Time Domain Integral Equations for Computational Electromagnetism

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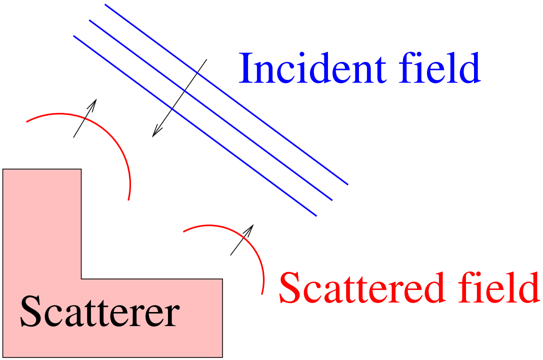
The scattering problem



Forward Problem: Given properties of the scatterer, the incident field, and the background, predict the scattered field.

Maxwell's Equations: Metallic Scatterer

Let D be a bounded domain (scatterer) with connected complement, boundary Γ and unit outward normal $\boldsymbol{\nu}$.

Suppose $\mathbf{E}^{inc}$ is a given incident wave (solution of Maxwell's equations vanishing on D for time $t < 0$). The scattered electric field $\boldsymbol{E} = \boldsymbol{E}(\mathbf{x}, t)$ satisfies

$$\begin{aligned} \frac{1}{c^2}\ddot{\boldsymbol{E}} + \nabla \times \nabla \times \boldsymbol{E} &= 0 \text{ in } \Omega := \mathbb{R}^3 \setminus \overline{D} \text{ for } t \in (0, T), \\ \boldsymbol{E} \times \boldsymbol{\nu} &= \boldsymbol{g} \text{ on } \Gamma \text{ for } t > 0, \\ \boldsymbol{E} = \dot{\boldsymbol{E}} &= 0 \text{ at } t = 0 \text{ in } \Omega. \end{aligned}$$

Here $\ddot{\boldsymbol{E}} = \partial^2 \boldsymbol{E}/\partial t^2$, c is the speed of light, and $\boldsymbol{g} = -\boldsymbol{E}^{inc} \times \boldsymbol{\nu}$.

Towards a time domain integral equation

We now derive the Convolution Quadrature semi-discrete boundary integral equation for the solution.

Write the problem as a first order system. Let $(\boldsymbol{E}, \boldsymbol{H})$ satisfy

$$\begin{cases} \frac{1}{c}\dot{\boldsymbol{H}} & = -\nabla \times \boldsymbol{E}, \text{ in } \Omega \text{ for } t > 0, \\ \frac{1}{c}\dot{\boldsymbol{E}} & = \nabla \times \boldsymbol{H}, \text{ in } \Omega \text{ for } t > 0, \\ \boldsymbol{E}(\boldsymbol{x}, 0) & = \boldsymbol{H}(\boldsymbol{x}, 0) = 0, \text{ in } \Omega, \\ \boldsymbol{E} \times \boldsymbol{\nu} & = \boldsymbol{g}, \text{ on } \Gamma \text{ for } t > 0. \end{cases}$$

Discretize only in time

For simplicity, consider the Backward Euler scheme (not the best in practice!). Define time steps $t_n = n\Delta t, n = 0, 1, \ldots, \Delta t > 0$, then let $\boldsymbol{E}^n := \boldsymbol{E}^n(\boldsymbol{x}) \approx \boldsymbol{E}(\boldsymbol{x}, t_n)$ and $\boldsymbol{H}^n := \boldsymbol{H}^n(\boldsymbol{x}) \approx \boldsymbol{H}(\boldsymbol{x}, t_n)$ for $n \geq 0$:

$$
\begin{cases}
\dfrac{\boldsymbol{H}^{n+1} - \boldsymbol{H}^n}{c\Delta t} & = -\nabla \times \boldsymbol{E}^{n+1}, \text{ in } \Omega \text{ for } n \geq 0, \\
\dfrac{\boldsymbol{E}^{n+1} - \boldsymbol{E}^n}{c\Delta t} & = \nabla \times \boldsymbol{H}^{n+1}, \text{ in } \Omega \text{ for } n \geq 0, \\
\boldsymbol{E}^0 & = \boldsymbol{H}^0 = 0, \text{ in } \Omega, \\
\boldsymbol{E}^{n+1} \times \boldsymbol{\nu} & = \boldsymbol{g}^{n+1} := \boldsymbol{g}(\cdot, t_{n+1}), \text{ on } \Gamma.
\end{cases}
$$

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Formal series

Let $\mathcal{E} := \sum_{n=0}^{\infty} \boldsymbol{E}^n \xi^n$ and $\mathcal{H} := \sum_{n=0}^{\infty} \boldsymbol{H}^n \xi^n$ where $\xi \in \mathbb{C}$ is a complex parameter.

Multiplying each discrete equation by ξ^{n+1} and adding these equations, as well as using the initial conditions:

$$\begin{cases} \left(\dfrac{1-\xi}{c\Delta t}\right)\mathcal{H} & = -\nabla \times \mathcal{E}, \text{ in } \Omega, \\ \left(\dfrac{1-\xi}{c\Delta t}\right)\mathcal{E} & = \nabla \times \mathcal{H}, \text{ in } \Omega, \\ \mathcal{E} \times \boldsymbol{\nu} & = \mathcal{G} \times \boldsymbol{\nu} := \left(\sum_{n=0}^{\infty} \boldsymbol{g}_n \xi^n\right) \times \boldsymbol{\nu} \text{ on } \Gamma. \end{cases}$$

Single Layer Ansatz

Eliminating $\mathcal{H}$ we obtain

$$\frac{1}{c^2}\left(\frac{1-\xi}{\Delta t}\right)^2 \mathcal{E} + \nabla\times(\nabla\times\mathcal{E}) = 0, \text{ in } \Omega.$$

We seek a solution using the following Anstaz:

$$\mathcal{E} = \mathrm{S}(s)\phi, \qquad s = \left(\frac{1-\xi}{\Delta t}\right),$$

where ϕ is an unknown tangential vector field on Γ,

$$(\mathrm{S}(s)\phi)(x) = -\frac{s^2}{c^2}\int_\Gamma K(x-y,s)\phi(y)\,d\sigma_y + \nabla\int_\Gamma K(x-y,s)\,\mathrm{div}_\Gamma\,\phi$$

and the fundamental solution of the Helmholtz equation is

$$K(d,s) := \frac{\exp(-s\|d\|/c)}{4\pi\|d\|}, \qquad \Re(s) > 0.$$

Boundary integral equation

Taking the tangential trace on the boundary Γ of D we see that ϕ satisfies

$$\mathbb{C}\left(\frac{1-\xi}{\Delta t}\right)\phi = \mathcal{G}.$$

where

$$\begin{aligned}\mathbb{C}(s)\phi &= -\frac{s^2}{c^2}\int_\Gamma K(x-y,s)\phi(y)\times\boldsymbol{\nu}(\boldsymbol{x}) \\ &\quad +\nabla_\Gamma\int_\Gamma K(x-y,s)\,\mathrm{div}_\Gamma\,\phi(\boldsymbol{y})\times\boldsymbol{\nu}(\boldsymbol{x})\end{aligned}$$

This is the electric field integral equation (EFIE).

Important Previous Work on the EFIE

1. A. Bendali, Numerical analysis of the exterior boundary value problem for the time harmonic Maxwell equations by a boundary finite element method. Part 1: The continuous problem, *Mathematics of Computation*, **43**, pp. 29-46 (1984).
2. A. Bendali, Numerical analysis of the exterior boundary value problem for the time harmonic Maxwell equations by a boundary finite element method. Part II: The discrete problem, *Mathematics of Computation*, **43**, pp. 47-68 (1984).

Marching on in Time

To write the integral equation as a discrete convolution, we expand the operator and ϕ as Taylor series:

$$\mathbb{C}\left(\frac{1-\xi}{\Delta t}\right) = \sum_{n=0}^{\infty} \boldsymbol{w}_n^{\Delta t}\xi^n, \qquad \text{and } \phi = \sum_{n=0}^{\infty} \phi_n \xi^n.$$

Using these representations

$$\begin{aligned}\mathbb{C}\left(\frac{1-\xi}{\Delta t}\right)\phi &= \left(\sum_{n=0}^{\infty} \boldsymbol{w}_n^{\Delta t}\xi^n\right)\left(\sum_{n=0}^{\infty} \phi_n \xi^n\right)\\ &= \sum_{n=0}^{\infty}\left(\sum_{m=0}^{\infty} \boldsymbol{w}_{n-m}^{\Delta t}\phi_m\right)\xi^n.\end{aligned}$$

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Backward Euler CQ weights

Recall $K(\boldsymbol{d}, s) = \exp(-s\|\boldsymbol{d}\|/c)/4\pi\|\boldsymbol{d}\|$. Expanding $K(\boldsymbol{x}-\boldsymbol{y}, (1-\xi)/(\Delta t))$ as a Taylor series in ξ:

$$\boldsymbol{w}_m^{\Delta t}\phi(\boldsymbol{x}) = -\frac{\Pi_T}{c^2}\int_\Gamma K_m^{2,\Delta t}(\boldsymbol{x}-\boldsymbol{y})\phi(\boldsymbol{y}) - \nabla_\Gamma \int_\Gamma K_m^{0,\Delta t}(\boldsymbol{x}-\boldsymbol{y})\,\mathrm{div}_\Gamma\,\phi(\boldsymbol{y})$$

where

$$K_m^{0,\Delta t}(\boldsymbol{x}-\boldsymbol{y}) = \frac{\exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{y}\|}{c\Delta t}\right)}{m!\,4\pi\|\boldsymbol{x}-\boldsymbol{y}\|}\left(\frac{\|\boldsymbol{x}-\boldsymbol{y}\|}{c\Delta t}\right)^m$$

and $K_m^{2,\Delta t}(\boldsymbol{x}-\boldsymbol{y})$ is obtained by differencing using the underlying ordinary differential equation solver (here Backward Euler).

Two approaches to solving the TDBIE

1. Marching on in Time (MoT): solve sequentially boundary integral equations

$$\boldsymbol{w}_0^{\Delta t}\phi_n = \boldsymbol{g}_n - \sum_{m=0}^{n-1} \boldsymbol{w}_{n-m}^{\Delta t}\phi_m$$

   We have arrived at an application of Convolution Quadrature[1] (CQ) to approximating the time domain electric field integral equation..

2. Parallel “frequency domain” approach: Choose a discrete set of ξ. Solve the corresponding frequency domain problem, and synthesize the time domain solution.[2]

Compare to the space-time Galerkin approach[3].

[1] C. Lubich, *Numer. Math.* **67**, 365-389 (1994).

[2] L. Banjai and S. Sauter, *SIAM J. Numer. Anal.* **47** (2008), pp. 227-249.

[3] I. Terrasse, PhD Thesis, Ecole Polytechnique, France (1993).

Semi-discrete weak form

After integration by parts, we get the following weak form: for each n we seek $\phi_n \in H^{-1/2}(\mathrm{Div};\Gamma)$ such that

$$
\begin{aligned}
&\sum_{j=0}^{n}\int_\Gamma\int_\Gamma\left\{\frac{K_{n-j}^{2,\Delta t}(\boldsymbol{x}-\boldsymbol{y})}{c^2}\boldsymbol{\phi}_j(\boldsymbol{y})\cdot\boldsymbol{\xi}(\boldsymbol{x})+K_{n-j}^{0,\Delta t}(\boldsymbol{x}-\boldsymbol{y})(\nabla_\Gamma\cdot\boldsymbol{\phi}_j)(\boldsymbol{y})(\nabla_\Gamma\cdot\boldsymbol{\xi})(\boldsymbol{x})\right\}dA(\boldsymbol{y})\,dA(\boldsymbol{x})\\
=&\quad -\int_\Gamma \boldsymbol{\nu}\times\boldsymbol{g}_n\cdot\boldsymbol{\xi}\,dA
\end{aligned}
$$

for all $\xi \in H^{-1/2}(\mathrm{Div};\Gamma)$ and $n = 0, 1, 2, \cdots, N$.

Spatial discretization on Γ is by mth order Raviart-Thomas elements in $H(\mathrm{Div};\Gamma)$ using the basis of Graglia, Wilton and Peterson (IEEE AP, 1997) or Rao, Wilson, Glisson (at lowest order).

Analysis of CQ

Classically, CQ is analyzed in the Laplace domain. Let $\mathcal{E} = \mathrm{S}(s)\phi$ where $\Re s = \sigma - \mathrm{i}\omega$, $\sigma > \sigma_0 > 0$. This satisfies

$$\nabla \times \nabla \times \mathcal{E} + \frac{s^2}{c^2}\mathcal{E} = 0 \text{ in } \Omega \text{ and } D$$

Critically, if

$$\gamma_N^+(\mathcal{E}) = (c/s)\nabla \times \mathcal{E}|_\Omega \times \boldsymbol{\nu}, \qquad \gamma_N^-(\mathcal{E}) = (c/s)\nabla \times \mathcal{E}|_D \times \boldsymbol{\nu},$$

then $[\![\gamma_N(\mathcal{E})]\!] = \gamma_N^-(\mathcal{E}) - \gamma_N^+(\mathcal{E}) = (s/c)\phi$ and $\gamma_D(\mathcal{E}) \times \boldsymbol{\nu} = \mathbb{C}(s)\boldsymbol{\phi}$ so since

$$-\int_\Gamma [\![\gamma_N(\mathcal{E})]\!] \cdot \gamma_D(\overline{\mathcal{E}}) \times \boldsymbol{\nu}\, dA = \int_{\Omega\cup D} s\|\mathcal{E}\|^2 + \frac{1}{s}\|\nabla \times \mathcal{E}\|^2\, dV$$

we obtain

$$\Re\left(\frac{s}{c}\int_\Gamma \phi \cdot \overline{\mathbb{C}(s)\boldsymbol{\phi}}, dA\right) = -\int_{\Omega\cup D} \sigma\|\mathcal{E}\|^2 + \frac{\sigma}{|s|^2}\|\nabla \times \mathcal{E}\|^2\, dV$$

This previous results show that $\mathbb{C}(s)$ is coercive and that as a map from $H^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$ to $H^{-1/2}(\mathrm{div}_\Gamma,\Gamma)$ the following bound holds

$$\|\mathbb{C}^{-1}\| \leq C|s|^1, \quad \|\mathbb{C}\| \leq C|s|^3.$$

This is sufficient to apply Lubich's theory to the semi discrete problem and find that for a pth order A-stable and L-stable method, then for $m \geq p+3$,

$$\|\boldsymbol{E}(\cdot,t_n) - \boldsymbol{E}^n\|_{H^{-1/2}(\mathrm{div}_\Gamma,\Gamma)} \leq C(\Delta t)^p \int_0^{t_n} \|\partial^m \boldsymbol{g}/\partial t^m\|_{H^{-1/2}(\mathrm{div}_\Gamma;\Gamma)}\, dt$$

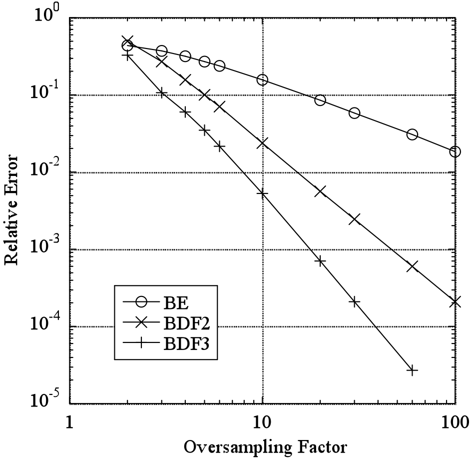
The analysis can be extended to the fully-discrete problem[4], and to IRK CQ discretization.[5]

[4] Q. Chen, P. Monk, D. Weile, Communications in Computational Physics, 11 (2012):383-399

[5] Ballani et al., Numer. Math. (2013) **123**, pp. 643-670

Convergence: 1m Diameter Conducting Sphere

Numerical results for the far field pattern[6]



- Error is in the L_1 norm for the RCS
- BE convergence is linear
- BDF2 convergence is quadratic
- BDF3 convergence is cubic and conditional
- The BDF3 kernel was computed using FFT.

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[6] X. Wang, D. Weile, R. Wildman and P. Monk.: *IEEE Trans. Ant. and Propagat.*, **56** 2442-2452 (2008).

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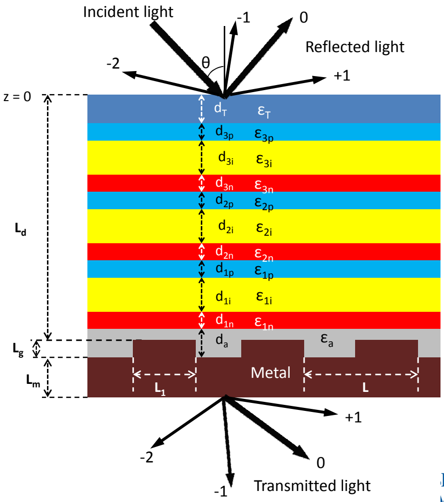
Model multiplasmonic solar cell

Thin film solar cell[7]

Wavelength of light of interest: 400-1200nm
Grating period $L \approx 400$nm
Height ≈ 2000nm

At this size and frequency, the field enters the metal.

Physical properties are generally frequency dependent (we assume a passive causal medium).



[7] M. Solano et al, Applied Optics, **52** (2013) 966-979

The Mathematical Model

Assume $\mu = \mu_0$ constant and $\epsilon_r := (\epsilon(x, z, t)/\epsilon_0)$. We seek solutions of Maxwell's equations that are independent of y. We can then split the solution into two *polarizations*. We shall consider the simplest:

- s-polarization: $u := E_2$ satisfies

$$\Delta u = \frac{\epsilon_r}{c^2} \star \frac{\partial^2 u}{\partial t^2}$$

Here $\star$ denotes time convolution and

$$u = u^i + u^s$$

where u^i is a known incident field and u^s is an unknown scattered field.

Incident field

We assume that u^i is a plane wave satisfying the wave equation with $\epsilon_r = \delta(t)$. In particular

$$u^i(x, z, t) = f(t - \mathbf{x} \cdot \mathbf{d}/c)$$

where $\mathbf{d} = (\sin\theta, \cos\theta)$, and f is such that $u^i(x, z, t) = 0$ for $t < 0$ and $(x, z) \in [0, L] \times [0, H]$ (H is the height of the grating).
The incident field u^i is not periodic in x, but

$$u^i(x + L, z, t) = f(t - d_1 L/c - \boldsymbol{d} \cdot \boldsymbol{x}/c) = u^i(x, z, t - d_1 L/c)$$

for any x, z and t so we impose, for all x and z,

$$u(x + L, z, t) = u(x, z, t - d_1 L/c).$$

This is the time domain counterpart of quasi-periodicity in the frequency domain.

The Time Domain (s-polarization)

Let $S=(0,L)\times\mathbb{R}$. We obtain the following equations for s-polarized light: given the incident field $u^i=u^i(x,z,t)$, the scattered field $u^s=u^s(x,z,t)$ satisfies

$$
\begin{aligned}
\frac{1}{c^2}\epsilon_r\star u^s_{tt} &= \Delta u^s+\frac{1}{c^2}(\epsilon_r-\delta)\star u^i_{tt} \text{ in } S\times\mathbb{R}\\
u^s(\cdot,0) &= 0 \text{ in } S\\
u^s_t(\cdot,0) &= 0 \text{ in } S\\
u^s(L,z,t) &= u^s(0,z,t-d_1L/c) \text{ in } \mathbb{R}\times\mathbb{R},\\
\frac{\partial u^s}{\partial x}(L,z,t) &= \frac{\partial u^s}{\partial x}(0,z,t-d_1L/c) \text{ in } \mathbb{R}\times\mathbb{R}.
\end{aligned}
$$

Change of variables

Use the change of variables[8]

$$w(x,z,t) = u^s(x,z,t+(x-L)d_1/c)$$

Then recalling $S=(0,L)\times\mathbb{R}$ we see that with $w^i(x,z,t)=f(t-d_2z/c)$:

$$\begin{aligned}
\frac{\epsilon_r - d_1^2\delta}{c^2}\star w_{tt} &= \Delta w - 2\frac{d_1}{c}w_{xt} + \frac{\epsilon_r-\delta}{c^2}\star w^i_{tt} \text{ in } S\times\mathbb{R}\\
w(\cdot,0) &= 0 \text{ in } S\\
w_t(\cdot,0) &= 0 \text{ in } S\\
w(L,z,t) &= w(0,z,t) \text{ for } z\in\mathbb{R},\ \ t>0\\
\frac{\partial w}{\partial x}(L,z,t) &= \frac{\partial w}{\partial x}(0,z,t) \text{ in } \text{ for } z\in\mathbb{R},\ \ t>0.
\end{aligned}$$

[8] M. Veysoglu, R. Shin, J. Kong, A finite-dfference time-domain analysis of wave scattering from periodic surfaces: Oblique incidence case, Journal of Electromagnetic Waves and Applications 7 (1993) 1595–1607 and V. Mathis, Etude de la diffraction d'ondes électromagnétiques par des réseaux dans le domaine temporel, École Polytechnique, 1996.

Analysis in the time domain

We again use Lubich's Convolution Quadrature technique[9] and tools from Bamberger and Ha Duong's Laplace transform approach.[10]

To use the Laplace transform

$$\hat{w}(x, z, s) = \int_0^\infty w(x, y, t) \exp(-st)\, dt, \quad s = \sigma - i\omega,$$

where $\sigma \in \mathbb{R}$ is fixed and $\sigma > 0$, while $\omega \in \mathbb{R}$.

[9] C. Lubich, On the multistep time discretization of linear initial-boundary value problems and their boundary integral equations, Numer. Math. 67 (1994) 365–89.

[10] A. Bamberger, T. H. Duong, Formulation variationnelle espace-temps pour le calcul par potentiel retarde de la diffraction d'une onde acoustique (I), Math. Meth. Appl. Sci. 8 (1986) 405–?435.

Laplace domain problem

Let Ω denote a bounded domain. We will use the following Sobolev space:

$$H^1_{\rm p}(\Omega) = \{v \in H^1(\Omega) \mid v(L,.) = v(0,.)\}$$

Recalling $s \in \mathbb{C}$ and $s \neq 0$ the norm is

$$\|v\|^2_{H^1_{\rm p}(\Omega)} = \int_\Omega \left[|\nabla v|^2 + \frac{|s|^2}{c^2}|v|^2 \right] dA.$$

Problem: Find $\hat{w}^s \in H^1_{\rm p}(S)$ such that

$$\begin{aligned} s^2 \frac{\hat{\epsilon}_r - d_1^2}{c^2} \hat{w}^s &= \Delta \hat{w}^s - 2s\frac{d_1}{c}\hat{w}^s_x + s^2 \frac{\hat{\epsilon}_r - 1}{c^2}\hat{w}^i \text{ in } S, \\ \frac{\partial \hat{w}^s}{\partial x}(L,z,t) &= \frac{\partial \hat{w}}{\partial x}(0,z,t) \text{ in } \mathbb{R}\times\mathbb{R}. \end{aligned}$$

Here $\hat{w}^i(x,y) = \hat{f}(s)\exp(-sd_1 z/c)$.

The weak Laplace domain problem

For $\hat{w}^s, \xi \in H^1_{\mathrm{p}}(S)$ define

$$\begin{aligned} a(\hat{w}^s,\xi) &= \int_S \left(\nabla \hat{w}^s \cdot \nabla \overline{\xi} + s^2 \frac{\hat{\epsilon}_r - d_1^2}{c^2} \hat{w}^s \overline{\xi} + 2s \frac{d_1}{c} \hat{w}^s_x \overline{\xi} \right) dA \\ \text{and } \hat{F} &= s^2 \left(\frac{\hat{\epsilon}_r - 1}{c^2} \right) \hat{w}^i . \end{aligned}$$

Then $\hat{w}^s \in H^1_p(S)$ satisfies

$$a(\hat{w}^s,\xi) = \int_S \hat{F}\,\overline{\xi}\,dA \text{ for all } \xi \in H^1_{\mathrm{p}}(S).$$

Coercivity

Coercivity (Bamberger & HaDuong): Select $\xi = s\hat{w}^s$ then

$$a(\hat{w}^s, s\hat{w}^s) \;=\; \int_S \left(\overline{s}|\nabla \hat{w}^s|^2 + s|s|^2 \frac{\hat{\epsilon}_r - d_1^2}{c^2} |\hat{w}^s|^2 + 2|s|^2 \frac{d_1}{c} \hat{w}^s_x \overline{\hat{w}^s} \right) \, dA$$

Then provided $\Re(s(\hat{\epsilon}_r - d_1^2)) > \alpha\sigma > 0$ for some constant α

$$\Re a(\hat{w}^s, s\hat{w}^s) = \sigma \int_S \left(|\nabla \hat{w}^s|^2 + |s|^2 \frac{\alpha}{c^2} |\hat{w}^s|^2 \right) \, dA$$

so

$$\Re a(\hat{w}^s, s\hat{w}^s) \geq \sigma \min(1, \alpha) \|\hat{w}^s\|^2_{H^1_{\mathrm{p}}(\Omega)}.$$

Laplace domain result[11]

Lax-Milgram gives:

Theorem

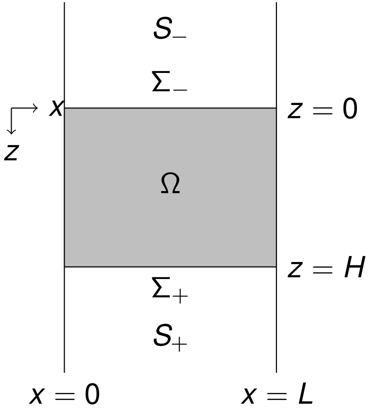
For each $s = \sigma - i\omega$, $\sigma > 0$, *suppose* $\Re(s(\hat{\epsilon}_r - d_1^2)) > \alpha\sigma > 0$, *then there exists a unique solution* $\hat{w}^s \in H^1_{\mathrm{p}}(S)$ *of the Laplace domain problem and*

$$\|\hat{w}^s\|_{H^1_{\mathrm{p}}(S)} \leq C\frac{1}{\sigma}\|\hat{F}\|_{L^2(S)}$$

Provided $\hat{\epsilon}_r$ is analytic in the right half of the complex plane, the inverse Laplace transform establishes existence of the time domain solution in suitable weighted space-time function spaces (time weight is $\exp(-2\sigma t)$). A good choice might be $\sigma = 1/T$ where T is the final time of interest.

[11] L.Fan and P. Monk, *Journal of Computational Physics*, **302** (2015) 97–113

Reduction to a bounded domain



A cartoon illustrating the parts of S. One period of the grating occupies Ω. In S_- and S_+ the parameters are constant.

Next we derive a Galerkin formulation for this elliptic problem[12] . Multiplying by a smooth test function ξ that is periodic in x, and integrating by parts we obtain

$$
\begin{aligned}
\int_\Omega \hat{F}\overline{\xi}\,dA &= \int_\Omega s^2\left(\left(\frac{\hat{\epsilon}_r - d_1^2}{c^2}\right)\hat{w}^s - \Delta \hat{w}^s + 2s\frac{d_1}{c}\frac{\partial \hat{w}^s}{\partial x}\right)\overline{\xi}\,dA \\
&= \int_\Omega \left[\nabla\,\hat{w}^s\cdot\nabla\overline{\xi} + s^2\left(\frac{\hat{\epsilon}_r - d_1^2}{c^2}\right)\hat{w}^s\overline{\xi} + 2s\frac{d_1}{c}\frac{\partial \hat{w}^s}{\partial x}\overline{\xi}\right]\,dA \\
&\quad - \int_{\Sigma_-\cup\Sigma_+}\frac{\partial \hat{w}^s}{\partial \nu}\overline{\xi}\,dx.
\end{aligned}
$$

To complete the derivation we need to use the fact that $\hat{w}^s$ is an H^1_{p} solution of the Helmholtz problem below Σ_- and above Σ_+.

[12] Li Fan and P. Monk, Time Dependent Scattering from a Grating using Convolution Quadrature and the Dirichlet-to-Neumann map, (2017) submitted for publication.

Towards the D-t-N map

Let κ_n be defined by

$$\kappa_n = \frac{s}{c}\sqrt{1 - \left(\frac{2in\pi c}{sL} - d_1\right)^2}$$

where we choose κ_n such that $\Re(\kappa_n) > 0$. Then for $y < 0$

$$\hat{w}^s(x,z) = \sum_{n\in\mathbb{N}} \hat{w}_n^s \exp(i2\pi nx/L)\exp(\kappa_n z), \text{ for } z < 0.$$

Then

$$\left.\frac{\partial \hat{w}^s}{\partial \nu}\right|_{\Sigma_-} = -\sum_{n\in\mathbb{N}} \hat{w}_n^s \kappa_n \exp(i2\pi nx/L).$$

We then have the following expression for the D-t-N map $T_-(s)$ on Σ_-

$$\begin{aligned}\hat{w}^s|_{z=0} &= \sum_{n\in\mathbb{N}} \hat{w}_n^s \exp(i2\pi nx/L),\\ T_-(s)\hat{w}^s &= -\sum_{n\in\mathbb{N}} \hat{w}_n^s \kappa_n \exp(i2\pi nx/L).\end{aligned}$$

Then

Lemma

The D-t-N map $T_-(s) : H_{\mathrm{p}}^{1/2}(\Sigma_-) \to H_{\mathrm{p}}^{-1/2}(\Sigma_-)$ and there is a constant C independent of s such that

$$\|T_-(s)u\|_{H_{\mathrm{p}}^{-1/2}(\Sigma_-)} \leq C\|u\|_{H_{\mathrm{p}}^{1/2}(\Sigma_-)}, \qquad \forall u \in H_{\mathrm{p}}^{1/2}(\Sigma_-).$$

This result also holds for $T_+(s)$.

We can now write a Galerkin formulation for the Laplace domain scattering problem. We seek $\hat{w}^s \in H^1_{\mathrm{p}}(\Omega)$ such that

$$b(\hat{w}^s, \xi) = \int_\Omega \hat{F}\,\overline{\xi}\, dA \text{ for all } \xi \in H^1_{\mathrm{p}}(\Omega),$$

where, for any $q, \xi \in H^1_{\mathrm{p}}(\Omega)$, we have

$$\begin{aligned} b(q,\xi) &= \int_\Omega \left[\nabla q \cdot \nabla\overline{\xi} + s^2\left(\frac{\hat{\epsilon}_r - d_1^2}{c^2}\right) q\overline{\xi} + 2s\frac{d_1}{c}\frac{\partial q}{\partial x}\overline{\xi}\right] dA \\ &\quad - \int_{\Sigma_-} (T_-(s)q)\overline{\xi}\, dx - \int_{\Sigma_+} (T_+(s)q)\overline{\xi}\, dx. \end{aligned}$$

Spatial discretization

1. $\mathcal{Q}_h$: mesh of quadrilaterals of maximum diameter h obtained by mapping from a reference square element using a bilinear mapping
2. Q_h: continuous finite elements on $\mathcal{Q}_h$ obtained by mapping a polynomial of degree at most q in each variable on the reference element by a bilinear mapping.
3. Trigonometric subspace of dimension $2N+1$ given by

$$\mathcal{P}_N := \mathrm{span}\left\{\exp(i2\pi nx/L) \mid -N \leq n \leq N,\ n \in \mathbb{Z}\right\}$$

4. $L^2(\Sigma_-)$ orthogonal projection $P_N : L^2(\Sigma_-) \to \mathcal{P}_N$ (similarly on Σ_+).

The discrete Laplace transformed field $\hat{w}^s_{h,N} \in Q_h$ is defined to satisfy

$$b_N(\hat{w}^s_{h,N}, \xi_h) = \int_S \hat{F}\,\overline{\xi}\,dA, \qquad \forall \xi_h \in Q_h.$$

where

$$\begin{aligned} b_N(\hat{w}^s_{h,N}, \xi_h) \;=\; & \int_\Omega \Bigg[\nabla\, \hat{w}^s_{h,N} \cdot \nabla \overline{\xi}_h + s^2 \left(\frac{\hat{\epsilon}_r - d_1^2}{c^2}\right) \hat{w}^s_{h,N}\overline{\xi}_h \\ & + 2s\frac{d_1}{c}\,\frac{\partial \hat{w}^s_{h,N}}{\partial x}\overline{\xi}_h\Bigg]\,dA - \int_{\Sigma_-} T_-(s) P_N \hat{w}^s_{h,N} P_N \overline{\xi}_h\,dx \\ & - \int_{\Sigma_+} T_+(s) P_N \hat{w}^s_{h,N} P_N \overline{\xi}_h\,dx. \end{aligned}$$

Multistep discretization in time

Suppose we use a k-step multistep method in time using a uniform time step $\Delta t > 0$. Let $t_m = m\Delta t$, $m \in \mathbb{Z}$. In particular, suppose that when applied to the initial value problem for the ordinary differential equation $y' = f(t, y)$, $t > 0$ where $y(0) = 0$, the method is

$$\sum_{j=0}^{k} \alpha_j y_{m-j} = \Delta t \sum_{j=0}^{k} \beta_j f(t_{m-j}, y_{m-j}), \quad m = 1, 2, \cdots$$

where we assume $\alpha_0/\beta_0 > 0$, $y_m = 0$ if $m \leq 0$ and we expect $y_m \approx y(t_m)$. Then define the rational function γ of $\zeta \in \mathbb{C}$ by

$$\gamma(\zeta) = \frac{\sum_{j=0}^{k} \alpha_j \zeta^k}{\sum_{j=0}^{k} \beta_j \zeta^j}.$$

BE: $\gamma(\zeta) = (1 - \zeta)$

The time-discrete Laplace transform domain scattered field $\hat{w}_{h,N}^{s,\Delta t} \in Q_h$ satisfies the weak problem with s replaced by $\gamma(\zeta)/\Delta t$:

$$\begin{aligned} & \int_\Omega \left[\nabla \hat{w}_{h,N}^{s,\Delta t} \cdot \nabla \overline{\xi} + \left(\frac{\gamma(\zeta)}{\Delta t} \right)^2 \left(\frac{\hat{\epsilon}_r - d_1^2}{c^2} \right) \hat{w}_{h,N}^{s,\Delta t} \overline{\xi} + 2 \frac{\gamma(\zeta)}{\Delta t} \frac{d_1}{c} \frac{\partial \hat{w}_{h,N}^{s,\Delta t}}{\partial x} \overline{\xi} \right] dA \\ & - \int_{\Sigma_-} T_-(\gamma(\zeta)/\Delta t) P_N \hat{w}_{h,N}^{s,\Delta t} \overline{\xi} \, dx - \int_{\Sigma_+} T_+(\gamma(\zeta)/\Delta t) P_N \hat{w}_{h,N}^{s,\Delta t} \overline{\xi} \, dx \\ = \quad & \int_\Omega \hat{F}(\gamma(\zeta)/\Delta t) \overline{\xi} \, dA, \qquad \forall \xi \in Q_h. \end{aligned}$$

This equation holds for all $|\zeta| < 1$ and $\zeta \in \mathbb{C}$.

Now we have fully discrete error estimate:

Theorem

Suppose we use a pth-order A-stable method such that $\gamma(\zeta)$ has no poles on the unit circle to discretize in time. For sufficiently smooth F, the time discrete finite element solution $w^s_{h,N}(t_n)$, $n = 0, 1, \cdots$, satisfies estimate

$$\begin{aligned}\|w^{s,\Delta t}_{h,N}(t_n) - w^s(t_n)\|_{H^1_{\mathrm{p}}(\Omega)} \quad \leq \quad & C\left((\Delta t)^p \int_0^T \left|\frac{\partial^{p+2}F}{\partial t^{p+2}}\right| dt + \|w^s - v_h\|_{H^2_0((0,T);H^1_{\mathrm{p}}(\Omega))}\right. \\ & \left. + \|P_N w^s - w^s\|_{H^2_0((0,T);H^{1/2}(\Sigma_-))} + \|P_N w^s - w^s\|_{H^2_0((0,T);H^{1/2}(\Sigma_+))}\right).\end{aligned}$$

for any $v_h \in H^2_0((0,T), Q_h)$. Here the constant C depends on T and Σ_- but is independent of u, h, N, Δt and v_h.

Time stepping

For simplicity assume that ϵ_r is frequency independent. We prefer to compute using the total field $\hat{w} = \hat{w}^s + \hat{w}^i$. The total field $\hat{w} \in H^1_{\rm p}(\Omega)$ satisfies

$$b(\hat{w}, \xi) = \int_{\Sigma_-} \left(\frac{\partial \hat{w}^i}{\partial \nu} - T_-(s)\hat{w}^i \right) \overline{\xi}\, dx, \qquad \forall \xi \in H^1_{\rm p}(\Omega).$$

The corresponding fully discrete Laplace domain problem is to find $\hat{w}^{\Delta t}_{h,N} \in Q_h$ such that

$$b_N(\hat{w}^{\Delta t}_{h,N}, \xi) = \int_{\Sigma_-} \left(\frac{\partial \hat{w}^i}{\partial \nu} - T_-(\gamma(\zeta)/\Delta t) P_N \hat{w}^i \right) \overline{\xi}\, dx, \qquad \forall \xi \in Q_h,$$

with $s = (\gamma(\zeta)/(\Delta t)$. To simplify the derivation we set

$$\hat{z}^{\Delta t}_{h,N} = (\gamma(\zeta)/(\Delta t))\hat{w}^{\Delta t}_{h,N}$$

The fully discrete Laplace domain problem becomes the problem of finding $(\hat{w}_{h,N}^{\Delta t}, \hat{z}_{h,N}^{\Delta t}) \in Q_h \times Q_h$ such that

$$\int_\Omega \left[\nabla \hat{w}_{h,N}^{\Delta t} \cdot \nabla \overline{\xi} + \left(\frac{\gamma(\zeta)}{\Delta t}\right)\left(\frac{b-d_1^2}{c^2}\right)\hat{z}_{h,N}^{\Delta t}\overline{\xi} + 2\frac{d_1}{c}\frac{\partial \hat{z}_{h,N}^{\Delta t}}{\partial x}\overline{\xi}\right] dA$$

$$-\int_{\Sigma_-} T_-(\gamma(\zeta)/\Delta t) P_N \hat{w}_{h,N}^{\Delta t}\overline{\xi} - \int_{\Sigma_+} T_+(\gamma(\zeta)/\Delta t) P_N \hat{w}_{h,N}^{\Delta t}\overline{\xi}$$

$$= \int_{\Sigma_-}\left(\frac{\partial \hat{w}^i}{\partial \nu} - T_-(\gamma(\zeta)/\Delta t) P_N \hat{w}^i\right)\xi, \qquad \forall \xi \in Q_h,$$

$$(\gamma(\zeta)/(\Delta t))\hat{w}_{h,N}^{\Delta t} = \hat{z}_{h,N}^{\Delta t}$$

for all $|\zeta| < 1$ and $\zeta \in \mathbb{C}$.

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To take the inverse discrete Laplace transform of the above equation set

$$\hat{w}_{h,N}^{\Delta t} = \sum_{m=0}^{\infty} w_{h,N}^{\Delta t,m} \zeta^n, \qquad \hat{z}_{h,N}^{\Delta t} = \sum_{m=0}^{\infty} z_{h,N}^{\Delta t,m} \zeta^n$$

where $w_{h,N}^{\Delta t,m} \in Q_h$ and $z_{h,N}^{\Delta t,m} \in Q_h$ are independent of ζ. Equating terms in ζ shows that the above equation gives the multistep scheme applied to $\partial w/\partial t = z$ or

$$\sum_{j=0}^{k} \alpha_j w_{h,N}^{\Delta t,m-j} = \Delta t \sum_{j=0}^{k} \beta_j z_{h,N}^{\Delta t,m-j}.$$

The same process gives the time stepping equivalent of the first equation. The only remaining difficulty is to expand $(\sum_{j=0}^{k} \beta_j \zeta^j) T_{\pm}(\gamma(\zeta)/\Delta t)$ as a power series in ζ.

This requires finding the Taylor series of

$$\tilde{\kappa}_n^{\Delta t} = \frac{\sum_{j=0}^{k} \alpha_j \zeta^j}{c} \sqrt{1 - \left(\frac{2in\pi c\Delta t}{L\gamma(\zeta)} - d_1 \right)^2} = \sum_{\ell=0}^{\infty} \tilde{\kappa}_{n,\ell}^{\Delta t} \zeta^\ell .$$

At level ℓ the discrete in time operator $\tilde{T}_-^{\Delta t,\ell} : \mathcal{P}_N \to \mathcal{P}_N$ is given for

$$u = \sum_{n=-N}^{N} u_n \exp(2\pi nx/L)$$

by

$$\tilde{T}_-^{\Delta t,\ell} u = \sum_{n=-N}^{N} \tilde{\kappa}_{n,\ell}^{s,\Delta t} u_n \exp(2n\pi ix/L)$$

and similarly for $\tilde{T}_+^{\Delta t,\ell}$.

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The first fully discrete equation gives, at the mth timestep,

$$
\begin{aligned}
&\int_\Omega \sum_{j=0}^{k} \left(\frac{b-d_1^2}{c^2}\right) \alpha_j z_{h,N}^{\Delta t, m-j} \overline{\xi} - \int_{\Sigma_-} \sum_{j=0}^{m} \left(\tilde{T}_-^{\Delta t, j} P_N w_{h,N}^{\Delta t, m-j}\right) \overline{\xi} \\
&\quad - \int_{\Sigma_+} \sum_{j=0}^{m} \left(\tilde{T}_+^{\Delta t, j} P_N w_{h,N}^{\Delta t, m-j}\right) \overline{\xi} \\
= &\quad -\Delta t \int_\Omega \sum_{j=0}^{k} \beta_j \left(\nabla w_{h,N}^{\Delta t, m-j} \cdot \nabla \overline{\xi} + \frac{2d_1}{c} \frac{\partial z_{h,N}^{\Delta t, m-j}}{\partial x} \overline{\xi}\right) + \Delta t \int_{\Sigma_-} \sum_{j=0}^{k} \beta_j \frac{\partial w^i}{\partial \nu}(\cdot, t_{m-j}) \overline{\xi} \\
&\quad - \int_{\Sigma_-} \sum_{j=0}^{m} \tilde{T}_-^{\Delta t, j} P_N w^i(\cdot, t_{m-j}) \overline{\xi} \quad \text{for all } \xi \in Q_h,
\end{aligned}
$$

for $m = 1, 2, \cdots$. The fields vanish if the index $m - j \leq 0$.

We need the coefficients $\tilde{\kappa}_{p,\ell}^{\Delta t}$. For BDF2

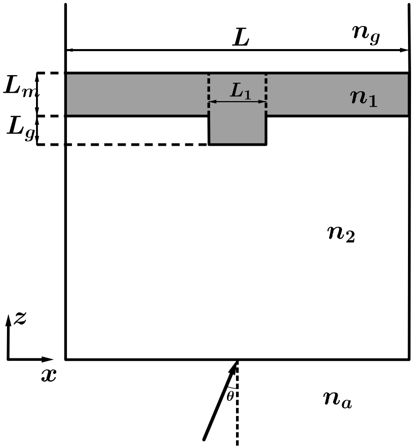
$$
\begin{aligned}
\tilde{\kappa}_{n,0}^{\Delta t} &= \frac{\sqrt{4\pi^2 c^2(\Delta t)^2 n^2 + (4i)L\pi c d_1(\Delta t)n - L^2 d_1^2 + L^2}}{Lc}, \\
\tilde{\kappa}_{n,1}^{\Delta t} &= \frac{2}{3}\frac{(-2\pi^2 c^2(\Delta t)^2 n^2 - (5i)L\pi c d_1(\Delta t)n + 2L^2 d_1^2 - 2L^2)}{Lc\sqrt{4\pi^2 c^2(\Delta t)^2 n^2 + (4i)L\pi c d_1(\Delta t)n - L^2 d_1^2 + L^2}}.
\end{aligned}
$$

In general we follow Banjai and Sauter and approximate the coefficients using a discrete approximation to the Cauchy integral formula:

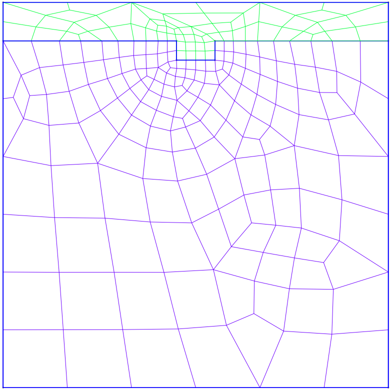
$$
\tilde{\kappa}_{n,\ell}^{s,\Delta t} = \frac{1}{2\pi i}\int_C \frac{\tilde{\kappa}_n^{s,\Delta t}(\zeta)}{\zeta^{\ell+1}}\, d\zeta
$$

where C is a circle of radius $\lambda < 1$ centered at the origin in the complex plane (using their choice of λ).

Frequency dependent model problem



Metallic grating, Drude model



Incoming wave with $\theta = 0^\circ$

$$f(t) = \begin{cases} 0 & \text{for } t < 0 \text{ or } t > \pi/ \\ \sin^4(4t) & \text{for } 0 < t < \pi/4. \end{cases}$$

In the fictitious "metal" we use the artificial choice

$$\epsilon_r = 4 + \frac{10}{s(1 + s/2)}$$

otherwise $\epsilon_r = 1$

Some references to CQ

- The CQ technique for TDIEs was first suggested by C. Lubich[3]. For a thorough introduction see the book of F.-J. Sayas.[13]
- Practical use in elastodynamics: M. Schanz and H. Antes[14].
- W. Kress and S. Sauter [15], and W. Hackbusch, W. Kress and S. Sauter[16].
- Error estimates for general Helmhotz problems have been proved by A. Laliena and F.-J. Sayas[17].

13 Francisco-Javier Sayas, Retarded Potentials and Time Domain Boundary Integral Equations, Springer 2016.

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15 *IMA J. Numer. Anal.* **28** 162-185, (2008)

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Further contributions to CQ-TDBIE for Maxwell

- First application to PEC Maxwell[18], and then to penetrable problems with requency dependent coefficients and IRK for Maxwell[19]
- Convergence of Maxwell Electric Field Integral Equation[20]
- Convergence of IRK for Maxwell[21], and penetrable homogeneous problems [22].
- Combined Field Integral Equation method for Maxwell's equations[23]
- Waveguides[24]

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[24] L. Fan, P. Monk and V. Selgas, in Trends in Differential Equations and Applications (2016) F. Ortegón, M. Redondo and J.R. Rodríguez, Eds., Springer, pp. 321-337.

Current work

- Inverse problems for penetrable media (with V. Selgas)
- 3D time dependent grating structures (i.e. full Maxwell).

Best wishes Professor Bendali!