Finite Element Methods for Maxwell's Equations

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75 years of Math. Comp.

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Time Harmonic Maxwell's Equations

$\boldsymbol{E}$: Electric field and $\boldsymbol{H}$: Magnetic field (both complex vector valued functions of position)

The linear time harmonic Maxwell system at angular frequency $\omega > 0$ is:

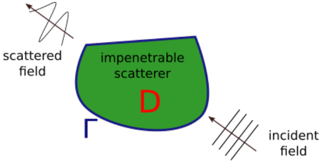
$$\begin{aligned} -i\omega\epsilon \boldsymbol{E} + \sigma \boldsymbol{E} - \nabla \times \boldsymbol{H} &= -\boldsymbol{J}, \\ -i\omega\mu \boldsymbol{H} + \nabla \times \boldsymbol{E} &= 0, \end{aligned}$$

where ϵ is the electric permittivity, μ the magnetic permeability, σ the conductivity and $\boldsymbol{J}$ is the applied current density. We assume $\mu = \mu_0 > 0$ and solve for $\boldsymbol{E}$:

$$\omega^2 \mu_0 \epsilon_0 \left(\frac{\epsilon}{\epsilon_0} + i \frac{\sigma}{\epsilon_0 \omega} \right) \boldsymbol{E} - \nabla \times \nabla \times \boldsymbol{E} = -i\omega\mu_0 \boldsymbol{J}$$

Define the wave number $\kappa = \omega\sqrt{\epsilon_0 \mu_0}$ and complex relative permitivitty $\epsilon_r = \left(\frac{\epsilon}{\epsilon_0} + i \frac{\sigma}{\epsilon_0 \omega} \right)$. In applications $\epsilon_r := \epsilon_r(\boldsymbol{x}, \omega)$.

Scattering Problem



- $\boldsymbol{E}^i$: Known incident field
- $\boldsymbol{E}^s$: Scattered electric field
- $\boldsymbol{E}$: Total electric field
- $\kappa > 0$: Wave-number
- $\epsilon_r = 1$: Outside D is air

Data (plane wave):

Known incident field: $\boldsymbol{E}^i = \boldsymbol{p} \exp(i\kappa \boldsymbol{d} \cdot \boldsymbol{x})$ $(\boldsymbol{d} \perp \boldsymbol{p}, |\boldsymbol{d}| = 1)$

Equations (no source, $\epsilon_r = 1$):

Maxwell's Equations: $\nabla \times \nabla \times \boldsymbol{E} - \kappa^2 \boldsymbol{E} = 0$ in $\mathbb{R}^3 \setminus \overline{D}$

Total field: $\boldsymbol{E} = \boldsymbol{E}^i + \boldsymbol{E}^s$ in $\mathbb{R}^3 \setminus D$

Boundary Conditions: ($\boldsymbol{\nu}$ is unit outward normal)

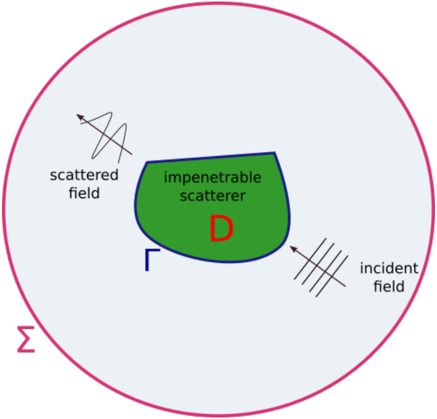
Perfect Electric Conductor (PEC): $\boldsymbol{\nu} \times \boldsymbol{E} = 0$ on Γ

Silver-Müller Radiation Condition: $\lim_{r\to\infty} ((\nabla \times \boldsymbol{E}^s) \times \boldsymbol{x} - i\kappa r \boldsymbol{E}^s) = 0.$

For a bounded Lipschitz domain D with connected complement, this problem is well posed.

Reduction to a Bounded Domain

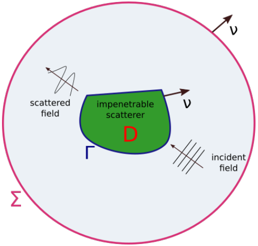
Introduce a closed surface Σ containing the scatterer (e.g. a sphere of radius R large enough) :



Let Ω be the region inside Σ and outside D

Need an appropriate boundary condition on the *artificial boundary* Σ.

Absorbing Boundary Condition (simplest case)



The simplest method is to apply the Silver-Müller Radiation Condition on Σ. Note $\boldsymbol{\nu}$ is the outward normal on Σ.
Abusing notation, $\boldsymbol{E}$ now denotes the approximate field on the truncated domain.

Incident Field: $\boldsymbol{E}^i(\boldsymbol{x}) = \boldsymbol{p}\exp(i\kappa\boldsymbol{x}\cdot\boldsymbol{d})$, $\boldsymbol{p}\cdot\boldsymbol{d} = 0$, and $|\boldsymbol{d}| = 1$

$$\begin{aligned}
\nabla\times(\nabla\times\boldsymbol{E}) - \kappa^2\boldsymbol{E} &= 0 \text{ in } \Omega\\
(\nabla\times\boldsymbol{E})\times\boldsymbol{\nu} - i\kappa\boldsymbol{E}_T &= \left(\nabla\times\boldsymbol{E}^i\right)\times\boldsymbol{\nu} - i\kappa\boldsymbol{E}^i_T \text{ on } \Sigma\\
\boldsymbol{E}\times\boldsymbol{\nu} &= 0 \text{ on } \Gamma
\end{aligned}$$

Here $\boldsymbol{E}_T = (\boldsymbol{\nu}\times\boldsymbol{E})\times\boldsymbol{\nu}$ is the tangential trace of $\boldsymbol{E}$.

Function Spaces

$$
\begin{aligned}
H(\mathrm{curl};\Omega) &= \left\{ \boldsymbol{u} \in (L^2(\Omega))^3 \mid \nabla \times \boldsymbol{u} \in (L^2(\Omega))^3 \right\} \\
X &= \left\{ \boldsymbol{u} \in H(\mathrm{curl};\Omega) \mid \boldsymbol{\nu} \times \boldsymbol{u}|_\Sigma \in (L^2(\Sigma))^3,\ \boldsymbol{\nu} \times \boldsymbol{u} = 0 \text{ on } \Gamma \right\}
\end{aligned}
$$

with norms

$$
\begin{aligned}
\|\boldsymbol{u}\|_{H(\mathrm{curl};\Omega)} &= \sqrt{\|\boldsymbol{u}\|^2_{(L^2(\Omega))^3} + \|\nabla \times \boldsymbol{u}\|^2_{(L^2(\Omega))^3}} \\
\|\boldsymbol{u}\|_X &= \sqrt{\|\boldsymbol{u}\|^2_{H(\mathrm{curl};\Omega)} + \|\boldsymbol{\nu} \times \boldsymbol{u}\|^2_{(L^2(\Sigma))^3}}
\end{aligned}
$$

Let

$$
(\boldsymbol{u}, \boldsymbol{v}) = \int_\Omega \boldsymbol{u} \cdot \overline{\boldsymbol{v}}\, dV, \qquad \langle \boldsymbol{u}, \boldsymbol{v} \rangle_\Sigma = \int_\Sigma \boldsymbol{u} \cdot \overline{\boldsymbol{v}}\, dA.
$$

To avoid complications, from now on we assume Ω has two connected boundaries, Σ, Γ, and D has connected complement.

Galerkin Method

Multiply by the conjugate of a test function ϕ such that $\phi \times \boldsymbol{\nu} = 0$ on Γ, and integrate over Ω:

$$\begin{aligned} 0 &= \int_\Omega \left(\nabla \times (\nabla \times \boldsymbol{E}) - \kappa^2 \boldsymbol{E}\right) \cdot \overline{\phi}\, dV \\ &= \int_\Omega \nabla \times \boldsymbol{E} \cdot \nabla \times \overline{\phi} - \kappa^2 \boldsymbol{E} \cdot \overline{\phi}\, dV + \int_{\partial\Omega} \boldsymbol{\nu} \times \nabla \times \boldsymbol{E} \cdot \overline{\phi}\, dA. \end{aligned}$$

The boundary terms are replaced using boundary data or the vanishing trace on Γ:

$$\begin{aligned} \int_{\partial\Omega} \boldsymbol{\nu} \times \nabla \times \boldsymbol{E} \cdot \overline{\phi}\, dA &= -\int_\Sigma i\kappa \boldsymbol{E}_T \cdot \overline{\phi}\, dA \\ &\quad + \int_\Sigma \left(\boldsymbol{\nu} \times \nabla \times \boldsymbol{E}^i - i\kappa \boldsymbol{E}^i_T\right) \cdot \overline{\phi}\, dA. \end{aligned}$$

We arrive at the variational problem of finding $\boldsymbol{E} \in X$ such that

$$(\nabla \times \boldsymbol{E}, \nabla \times \phi) - \kappa^2 (\boldsymbol{E}, \phi) - i\kappa \langle \boldsymbol{E}_T, \phi_T \rangle_\Sigma = \langle \boldsymbol{F}, \phi_T \rangle_\Sigma$$

for all $\phi \in X$ where $\boldsymbol{F} = (\nabla \times \boldsymbol{E}^i) \times \boldsymbol{\nu} + i\kappa \boldsymbol{E}^i_T$.

Existence and Approximation

Problem: curl has a large null space. We use the Helmholtz decomposition:

$$\text{Define:} \quad S = \left\{ p \in H^1(\Omega) \mid p = 0 \text{ on } \Gamma, \ p \text{ constant on } \Sigma \right\}$$

then $\nabla S \subset X$. Choosing $\phi = \nabla \xi$, $\xi \in S$ as a test function:

$$-\kappa^2(\boldsymbol{E}, \nabla \xi) = 0$$

so $\boldsymbol{E}$ is divergence free. Next we prove uniqueness. Then, using the subspace of divergence free functions $\tilde{X} \subset X$, the compact embedding of $\tilde{X}$ in L^2 and the Fredholm alternative we have:

Theorem

Under the previous assumptions on D, there is a unique solution to the variational problem for any $\kappa > 0$.

If Σ is a sphere of radius R, and B is a fixed domain inside Σ and outside D then for R large enough

$$\|\boldsymbol{E}_{true} - \boldsymbol{E}_{truncated}\|_{H(\mathrm{curl};B)} \leq \frac{C}{R^2}$$

Standard continuous elements [1980-90's]

Suppose that Ω has been covered by a regular tetrahedral mesh denoted by $\mathcal{T}_h$ (tetrahedra having a maximum diameter h).

An obvious choice: use three copies of standard continuous piecewise linear finite elements. If we construct a finite element subspace $X_h \subset X$ using these continuous elements (note $X_h \subset (H^1(\Omega))^3$), we find that the previously defined variational formulation gives incorrect answers due to lack of control of the divergence.

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We can try to add a penalty term. Choose $\gamma > 0$ sufficiently large and seek $\boldsymbol{E}_h \in X_h$ such that

$$(\nabla \times \boldsymbol{E}_h, \nabla \times \phi_h) + \gamma(\nabla \cdot \boldsymbol{E}_h, \nabla \cdot \phi_h) - \kappa^2(\boldsymbol{E}_h, \phi_h)$$
$$-i\kappa\langle \boldsymbol{E}_{h,T}, \phi_{h,T}\rangle_\Sigma = \langle \boldsymbol{F}, \phi_{h,T}\rangle \text{ for all } \phi_h \in X_h$$

A numerical analyst's nightmare

However, if Ω has reentrant corners, we may compute solutions that converge as $h \to 0$ but to the the wrong answer![1]

The correct space for the problem is $X_N = X \cap H(\mathrm{div}, \Omega)$ but $H_N = H^1(\Omega)^3 \cap X$ is a closed subspace of X_N in the curl+div norm.
If you want to use continuous elements, consult Costabel & Dauge (γ needs to be position dependent) or more recently Bonito's papers[2].

To handle this problem and discontinuous fields due to jumps in ϵ_r, we can use vector finite elements in $H(\mathrm{curl})$ due to Nédélec[3] (see also Whitney).

[1] M. Costabel, M. Dauge, Numer. Math. 93 (2002) 239-277.

[2] A. Bonito et al., Math. Model. Numer. Anal., 50, 1457–1489, 2016.

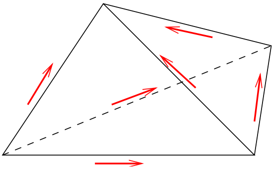
[3] J.C. Nédélec, Numer. Math. **35** (1980) 315-341.

Finite Elements in $H(\mathrm{curl})$ [Nédélec 1980, 1986]

The lowest order *edge finite element* space is

$$X_h = \{\boldsymbol{u}_h \in H(\mathrm{curl};\Omega) \mid \boldsymbol{u}_h|_K = \boldsymbol{a}_K + \boldsymbol{b}_K \times \boldsymbol{x}, \quad \boldsymbol{a}_K, \boldsymbol{b}_K \in \mathbb{C}^3, \quad \forall K \in \mathcal{T}_h\Big\}.$$

The degrees of freedom (unknowns) for this element are $\int_e \boldsymbol{u}_h \cdot \boldsymbol{\tau}_h \, ds$ for each edge e of each tetrahedron where $\boldsymbol{\tau}_e$ is an appropriately oriented tangent vector.



Note: Nédélec describes elements of all orders and in a later paper a second family of elements.[4] Engineering codes often use 2nd or higher order elements.

[4] P. Monk, *Finite Element Methods for Maxwell's Equations*, Oxford University Press, 2003.

Edge Element Method

Let X_h be the discrete space consisting of edge finite elements. We now seek $\boldsymbol{E}_h \in X_h$ such that

$$(\nabla \times \boldsymbol{E}_h, \nabla \times \phi_h) - \kappa^2(\boldsymbol{E}_h, \phi_h) - i\kappa\langle \boldsymbol{E}_{h,T}, \phi_{h,T}\rangle_\Sigma = \langle \boldsymbol{F}, \phi_{h,T}\rangle$$

for all $\phi_h \in X_h$.

Discrete Divergence Free Functions

Recall that if

$$S = \{p \in H^1(\Omega) \;\; p = 0 \text{ on } \Gamma, \; p = \text{constant on } \Sigma\}$$

then $\nabla S \subset X$ and this property enabled control of the divergence.

Discrete Divergence Free Functions

Recall that if

$$S = \{p \in H^1(\Omega) \;\; p = 0 \text{ on } \Gamma, \; p = \text{constant on } \Sigma\}$$

then $\nabla S \subset X$ and this property enabled control of the divergence.

An important property of Nédélec's elements is that they contain many gradients. In the lowest order case, if

$$S_h = \{p_h \in S \mid p_h|_K \in P_1, \quad \forall K \in \mathcal{T}_h\},$$

then $\nabla S_h \subset X_h$.

Discrete divergence free

We write a discrete Helmholtz decomposition

$$X_h = X_{0,h} \oplus \nabla S_h.$$

Functions in $X_{0,h}$ are said to be *discrete divergence free*.

$$X_{0,h} = \left\{ \boldsymbol{u}_h \in X_h \mid (\boldsymbol{u}_h, \nabla \xi_h) = 0, \quad \text{for all } \xi_h \in S_h \right\}.$$

Note

$$X_{0,h} \not\subset X_0.$$

Error Estimate

Using the properties of edge finite element spaces (in particular a discrete analogue of compactness[5]) and an extension theorem, Gatica and Meddahi[6] prove (earlier proofs required the mesh is quasi-uniform near Σ):

Theorem

If h is small enough then there exists a unique finite element solution $\boldsymbol{E}_h \in X_h$ and

$$\|\boldsymbol{E} - \boldsymbol{E}_h\|_{H(\mathrm{curl};\Omega)} \to 0 \text{ as } h \to 0$$

For sufficiently smooth solutions, lowest order Nédélec elements give $O(h)$ convergence, 2nd order give $O(h^2)$ etc if $\boldsymbol{E}$ is smooth enough. For another approach using mixed method techniques see Boffi[7]

[5] Kikuchi, F. (1989). On a discrete compactness property for the N?ed?elec finite elements. J. Fac. Sci. Univ. Tokyo, Sect. 1A Math., 36, 479?90

[6] G.N. Gatica and S. Meddahi, IMA J Numer. Anal., 32 534-552, 2012

[7] D. Boffi. Finite element approximation of eigenvalue problems. Acta Numerica, 19 (2010) 1-120.

An aside: the Discrete deRham diagram

The standard vertex and Nédélec finite element spaces satisfy the following discrete deRham diagram [8],[9]

$$
\begin{array}{ccccccc}
H^1(\Omega) & & H(\mathrm{curl};\Omega) & & H(\mathrm{div};\Omega) & & L^2(\Omega) \\
\cup & & \cup & & \cup & & \cup \\
C^\infty & \xrightarrow{\nabla} & (C^\infty)^3 & \xrightarrow{\nabla\times} & (C^\infty)^3 & \xrightarrow{\nabla\cdot} & C^\infty \\
\pi_h \downarrow & & \boldsymbol{r}_h \downarrow & & \boldsymbol{w}_h \downarrow & & P_{0,h} \downarrow \\
U_h & \xrightarrow{\nabla} & V_h & \xrightarrow{\nabla\times} & W_h & \xrightarrow{\nabla\cdot} & Z_h \\
Vertex & & Edge & & Face & & Volume.
\end{array}
$$

Here W_h is the Nédélec-Raviart-Thomas space in 3D. This connects to the Finite Element Exterior Calculus[10].

[8] A. Bossavit, *Computational Electromagnetism*, Academic Press, 1998

[9] R. Hiptmair, Acta Numerica, 11 237-339, 2002

[10] D.N. Arnold, R.S. Falk and R. Winther, Bulletin of the American Mathematical Society, 47 281-354, 2010

Challenges

- *Problem size*: need κh sufficiently small to get accuracy. For Helmholtz, if p is the degree of the finite element space

$$\frac{\kappa h}{p} = \eta \text{ fixed small enough, and } p = O(\log(\kappa))$$

  to maintain accuracy as κ increases[11]. We expect the same for Maxwell. So we need to use higher order edge elements.[12]
- *Solver*: How to solve the indefinite complex symmetric matrix problem resulting from discretization? Multigrid/Schwarz methods need a "sufficiently fine" coarse grid solve[13].
- *A posteriori error control*: standard techniques have bad κ dependence due to "phase error". For coercive problem estimators are available.[14]

[11] J.M. Melenk, S. Sauter, SIAM J. Numer. Anal. 49 (2011), pp. 1210-1243

[12] L. Demkowicz, Computing with hp-Adaptive Finite Elements, vol 1, CRC Press, 2006

[13] J. Gopalakrishnan and J. E. Pasciak. Math. Comp. 72 (2003) 1-15

[14] J. Schoeberl, Math. Comp., 77 633-649 (2008).

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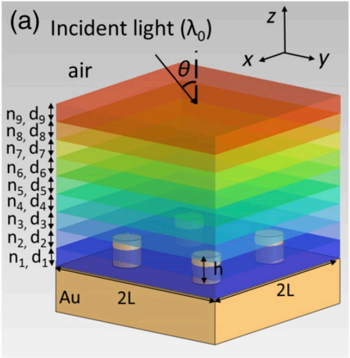
Thin Film Photo-Voltaic (PV) Device: a simplified model

A periodic metal grating substrate can be used to generate surface waves entrap light. A periodic photonic crystal generates multiple surface waves:[15]

Wavelengths of interest:
400-1200nm
Period of the grating:
$L \approx 400$nm
Height of structure:
≈ 2000nm



Note that the structure is periodic in x and y with period L. [16]

[15] M. Faryad and A. Lakhtakia, J. Opt. Soc. Am. B. **27** (2010) 2218-2223

[16] L. Liu et al., J. Nanophotonics, **9** (2015) 093593-1

The Mathematical Model

Assume the relative permeability $\mu_r = 1$ is constant and biperiodic relative permittivity ε_r. Now we must incorporate the effects of materials in the cell and so the time harmonic electric total field $\boldsymbol{E}$ satisfies

$$\nabla \times \nabla \times \boldsymbol{E} - \kappa^2 \varepsilon_r \boldsymbol{E} = 0$$

For a thin film grating, $\epsilon_r = 1$ if $x_3 > H$.

We are interested in the optimal design of solar cells, in particular allowing a spatially continuously varying ϵ_r and a well designed metallic grating.

Periodicity and the Incident Field

The permittivity is assumed to be bi-periodic so there are spatial periods $L_1 > 0$ and $L_2 > 0$ such that

$$\varepsilon_r(x_1 + L_1, x_2 + L_2, x_3) = \varepsilon_r(x_1, x_2, x_3)$$

for all $(x_1, x_2, x_3) \in \mathbb{R}^3$.

As before, the incident field is a plane wave with polarization $\boldsymbol{p} \neq 0$ and direction of propagation $\boldsymbol{d}$ with $|\boldsymbol{d}| = 1$ and $\boldsymbol{d} \cdot \boldsymbol{p} = 0$

$$\boldsymbol{E}^i(\boldsymbol{x}) = \boldsymbol{p} \exp(i\kappa \boldsymbol{d} \cdot \boldsymbol{x})$$

Unless $d_1 = d_2 = 0$ (normal incidence) the incident field is not periodic in x_1 and x_2. Instead

$$\boldsymbol{E}^i(x_1 + L_1, x_2 + L_2, x_3) = \exp(i\kappa(L_1 d_1 + L_2 d_2))\boldsymbol{E}^i(x_1, x_2, x_3)$$

for all $(x_1, x_2, x_3) \in \mathbb{R}^3$.

Quasiperiodicity

We seek the *quasi-periodic* scattered field $\boldsymbol{E}^s$ with the property

$$\boldsymbol{E}^s(x_1 + L_1, x_2 + L_2, x_3) = \exp(i\kappa(d_1 L_1 + d_2 L_2))\boldsymbol{E}^s(x_1, x_2, x_3)$$

for all $(x_1, x_2, x_3) \in \mathbb{R}^3$.
In view of the above discussion we can now restrict the problem to an infinite cylinder

$$C = \{(x_1, x_2, x_3) \mid 0 < x_1 < L_1,\ 0 < x_2 < L_2,\ x_3 > 0\}.$$

We then require that Maxwell's equations are satisfied in C together with appropriate boundary conditions enforcing the quasi-periodiciy of the solution in x_1 and x_2.

Radiation condition

We note that C has two components

$$C_+ = \{(x_1, x_2, x_3) \in C \mid x_3 > H\},$$
$$C_0 = \{(x_1, x_2, x_3) \in C \mid 0 < x_3 < H\}.$$

In C_+ the coefficients $\varepsilon_r = 1$ and $\mu_r = 1$.
Since $\boldsymbol{E}^s$ is quasiperiodic in x_1 and x_2, it has a Fourier expansion

$$\boldsymbol{E}^s(\boldsymbol{x}) = \sum_{\mathbf{n}\in\mathbb{Z}^2} \boldsymbol{u}_{\boldsymbol{\alpha},\mathbf{n}}(x_3) \exp(i(\boldsymbol{\alpha} + \boldsymbol{\alpha}_{\mathbf{n}}) \cdot \boldsymbol{x}),$$

where $\boldsymbol{\alpha} = \kappa(L_1 d_1 + L_2 d_2)$, $\boldsymbol{\alpha}_{\mathbf{n}} = (2\pi n_1/L_1, 2\pi n_2/L_2, 0)^T$ and $\mathbf{n} = (n_1, n_2) \in \mathbb{Z}^2$.

Propagating and Decaying Modes

We assume κ is not at a Rayleigh frequency meaning that

$$\kappa^2 \neq (\boldsymbol{\alpha}_{\mathbf{n}} + \boldsymbol{\alpha})^2 \quad \text{for any } \mathbf{n} \in \mathbb{Z}^2.$$

Substituting the Fourier series for $\boldsymbol{E}^s$ into Maxwell's equations we see that if

$$\beta_{\mathbf{n}}(\boldsymbol{\alpha}) = \begin{cases} \sqrt{\kappa^2 - (\boldsymbol{\alpha}_{\mathbf{n}} + \boldsymbol{\alpha})^2} & \text{if } |\boldsymbol{\alpha}_{\mathbf{n}} + \boldsymbol{\alpha}| < \kappa^2 \text{ (propagating)} \\ i\sqrt{(\boldsymbol{\alpha}_{\mathbf{n}} + \boldsymbol{\alpha})^2 - \kappa^2} & \text{if } |\boldsymbol{\alpha}_{\mathbf{n}} + \boldsymbol{\alpha}| > \kappa^2 \text{ (evanescent)} \end{cases}$$

then the scattered field should be expanded as

$$\boldsymbol{E}^s(\boldsymbol{x}) = \sum_{\mathbf{n} \in \mathbb{Z}^2} \boldsymbol{u}^{0,+}_{\alpha,\mathbf{n}} \exp(i\beta_{\mathbf{n}}(\boldsymbol{\alpha}) x_3 + i(\boldsymbol{\alpha} + \boldsymbol{\alpha}_{\mathbf{n}}) \cdot \boldsymbol{x}).$$

Here we choose $\boldsymbol{E}^s$ to consist of upward propagating modes or decaying modes as $x_3 \to \infty$.

Summary of the Equations

Let

$$X_{qp} = \{\boldsymbol{u} \in H_{loc}(\mathrm{curl}; C) \mid \boldsymbol{u} \text{ is quasi periodic}\}$$

We seek $\boldsymbol{E}^s \in X_{qp}$ such that

$$\nabla \times \nabla \times \boldsymbol{E}^s - \kappa^2 \epsilon_r \boldsymbol{E}^s = \kappa^2 (1 - \epsilon_r) \boldsymbol{E}^i \text{ in } C$$

together with the boundary condition

$$\boldsymbol{E}^s \times \boldsymbol{\nu} = -\boldsymbol{E}^i \times \boldsymbol{\nu} \text{ on } x_3 = 0 \text{ (PEC on the lower face)}$$

and such that $\boldsymbol{E}^s$ has the Fourier expansion given on the previous slide.

Existence

Let $\Omega = [0, L_1] \times [0, L_2] \times [0, H]$ contain the inhomogeneous structure.[17]

Theorem (Ammari & Bao)

For all but a discrete set of wavenumbers, the solar cell scattering problem has a unique solution $\boldsymbol{E}$ in X_{qp} .

This problem is more tricky than before. We can no longer show that the solution is unique (due to the evanescent modes). Instead the analytic Fredholm theory is used.

[17] H. Ammari and G. Bao, Math. Nachr. 251, 3-18 (2003)

How to discretize?

We can use edge elements in C_0, but need to truncate the domain:

1. The Silver-Müller condition is no longer sufficient.
2. We can use the Fourier expansion to derive a "Dirichlet-to-Neumann" map and use it as a non-local boundary condition. This works well in 2D but introduces a large dense block into the matrix in 3D.
3. We use the Perfectly Matched Layer (PML)[18] to absorb upward propagating and evanescent waves above the structure (evanescent waves are an extra concern here). It took some time for a theoretical understanding to emerge.[19].

[18] J. Berenger, J. Comp. Phys., 114 185-200 (1996)

[19] J.H. Bramble and J.E. Pasciak. Math. Comp. 76 (2007) 597-614

At last a discrete problem

Assuming a periodic constraint on the mesh, let

$$X_{qp,h} = \{\boldsymbol{u}_h \in X_h \mid \boldsymbol{u}_h \text{ is quasi periodic, and } \boldsymbol{u}_h \times \boldsymbol{\nu} = 0 \text{ at } x_3 = L + \delta\}$$

We seek $\boldsymbol{E}_h^s \in X_{qp,h}$ such that

$$\boldsymbol{E}_h^s \times \boldsymbol{\nu} = -\boldsymbol{r}_h(\boldsymbol{E}^i) \times \boldsymbol{\nu} \text{ on } x_3 = 0$$

where $\boldsymbol{r}_h$ is the interpolant into $X_{qp,h}$, and

$$(\tilde{\mu}_r^{-1}\nabla \times \boldsymbol{E}_h^s, \nabla \times \boldsymbol{\xi}) - \kappa^2(\tilde{\epsilon}_r \boldsymbol{E}_h^s, \boldsymbol{\xi}) = \kappa^2((1 - \epsilon_r)\boldsymbol{E}^i, \boldsymbol{\xi})$$

for all $\boldsymbol{\xi} \in \{\boldsymbol{u}_h \in X_{qp,h} \mid \boldsymbol{u}_h \times \boldsymbol{\nu} = 0 \text{ when } x_3 = 0\}$ and where we denote by

$$\tilde{\epsilon}_r = \begin{cases} \epsilon_r & \text{outside the PML} \\ \epsilon_{PML} & \text{in the PML} \end{cases} \qquad \tilde{\mu}_r = \begin{cases} 1 & \text{outside the PML} \\ \epsilon_{PML} & \text{in the PML} \end{cases}$$

Some comments on the discrete problem

In the context of solar cells we have several issues:

1. The problem needs to be solved for many values of κ and many choices of $\boldsymbol{d}$ (the matrix changes whenever κ or $\boldsymbol{d}$ changes).
2. The problem is still generally indefinite and we need "sufficiently many" grid points per wavelength.
3. Because the matrix is not Hermitian or complex symmetric, we often use a direct method to solve the linear system. GMRES can be used but we still need a good preconditioner.
4. For a posteriori analysis of the FEM with (a different) PML see Wang and Bao[20]

[20] Z. Wang, G. Bao, et al.,5) SIAM Journal on Numerical Analysis, 53(2015), 1585-1607.

Numerical results

Nédélec elements have gone from being "exotic" in the early 2000s to an available standard in many packages.[21] For example the open source software: deal.ii, FEniCS, FELICITY, NGSolve to name a few...

We use *NGSolve*[22].

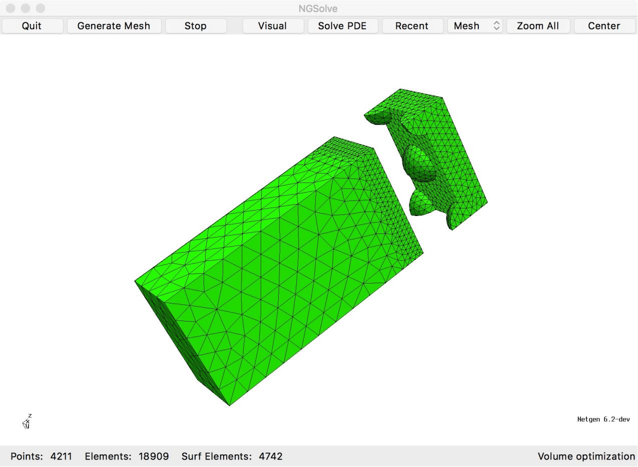
1. Python front end, C++ back end. Motivated by FEniCS but with complex arithmetic.
2. Has all elements in the de Rham diagram at all orders
3. Mesh generator, surface differential operators, etc
4. Currently under intensive development.

[21] M. AInsworth and J. Coyle, Hierarchic finite element bases on unstructured tetrahedral meshes, International Journal of Numerical Methods in Engineering, https://doi.org/10.1002/nme.847 (2003)

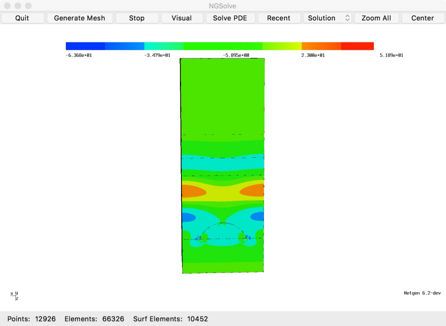
[22] J. Schöberl, https://ngsolve.org, Thanks to Christopher Lackner (TU Vienna)

An Example

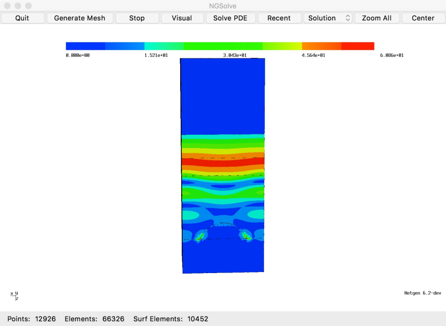
We are interested in using a hexahedral pattern of spherical metal caps in a metallic back reflector ($L_x = 350nm$, $L_y = \sqrt{3}L_x$, $\lambda_0 = 635\text{nm}$).



Some results: $|\mathbf{E}^s|$ and $|\mathbf{E}|$



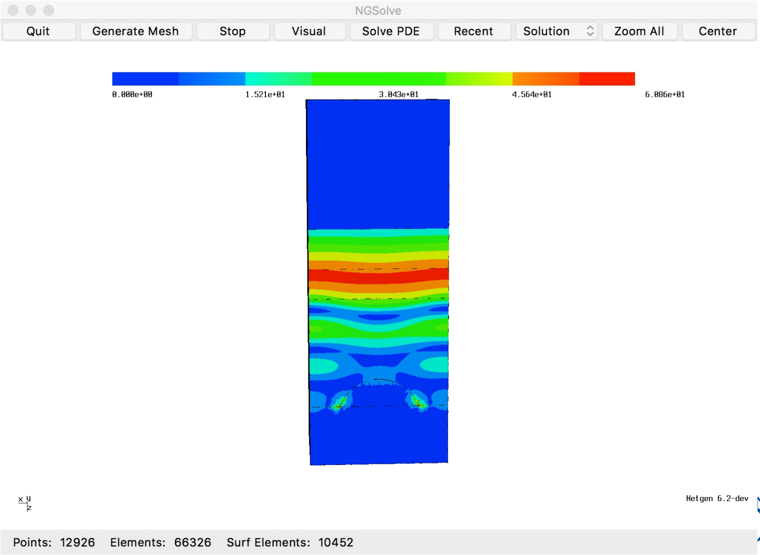
Density plot of $|\mathbf{E}^s|$



Density plot of $|\mathbf{E}|$

The total field in the physical domain

First component of the total electric field



Challenges and Opportunities

1. Problems become large quickly (in terms of storage and calculation). The main problem is to solve the linear algebra problem.
2. We are working on Reduced Basis methods to cut down the number of solves need to compute the electron generation rate $\Im(\epsilon_r)|\boldsymbol{E}|^2$ as a function of wave-length and incident direction (with Yanlai Chen and Manuel Solano).
3. An adaptive scheme is needed to refine the mesh to obtain a good estimate of the electron generation rate in the semiconductor layers.
4. There are interesting new Discontinuous Galerkin schemes that may help (HDG,...).

Thanks for the opportunity to visit and speak at ICERM!