathbf{z}$  and  $\mathbf{E} = \mathbf{E}(x, y) = E_x(x, y)\mathbf{x} + E_y(x, y)\mathbf{y}$ 

We are looking for non trivial solution of the source-free Helmholtz equation:

• *i.e.* the eigenvalues  $\omega_n$  and associated eigenvectors  $\mathbf{E}_n$  of the operator  $\mathscr{L}_e^{3D}$ 

•  $\mathscr{L}_{e}^{3D}(\mathbf{E})$  depends of  $\boldsymbol{\omega}$  we are looking for!

Two possible solutions:

- Physical linearization: construction of an augmented system where auxiliary fields are added to (E, H)<sup>1</sup>
- Numerical linearization <sup>2</sup>

<sup>&</sup>lt;sup>1</sup>Y. Brûlé, B. Gralak, and G. Demésy, "Calculation and analysis of the complex band structure of dispersive and dissipative two-dimensional photonic crystals", J. Opt. Soc. Am. B **33**, 691-702 (2016)

<sup>&</sup>lt;sup>2</sup>J. E. Roman, C. Campos, E. Romero and A. Tomas. SLEPc Users Manual. Tech. Rep. DSIC-II/24/02 - Revision 3.7, Universitat Politècnica de València, 2016.



## Toy example: the "bi-Drudy Bi-box"



Dispersion relation: Semi-analytical transcendental equation

s-polarization:
$$\frac{1}{\beta_{1}(\omega_{n})} \tan[\beta_{1}(\omega_{n})a] + \frac{1}{\beta_{2}(\omega_{n})} \tan[\beta_{2}(\omega_{n})a] = 0$$
p-polarization:
$$\frac{\beta_{1}(\omega_{n})}{\varepsilon_{1}(\omega_{n})} \tan[\beta_{1}(\omega_{n})a] + \frac{\beta_{2}(\omega_{n})}{\varepsilon_{2}(\omega_{n})} \tan[\beta_{2}(\omega_{n})a] = 0$$

With  $eta_1$  and  $eta_2$  two complex functions of  $\omega$  :

$$\beta_j(\omega_n) = \sqrt{\frac{\omega_n^2}{c^2} \varepsilon_j(\omega_n) - \frac{q^2 \pi^2}{a^2}} \quad \text{with} \quad j \in \{1, 2\},$$
(3)

where  $q \in \mathbb{N}^{\star}$  for s-polarization and  $q \in \mathbb{N}$  for p-polarization.






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0

8

803

- $\omega_1: |\varepsilon_1(\omega)| \to \infty$
- $\omega_2: \varepsilon_1(\omega_2) = -\varepsilon_2$  plasmons
- $\omega_3 : \varepsilon_1(\omega_3) = 0$  spurious
- high frequencies:  $arepsilon_1(\omega) o arepsilon_\infty$



p-polarization

80

0

r



















































































Resonances in frequency dispersive media (ANR RESONANCE)

with F. Zolla, A. Nicolet and B. Gralak (PI: P. Lalanne, LP2N)



G. Demésy et al. https://arxiv.org/abs/1802.02363v1



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#### Structured waveguides (ANR LOUISE)

with G. Renversez (PI: V. Nazabal, Institut des Sciences Chimiques de Rennes)

A leaky mode... as an incident field for a scattering problem.





#### Oscillating particle

#### Mauricio Garcia-Vergara's PhD

Oscillating charge: A multiharmonic problem





#### Other examples (scattering)



A trimer in a photoresist.

ACS Photonics, 2018, 5 (3), pp 918-928



T matrix of an arbitrary scatterer. GNU Model.

https://arxiv.org/abs/1802.00596v2



#### Metallic grating academical case

Comparison to the results of a independent modal method (FMM)





N <sub>M</sub>	$R_0^{TM}$	$R_0^{TE}$
4	0.7336765	0.8532342
6	0.7371302	0.8456592
8	0.7347466	0.8482817
10	0.7333739	0.8500710
12	0.7346569	0.8494844
14	0.7341944	0.8483238
16	0.7342714	0.8484774
Result given by Granet <i>et al.</i> 1	0.7342789	0.8484781

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#### Test Structures presentation







#### Optical measurement bench





#### Photodiode toped with a dielectric multilayered stack



Very good agreement without any adjustment parameter, provided the precise knowing of:

- The thickness of each layer (SEM views of cross-sections)
- The dispersion of each material (ellipsometric measurements)
- Validates both:
  - the use of the measured  $\varepsilon(\lambda)$ , on which is based the ancillary problem,
  - the validity of the approximation of QE calculation.



Photodiode with an embedded copper grating







<sup>1</sup>Demésy et al., Optical Engineering 48, p.058002 (may 2009)



#### Photodiode with an embedded copper grating



<sup>1</sup>Demésy et al., Optical Engineering 48, p.058002 (may 2009)


## Energy balance – TE case – $\lambda$ = 720 nm







With Ta/TaN barrier

### Without Ta/TaN barrier







# Field maps – TE case – $\lambda=$ 720 nm

### With Ta/TaN barrier





#### Without Ta/TaN barrier

