Scattering from finite structures: An extended Fourier modal method

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Outline

1. Motivation
2. Overview of PhD
3. Alternative discretization
4. Results
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Profile reconstruction

Currently used models assume infinitely periodic gratings...
Profile reconstruction

... but in reality the gratings are finite.
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⇒ scattering from structures with a finite number of periods.
Methods for solving Maxwell’s equations

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Why FMM?
Motivation Overview of PhD Alternative discretization Results

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- No one has done it yet!
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- No one has done it yet!
- Faster than other methods for periodic structures
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Overview of PhD

Alternative discretization

Results

Methods for solving Maxwell’s equations

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Why FMM?
- No one has done it yet!
- Faster than other methods for periodic structures
- Well-known and widely used inside ASML
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Progress

Progress


  ![FMM to aFMM-CFF](image1)


  ![Generalization to arbitrary shapes](image2)
Progress


- Alternative discretization [J. Comp. Phys., in prep.] (Today)
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Horizontal and vertical problems

Discretization:
- $z$ direction - *spatial discretization* into layers
- $x$ direction - *spectral discretization* with harmonics

\[
\mathcal{T} = \mathcal{O}(\bar{N}_x^3 \bar{N}_z) \quad \bar{\mathcal{T}} = \mathcal{O}(\bar{N}_x^3 \bar{N}_z)
\]

Use slicing in the longer direction and harmonics in the shorter dir.
Discretization:

$z$ direction - *spatial discretization* into layers

$x$ direction - *spectral discretization* with harmonics

$$\bar{T} = O(\bar{N}_x^3 \bar{N}_z) \quad \bar{T} = O(\bar{N}_x^3 \log_2 \bar{N}_z)$$

Use slicing in the longer direction and harmonics in the shorter dir.
1. Continuous Maxwell’s equations (for contrast field):

\[ \nabla \times \mathbf{e}^c(x) = -k_0 \mathbf{h}^c(x), \]
\[ \nabla \times \mathbf{h}^c(x) = -k_0 \epsilon(x, z)\mathbf{e}^c(x) - k_0 (\epsilon(x, z) - \epsilon^b(x, z))\mathbf{e}^b(x), \]
The aperiodic Fourier modal method

2. Add PML

\[ \frac{\partial}{\partial x} \rightarrow \frac{1}{f'(x)} \frac{\partial}{\partial x}, \text{ with } f(x) = x + i\beta(x). \]
The aperiodic Fourier modal method

3. Discretize in \( z \) (slicing)

\[ \epsilon_l(x) = \epsilon(x, z_l), \quad \epsilon_l^b(x) = \epsilon^b(x, z_l), \quad \text{with} \quad z_l = [h_{l-1}, h_l]. \]
The aperiodic Fourier modal method

4. Discretize in $x$, $y$ (Fourier harmonics, $\phi_n(x, y) = e^{-i(k_n x + k_y y)}$)

$$e_{c/b,N}^{\alpha,l}(x, y, z) = \sum_{n=-N}^{N} s_{\alpha,l,n}(z) \phi_n(x, y)$$

$$h_{c/b,N}^{\alpha,l}(x, y, z) = \sum_{n=-N}^{N} u_{\alpha,l,n}(z) \phi_n(x, y)$$
Transmission problem

System of ODEs in $z$

$$\frac{d^2}{dz^2} v^c_l(z) = A_l v^c_l(z) + A^b_l v^b_l(z)$$

General solution (homogeneous + particular)

$$v^c_l = W^l (e^{-k_0 Q_l (z-h_l)} c^+_l + e^{k_0 Q_l (z-h_{l+1})} c^-_l) + p_l v^b_l(z)$$

Interface conditions yield recursive linear systems

$$\begin{bmatrix} W_l X_l & W_l \\ V_l X_l & -V_l \end{bmatrix} \begin{bmatrix} c^+_l \\ c^-_l \end{bmatrix} = \begin{bmatrix} W_{l+1} & W_{l+1} X_{l+1} \\ V_{l+1} & -V_{l+1} X_{l+1} \end{bmatrix} \begin{bmatrix} c^+_{l+1} \\ c^-_{l+1} \end{bmatrix} + g_{l+1}, \ l = 1, ..., M - 1$$

with $c^+_1 = c^-_M = 0$
**Interface matrix**

**T-matrix**

\[
\begin{bmatrix}
  c_2^+ \\
  c_2^-
\end{bmatrix} = \begin{bmatrix}
  T_{1,2}^{11} & T_{1,2}^{12} \\
  T_{1,2}^{21} & T_{1,2}^{22}
\end{bmatrix} \begin{bmatrix}
  c_1^+ \\
  c_1^-
\end{bmatrix} + \begin{bmatrix}
  g_{1,2}^1 \\
  g_{1,2}^2
\end{bmatrix}
\]

\[
(T_{1,2}, g_{1,2})
\]

**S-matrix**

\[
\begin{bmatrix}
  c_2^+ \\
  c_2^-
\end{bmatrix} = \begin{bmatrix}
  S_{1,2}^{11} & S_{1,2}^{12} \\
  S_{1,2}^{21} & S_{1,2}^{22}
\end{bmatrix} \begin{bmatrix}
  c_1^+ \\
  c_1^-
\end{bmatrix} + \begin{bmatrix}
  f_{1,2}^1 \\
  f_{1,2}^2
\end{bmatrix}
\]

\[
(S_{1,2}, f_{1,2})
\]

**UNSTABLE**

**STABLE**
Stability: an example

Cylinder illuminated by a TE-polarized plane wave at an angle $\theta = 0^\circ$.

Geometry

Exact solution

Numerical solution

Convergence
Merging interfaces: Redheffer product

\[ \begin{bmatrix} c_3^+ \\ c_1^- \end{bmatrix} = S_{1,3} \begin{bmatrix} c_1^+ \\ c_3^- \end{bmatrix} + f_{1,3} \]

Define an extended Redheffer product

\[(S_{1,2}, f_{1,2}) \ast (S_{2,3}, f_{2,3}) = (S_{1,3}, f_{1,3}) \quad \text{(not commutative, associative)}\]

\[
S_{1,3} = \begin{bmatrix} S_{2,3}^{11} (I - S_{1,2}^{12} S_{2,3}^{21})^{-1} S_{1,2}^{11} \\ S_{1,2}^{21} + S_{1,2}^{22} S_{2,3}^{21} (I - S_{1,2}^{12} S_{2,3}^{21})^{-1} S_{1,2}^{11} \end{bmatrix} \quad \begin{bmatrix} S_{2,3}^{12} + S_{2,3}^{11} S_{1,2}^{12} (I - S_{2,3}^{21} S_{1,2}^{12})^{-1} S_{2,3}^{22} \\ S_{1,2}^{22} (I - S_{2,3}^{21} S_{1,2}^{12})^{-1} S_{2,3}^{22} \end{bmatrix} 
\]

\[
f_{1,3} = \begin{bmatrix} S_{2,3}^{11} (I - S_{1,2}^{12} S_{2,3}^{21})^{-1} (S_{1,2}^{12} f_{2,3}^2 + f_{1,2}^1) + f_{2,3}^1 \\ S_{1,2}^{22} S_{2,3}^{21} (I - S_{1,2}^{12} S_{2,3}^{21})^{-1} (S_{1,2}^{12} f_{2,3}^2 + f_{1,2}^1) + S_{1,2}^{22} f_{2,3}^2 + f_{1,2}^2 \end{bmatrix} \]
Fast recursion

Standard recursion, update relation:

\[(S_{1,l+1}, f_{1,l+1}) = (S_{1,l}, f_{1,l}) \ast (S_{l,l+1}, f_{l,l+1})\]
Fast recursion

Standard recursion, all interfaces:

\[(S_{1,M}, f_{1,M}) = [\ldots[((S_{1,2}, f_{1,2}) \ast (S_{2,3}, f_{2,3})) \ast (S_{3,4}, f_{3,4})) \ast \ldots \ast (S_{M-1,M}, f_{M-1,M})] \]
Fast recursion, exploit periodicity:

\[(S_{3,5}, f_{3,5}) = (S_{1,3}, cf_{1,3})\]
Fast recursion, exploit associativity:
\[(S_{1,5}, f_{1,5}) = (S_{1,3}, f_{1,3}) \ast (S_{3,5}, f_{3,5}) = (S_{1,3}, f_{1,3}) \ast (S_{1,3}, c f_{1,3})\]
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Near-field comparison

Resist grating with 8 rectangular lines illuminated by TE-polarized light ($\lambda = 628.3$ nm) at an angle $\theta = 30^\circ$. 

![Slicing along the grating](image1)

![Slicing perpendicular to the grating](image2)
Convergence and computational cost

Resist grating with 32 rectangular lines illuminated by TE-polarized light ($\lambda = 628.3$ nm) at an angle $\theta = 30^\circ$.
Speed-up and memory saving (1)

**Speed-up**
\[ \eta_T = \frac{\bar{T}}{\bar{T}} \]

**Memory saving**
\[ \eta_M = \frac{\bar{M}}{\bar{M}} \]

Graphs showing speed-up factor, \( \eta_T \), and memory use factor, \( \eta_M \), for different line counts: 16 lines, 32 lines, and 64 lines. The graphs plot error against speed-up and memory use factor on a log scale.
Speed-up and memory saving (2)

**Speed-up**

\[ \eta_T = \frac{T}{\bar{T}} \]

**Memory saving**

\[ \eta_M = \frac{M}{\bar{M}} \]
Large structure

Resist grating with 1024 (!) lines

This example requires only 5 times more work and memory than a grating with 32 lines
Conclusions

- The FMM has been extended to finite structures (aFMM-CFF).
- A stable recursive algorithm has been developed for aFMM-CFF.
- Swapping the discretization directions yields significant speed-ups (up to 35) and considerable memory savings (up to 100).
- The speed-up and memory saving are higher for larger structures and materials with low refraction index.
- Very large structures with repeating patterns can now be considered.
Thank You! Questions?