Exact simulation of the diffraction of large, high-NA DOE-sections with $O(N\log N)$ time and memory resort

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OUTLINE

→ DOE simulation
→ Generalized Source Method
→ Three breakthroughs that make GSM ultrafast and memory sparing
→ Numerical benchmarks
→ Conclusions
DOE SIMULATION

Quartz $n = 1.46 \, k = 0$

$n = 1.46 - 2.35 \, k < 0.01$

 Thickness $< 1000 \, \text{nm}$
Requirements on a new method for today’s objectives in *DOE simulation*:

- Rigorous
- Fast and memory-sparing

**Challenge:**

DOE reference method $\equiv$ DOE fast tool

Current exact methods (FDTD, FMM (RCWA)) are very far from this objective
A DOE is a planar structure

Plane waves are a basic solutions characterized by their in-plane wavevector projections $k_x, k_y$

An efficient resolution technique has to operate

# in-plane in the reciprocal $k$-space $k_x, k_y$
# in the direct space normally to the plane, along $z$
The electromagnetic problem is characterized by the spatial permittivity distribution:

\[ \varepsilon = \varepsilon(r) \]

1. Replace the initial problem with another one with which has an exact analytical solution for any source distribution:

\[ \nabla \times \nabla \times \mathbf{E} - \omega^2 \mu_0 \varepsilon_b(r) \mathbf{E} = i\omega \mu_0 \mathbf{J} \quad \Rightarrow \quad \mathbf{E} = \mathbf{\mathcal{K}}_b(\mathbf{J}) \]

2. Take all nonzero differences between permittivities as generalized sources

\[ \mathbf{J}_g = -i\omega(\varepsilon - \varepsilon_b)\mathbf{E} \]

3. This leads to an implicit equation for unknown \( \mathbf{E} \)

\[ \mathbf{E} = \mathbf{E}_0 - \mathbf{\mathcal{K}}_b[i\omega(\varepsilon - \varepsilon_b)\mathbf{E}] \]

Example of a binary corrugation

\[ y_{ik} + x_{ik} + z_{x,y,z} \exp(jJ) = \]

**Problem**

DOE pattern on substrate

\[ \varepsilon_3 \]

\[ \varepsilon_1 \]

\[ \varepsilon_2 \]

**Basis problem**

Homogeneous layer

\[ \varepsilon_b \]

\[ \varepsilon_1 \]

\[ \varepsilon_2 \]

**Perturbation**

Permittivity difference creates generalized sources:

\[ J(x,y,z) = j(z) \exp(ik_x x + ik_y y) \]

**Solution unknown**

Complete solution known once for all
Maxwell equations are reduced finally to the implicit integral equation:

\[
\begin{pmatrix}
  a_n^{e+}(z)
  \\ a_n^{h+}(z)
\end{pmatrix}
= \delta_{n0}
\begin{pmatrix}
  a_{inc}^{e+}(z)
  \\ a_{inc}^{h+}(z)
\end{pmatrix}
+ \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \sum_{\beta=x,y,z} \sum_{m=-\infty}^{\infty} P_{n\alpha}^{\pm} R_{n\alpha}^{\pm}(z,z') V_{nm}^{\alpha\beta}(z') \left[ Q_{m\beta}^{+}\begin{pmatrix}
  a_m^{e+}(z')
  \\ a_m^{h+}(z')
\end{pmatrix}
+ Q_{m\beta}^{-}\begin{pmatrix}
  a_m^{e-}(z')
  \\ a_m^{h-}(z')
\end{pmatrix}\right] dz'
\]
Integral equation:

\[
\begin{pmatrix}
a_n^{e\pm}(z) \\
a_n^{h\pm}(z)
\end{pmatrix}
= \delta_{n0} \begin{pmatrix}
a_{inc}^{e\pm}(z) \\
a_{inc}^{h\pm}(z)
\end{pmatrix} + \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \left\{ \sum_{m=\infty}^{\infty} \sum_{\beta=x,y,z} P^\pm_{n\alpha} R^\pm_{n\alpha}(z, z') V^{\alpha\beta}_{nm}(z') \left[ Q^+_{m\beta} \begin{pmatrix} a_m^{e+}(z') \\ a_m^{h+}(z') \end{pmatrix} + Q^-_{m\beta} \begin{pmatrix} a_m^{e-}(z') \\ a_m^{h-}(z') \end{pmatrix} \right] \right\} dz'
\]

**Incident field harmonics**
Integral equation:

\[
\begin{pmatrix}
a_n^{e \pm}(z)
a_n^{h \pm}(z)
\end{pmatrix} = \delta_{n0} \begin{pmatrix}
a_{\text{inc}}^{e \pm}(z)
a_{\text{inc}}^{h \pm}(z)
\end{pmatrix} + \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \left\{ \sum_{m=\infty}^{\infty} \sum_{\beta=x,y,z} P_{n\alpha}^\pm R_{n\alpha}^\pm (z, z') V_{nm}^{\alpha\beta}(z') \left[ Q_{m\beta}^+ \begin{pmatrix}
a_m^{e+}(z')
a_m^{h+}(z')
\end{pmatrix} + Q_{m\beta}^- \begin{pmatrix}
a_m^{e-}(z')
a_m^{h-}(z')
\end{pmatrix} \right] \right\} dz'
\]

**Unknown** amplitudes of TE- and TM-polarized harmonics.
Integral equation:

\[
\begin{pmatrix}
a_n^{e+}(z) \\
a_n^{h\pm}(z)
\end{pmatrix} = \delta_{n0} \begin{pmatrix}
a_{inc}^{e+}(z) \\
a_{inc}^{h\pm}(z)
\end{pmatrix} + \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \left\{ \sum_{m=-\infty}^{\infty} \sum_{\beta=x,y,z} P_{n\alpha}^\pm R_{n\alpha}^{\pm}(z, z') V_{nm}^{\alpha\beta}(z') \begin{bmatrix}
a_m^{e+}(z') \\
a_m^{h+}(z')
\end{bmatrix} \right\} + Q_{n\beta}^- \begin{bmatrix}
a_m^{e-}(z') \\
a_m^{h-}(z')
\end{bmatrix} \right\} dz'
\]

Transition matrix from TE- and TM-harmonics amplitudes to x-, y- and z-components of the electric field

\[
Q_n^\pm = \begin{pmatrix}
k_{y0} & \pm k_{xn} k_{zn} \\
k_{xn} & \pm \frac{k_{y0} k_{zn}}{\omega \varepsilon_b \gamma_n} \\
\gamma_n & \frac{k_{y0}}{\omega \varepsilon_b} \\
0 & \frac{\gamma_n}{\omega \varepsilon_b}
\end{pmatrix}
\]
Integral equation:

\[
\left( a_n^{e\pm}(z) \right) = \delta_{n0} \left( a_{inc}^{e\pm}(z) \right) + \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \left\{ \sum_{m=-\infty}^{\infty} \sum_{\beta=x,y,z} P_{n\alpha}^\pm R_{n\alpha}^\pm (z, z') V_{nm\alpha}^{\alpha\beta} (z') \right\} \left[ Q_{m\beta}^+ \left( a_m^{e+}(z') \right) + Q_{m\beta}^- \left( a_m^{e-}(z') \right) \right] dz'
\]

Transition matrix from x-, y- and z-components of the electric field to TE- and TM-harmonics amplitudes

\[
P_n^\pm = \begin{pmatrix}
-\frac{\omega \mu_0 k_{y0}}{2\gamma_n k_{zn}} & \frac{\omega \mu_0 k_{xn}}{2\gamma_n k_{zn}} & 0 \\
\frac{k_{xn}}{2\gamma_n} & \frac{k_{zn}}{2\gamma_n} & -\frac{\gamma_n}{2k_{zn}} \\
\pm \frac{k_{xn}}{2\gamma_n} & \pm \frac{k_{y0}}{2\gamma_n} & \frac{\gamma_n}{2k_{zn}}
\end{pmatrix}
\]
Along z the integral is divided into slices:

\[
\int_{-\infty}^{\infty} (\ldots) \, dz
\]

The resulting equation is written in the form

\[
a^{\pm}_n(z_1, z_2) = \delta_{n0} a^{\text{inc} \pm}_n(z_1, z_2) + \sum_{\alpha=x,y,z} \sum_{\beta=x,y,z} T^{\pm}_{nq} P_{n\alpha}^{\pm} V^{\alpha\beta}_{nmq} Q_{m\beta}^{\pm} \left( A_{nmpq}^{\pm} \right)^{-1} \delta_{m0} a^{\text{inc} \pm}_n(z_1, z_2)
\]

Where the **final matrix to be inverted** is

\[
A_{nmpq}^{\pm} = I_{nmpq}^{\pm} - \sum_{\alpha=x,y,z} \sum_{\beta=x,y,z} R^{\pm}_{nq} P_{n\alpha}^{\pm} V^{\alpha\beta}_{nmq} Q_{m\beta}^{\pm}
\]
LINEAR SYSTEM OF ALGEBRAIC EQUATIONS

\[
A_{nmpq}^{\pm} = I_{nmpq}^{\pm} - \sum_{\alpha=x,y,z} \sum_{\beta=x,y,z} R_{nmpq}^{\pm} P_{nq}^{\pm} V_{nmq}^{\alpha} Q_{m\beta}^{\pm}
\]

Matrix containing exponential factors that describe the wave propagation along z-axis

The 1^{\text{st}} clue for ultra-fast computing:
Despite multiple reflections at interfaces matrix R keeps a Toeplitz structure

Fast numerical techniques applicable
3D boundary conditions affect matrix multiplications

\[
J = -i\omega(D - D_b)
\]

\[
[\varepsilon]_{n-m}(E_{||})_m = (D_{||})_n \quad (E_{\perp})_n = \left[\frac{1}{\varepsilon}\right]_{n-m} (D_{\perp})_m
\]

2\textsuperscript{nd} clue for ultra-fast computing:
Matrix containing Fourier components of
\# permittivity
\# fields
\# local slope functions of boundaries
has Toeplitz structure

High accuracy achievable
Last task: inversion of matrix $A$

$$A_{nmpq} = I_{nmpq} - \sum_{\alpha=x,y,z} \sum_{\beta=x,y,z} R_{npq}^\pm P_{n\alpha}^\pm V_{nmq}^{\alpha\beta} Q_{m\beta}^\pm$$

Assuming
- # number of slices: 100
- # number of diffraction orders: 100 and 100

size of matrix $A$ is $\sim 10^6$ !!

3rd clue for ultra-fast computing:

**GMRES resolves a linear system in Krylov space in a few tens of iterative multiplications of a matrix by a vector**

Fast and stable convergence attained
Comparison with Fourier-modal method (FMM, RCWA) versus number of slices $N_L$

The dependencies resemble each other for different types of structures.

8th EOS Topical Meeting on Diffractive Optics, Monday, 27 February 2012
Comparison with Fourier-modal method (FMM, RCWA):

2D lamellar grating
NUMERICAL BENCHMARKS

Convergence versus number of slices and diffraction orders

- Period: 4 μm
- Depth: 0.4 μm
- Wavelength: 0.633 μm
- DOE refractive index: 2.1
- Cover refractive index: 1.0
NUMERICAL BENCHMARKS

**Period:** 4 μm  
**Depth:** 0.4 μm  
**Wavelength:** 0.6328 μm  
**DOE refractive index:** 2.1  
**Cover refractive index:** 1.0  

**Processor:** 2.5 GHz  
**Memory:** 4 GB (Windows OS)

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![Graph showing numerical benchmarks with data points and lines for GSM, FMM, and O(N^2) and O(N).](image-url)
GSM needs 16 Gb of computer memory to calculate such DOE part with accuracy better than $10^{-3}$.

Parallel calculation by a GPU reduces 1 hour to 2-3 minutes!
The GSM breaks through the time & memory limits of existing exact methods.

The GSM permits exact modeling to invade the land occupied by scalar methods.

It makes it in three important application fields of diffraction/scattering:
- Reticle and wafer latent image in advanced photolithography
- Scattering layers for light extraction from (O)LEDs
- Diffractive optics, e.g., high NA diffractive lenses

As from now on, a big effort is needed to adapt and optimize the method to various application domains. (Ref. Th. Kämpfe presentation in this conference)
THANK YOU!