An iterative solver enhanced with extrapolation for steady-state high-frequency Maxwell problems

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Basic Outline

1. Model and Discretization
2. Iterative Solver
3. Extrapolation
4. Numerical Results
Overview of the model problem

- High-frequency Maxwell problem (optical regime, \(2.7 \cdot 10^{14} \text{Hz} < f < 10^{15} \text{Hz},\) \(0.3 \mu m < \lambda < 1.1 \mu m\) resp.)
- Simple box-shaped domain geometries
- Both media of positive and negative permittivities
- Rough interfaces between media
- Periodic and absorbing boundaries (PML)

Figure: Schematic of a multi-junction thin-film silicon solar cell

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Overview of the numerical scheme

- Finite Difference Frequency Domain discretization (FDFD)
- Spatial discretization based on Yee cells
- Finite Integration Technique (FIT)
- Explicit leap-frog time stepping scheme
- Algebraically speaking a Richardson method
- Prony’s extrapolation method

Figure: EM field in a solar cell structure
Under model assumptions valid for optical applications (linearity, isotropy and non-dispersivity), Maxwell’s equations can be stated as follows:

- **Faraday’s Law:**
  \[ \mu \frac{\partial}{\partial t} H = -\nabla \times E - \sigma^* H \]  
  (1)

- **Ampère’s Law:**
  \[ \epsilon \frac{\partial}{\partial t} E = \nabla \times H - \sigma E \]  
  (2)

- **Gauß’s Law for Electric Fields:**
  \[ \nabla \cdot (\epsilon E) = 0 \]  
  (3)

- **Gauß’s Law for Magnetic Fields:**
  \[ \nabla \cdot H = 0 \]  
  (4)
In a time-harmonic setting of (1),(2), we seek a solution:

\[ H(\xi,t) = \hat{H}(\xi) \exp(i\omega t) \]
\[ E(\xi,t) = \hat{E}(\xi) \exp(i\omega t) \]

Therefore, the problem with source terms \( S_{\hat{E}}, S_{\hat{H}} \) of frequency \( \omega \) can be stated as: Find \((\hat{H}, \hat{E})\) that satisfies:

\[ i\omega \mu(\xi) \hat{H}(\xi) = -\nabla \times \hat{E}(\xi) - \sigma^*(\xi) \hat{H}(\xi) + \mu(\xi) S_{\hat{H}}(\xi) \]
\[ i\omega \epsilon(\xi) \hat{E}(\xi) = \nabla \times \hat{H}(\xi) - \sigma(\xi) \hat{E}(\xi) + \epsilon(\xi) S_{\hat{E}}(\xi) \]

with \( \xi \in \Omega \subset \mathbb{R}^3 \) a box-shaped domain.
After discretization in time and space (FDFD, Yee cells, explicit leap-frog), we get the following iterative scheme:

\[
\frac{\mu}{\tau} \left( \alpha^2 \hat{H}^{k+1} - \hat{H}^k \right) = -\alpha \nabla_h \times \hat{E}^k - \frac{\sigma^*}{2} \left( \hat{H}^k + \alpha^2 \hat{H}^{k+1} \right) + \mu S \hat{H}
\]

\[
\frac{\varepsilon}{\tau} \left( \alpha^2 \hat{E}^{k+1} - \hat{E}^k \right) = \alpha \nabla_h \times \hat{H}^{k+1} - \frac{\sigma}{2} \left( \hat{E}^k + \alpha^2 \hat{E}^{k+1} \right) + \varepsilon S \hat{E}
\]

for time steps \( \tau > 0 \), where

\[
\alpha := \alpha(\tau) = \exp \left( i\omega \frac{1}{2\tau} \right)
\]

and

\[
H^k(\xi, k\tau) = \hat{H}^k(\xi)\alpha^{2k}, \quad E \left( \xi, \frac{2k + 1}{2\tau} \right) = \hat{E}^k(\xi)\alpha^{2k+1}
\]

\[
H \left( \xi, \frac{2k + 1}{2\tau} \right) \approx \frac{1}{2} \alpha^{2k} \left( \hat{H}^k(\xi) + \alpha^2 \hat{H}^{k+1}(\xi) \right)
\]
Introduce a local modification to the iteration scheme (THIIM) to deal with instabilities in media of negative permittivity $\varepsilon < 0$:

$$\frac{\varepsilon}{\tau} \left( \alpha^2 \hat{E}^k - \hat{E}^{k+1} \right) = \alpha \nabla_h \times \hat{H}^{k+1} - \frac{\sigma}{2} \left( \alpha^2 \hat{E}^k + \hat{E}^{k+1} \right) + \varepsilon S \hat{E}$$

This yields a sparse system matrix consisting of blocks of the following kind:

$$M := \begin{pmatrix}
\frac{2\mu - \tau \sigma^*}{\alpha^2 (2\mu + \tau \sigma^*)} & \frac{-2\tau}{\alpha (2\mu + \tau \sigma^*)} & \nabla_h \\
\frac{2\tau}{\alpha (2\varepsilon + \tau \sigma)} & \frac{2\mu - \tau \sigma^*}{\alpha^2 (2\varepsilon + \tau \sigma)} & \nabla_h \\
\frac{2\tau \alpha}{2|\varepsilon| + \tau \sigma} & \frac{2\mu - \tau \sigma^*}{\alpha^2 (2\mu + \tau \sigma^*)} & \nabla_h \\
\end{pmatrix}$$

with eigenpairs $(\lambda_m, e_m), \|e_m\| = 1, |\lambda_m| < 1 \forall m$ for $0 < \tau$ sufficiently small and

$$M(\tau) = \sum_m e_m \lambda_m e_m^T \xrightarrow{\tau \to 0} \text{Id}.$$
Define algebraic state variables and load vectors:

\[ x^k := \left( \hat{H}^k, \hat{E}^k \right)^T = \left( \hat{H}^k, \hat{E}^k \bigg|_{\varepsilon > 0}, \hat{E}^k \bigg|_{\varepsilon < 0} \right)^T, \quad b := \tau \left( S_{\hat{H}}, S_{\hat{E}} \right)^T \]

and restate the discretized time-harmonic Maxwell problem:
Find a solution \( x^* = (\hat{H}, \hat{E})^T \subseteq \mathbb{R}^d \) such that:

\[ x^* = M x^* + b \]

or equivalently: Solve the system

\[ (\text{Id} - M) x^* = b \]
Explicit FDFD iteration scheme:

\[
x^0 = 0
\]

\[
x^{k+1} = M x^k + b = \sum_{\kappa=0}^{k-1} M^\kappa b
\]

converges slowly\(^2\). Approximation error:

\[
x^* - x^k = M (x^* - x^{k-1}) = M^k (x^* - x^0) = M^k x^* = \sum_{\kappa=k}^{\infty} M^\kappa b
\]

\(^2\)Recall the corresponding Neumann series: \(\sum_{\kappa=0}^{\infty} M^\kappa = (\text{Id} - M)^{-1}\)
High iteration numbers (typically \(10^4 - 10^6\)) to convergence up to a suitable prescribed tolerance

Figure: Transient signal and iterations to convergence up to a tolerance of \(10^{-4}\)
How to speed up convergence?

\[ x^{k+1} - x^k = M^k b = \sum_m e_m \lambda_m^k e_m^T \]

Idea: Use low order model to capture the (few) dominant eigenvalue contributions of the system matrix to the iterates.

\[ M \approx \sum_{m \in \{ n \in \mathbb{N} : |\lambda_n| > \theta \}} e_m \lambda_m^k e_m^T \]

Problem: How to get an estimate of the dominant eigenpairs (or their effect on given iterates)?

Approach: Use an extrapolation method based on component-wise samples of successive iterates

Pros: Allows for observation of oscillatory behavior caused by resonant modes.

Cons: Decouples the degrees of freedom.
Step 1: Establish dependence of iterates on previous iterates

\[ P_s := \begin{pmatrix} x_s^{k_l} & x_s^{k_{l-1}} & \cdots & x_s^{k_1} \\ x_s^{k_{l+1}} & \cdots & \cdots & x_s^{k_2} \\ \vdots & \cdots & \cdots & \vdots \\ x_s^{k_{n-1}} & x_s^{k_{n-2}} & \cdots & x_s^{k_{n-l}} \end{pmatrix}, \quad u := \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_l \end{pmatrix}, \quad r_s := \begin{pmatrix} -x_s^{k_{l+1}} \\ -x_s^{k_{l+2}} \\ \vdots \\ -x_s^{k_n} \end{pmatrix} \]

We solve for \( u \):

\[ P_s u = r_s \]

Equivalent to:

\[ \sum_{m=0}^{l} u_m x_s^{k_{t-m}} = 0 \quad \forall t = l + 1 \ldots n, \text{ where } u_0 = 1 \quad (5) \]
Step 2: Exponential basis

- Represent \( x_s^k \) as linear combination of exponentials \( z^k = \exp(i f k) \)

- Complex-valued \( f \) relates to frequency (\( \text{Re} f \)) and attenuation (\( -\text{Im} f \))

Determine roots \( \{ z_m : p(z_m) = 0 \} \) of:

\[
p(z) = 1 + \sum_{m=1}^{l} u_m z^{l+1-m}
\]  \( (6) \)

Roots \( z_m = \exp(i f_m) \) represent distinct frequencies of the system (as detected in the respective degree of freedom \( s \) corresponding to some spatial position \( \xi \in \Omega \)).
Step 3: Determine amplitudes

\[ Q_s := \begin{pmatrix} z_{k1}^1 & z_{k1}^2 & \cdots & z_{k1}^l \\ z_{k2}^1 & \cdots & \cdots & z_{k2}^l \\ \vdots & \ddots & \ddots & \vdots \\ z_{kn}^1 & z_{kn}^2 & \cdots & z_{kn}^l \end{pmatrix}, \quad a := \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_l \end{pmatrix}, \quad w_s := \begin{pmatrix} x_{s1}^{k_1} \\ x_{s2}^{k_2} \\ \vdots \\ x_{sn}^{k_n} \end{pmatrix} \]

- Denote iterates \( x_{s}^{k_t} \) as a superposition of frequencies:

\[ x_{s}^{k_t} = \sum_{m=1}^{l} a_m \exp(ift) \]

- Solve system to get corresponding amplitudes:

\[ Q_s a = w_s \]

- Filter amplitude-frequency pairs to get behavior for \( t \to \infty \)
Remarks

- *System generally overdetermined* \((n \geq 2l)\)
- *Solve in the least squares sense*
- *Leads to singular value decomposition (SVD)*
- *Minimizes:*
  \[
  \|P_s u - r_s\|_2 = \inf_{v \in \mathbb{R}^l} \|P_s v - r_s\|_2 \tag{7}
  \]
  \[
  \|Q_s a - w_s\|_2 = \inf_{v \in \mathbb{R}^l} \|Q_s v - w_s\|_2 \tag{8}
  \]
- *Numerically robust*
Typical distribution of amplitude and frequency pairs as determined by Prony’s method

Figure : The signal’s frequency-amplitude pairs (abs)

Stabilization: Attenuation \( a = -\text{Im} f \). Discard frequencies with \( a > \varepsilon \), assume that frequencies \( a \leq \varepsilon \) are 0.
Convergence of a single degree of freedom:

![Error: Iterated vs extrapolated signal](image)

Order 6 extrapolation error vs iterative error, filter by frequency, 0.97 frequencies used on average

Figure: Error: Iterated vs extrapolated signal

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Convergence of the whole simulation domain:

Figure: $\|\cdot\|_2$ Error: Iterated vs extrapolated signal

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Numerical Results

Figure: Experimental and simulation results

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Figure: Absorption for smooth and rough interfaces

Figure: Quantum efficiency under different angles of incidence
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Summary

- Explicit iteration scheme for high-frequency Maxwell problems
- Stable for negative permittivity
- Extrapolation reduces error

Future work

- How to improve the extrapolation accuracy? (e.g. by choice of better samples)
- Can a hierarchical basis approach reduce local inaccuracies?
- What about the divergence of the extrapolated signal? (a constraint in the original system of PDEs)
- How to make use of multigrid methods?
Thank you for your attention.

References:

- A. Taflove, S. Hagness: Computational Electrodynamics, Artech House, 2005