RCWA: extension to finite structures

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Outline

Motivation

An overview of the standard RCWA

Finite structures: RCWA+PML

Finite structures: RCWA+PML+CFF

Computations and results
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Computations and results
Currently used models assume infinitely periodic gratings...
Profile reconstruction

... but in reality the gratings are finite.
A computational example: infinite vs. finite

Infinite grating (blue) and finite grating (red)
A computational example: infinite vs. finite

Infinite grating (blue) and finite grating (red)

Near-field (field on top of grating)
A computational example: infinite vs. finite

Infinite grating (blue) and finite grating (red)

Near-field (field on top of grating)

Far-field (reflection coefficients)
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Computations and results
RCWA in a nutshell

- Divide the computational domain into layers, s.t. $\epsilon$ does not depend on $z$ in each layer
- Derive the general solution in each layer
- Match the solutions at layer interfaces
The standard RCWA

Equation to be solved in one layer (TE-polarization)

\[ \frac{\partial^2}{\partial x^2} E_{y,i}(x, z) + \frac{\partial^2}{\partial z^2} E_{y,i}(x, z) + \epsilon_i(x) E_{y,i}(x, z) = 0 \]

The $x$-dependent quantities are expanded in Fourier modes

\[ E_{y,i}(x, z) = \sum_{n=-N}^{N} s_{i,n}(z) e^{-i k_n x}, \quad \epsilon_i(x) = \sum_{n=-N}^{N} \hat{\epsilon}_{i,n} e^{-i n \frac{2\pi}{\Lambda} x} \]

In matrix form

\[ s''_i(z) = A_i s_i(z), \quad \Rightarrow \quad s_i(z) = W_i (e^{-Q_i z} c_i^+ + e^{Q_i z} c_i^-) \]

M.G. Moharam, T.K. Gaylord (1981) - RCWA (periodic)
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Computations and results
P. Lalanne, et al. (2000), RCWA for waveguides
The idea of PML (Perfectly Matched Layer)

1. Analytical continuation

\[ \tilde{x} = f(x) = x + i\beta(x) \]

2. Write derivatives in \( \mathbb{R} \)

\[ \frac{\partial}{\partial \tilde{x}} = \frac{\partial x}{\partial \tilde{x}} \frac{\partial}{\partial x} = \frac{1}{f'(x)} \frac{\partial}{\partial x} \]

3. Solve the new PDE

Simple example - plane wave

\[ E(x) = e^{-ikx} \]

\[ \Rightarrow \tilde{E}(x) = E(x + i\beta(x)) = e^{-ikx} e^{k\beta(x)} \]

J.-P. Berenger (1994) - PML for absorption of waves
RCWA + PML

Periodic:
\[ \frac{\partial^2}{\partial x^2} E_{y,i} + \frac{\partial^2}{\partial z^2} E_{y,i} + \epsilon_i(x) E_{y,i} = 0 \]

Aperiodic:
\[ \frac{1}{f'(x)} \frac{\partial}{\partial x} \left( \frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_{y,i} \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_{y,i} + \tilde{\epsilon}_i(x) \tilde{E}_{y,i} = 0 \]

Besides \( E_{y,i} \) and \( \epsilon_i \), also \( 1/f' \) is expanded in Fourier modes

\[ \frac{1}{f'(x)} = \sum_{n=-N}^{N} \hat{f}_n e^{-i k_n x} \]

\[ s''_i(z) = A_i s_i(z), \quad A_i = (FK_x)^2 - E_i. \]

A computational example: radiating line source

\[ \frac{\partial^2}{\partial x^2} u + \frac{\partial^2}{\partial z^2} u + k_0^2 u = -\delta \]

Exact solution available

\[ u(x, z) = G(x, z) = \frac{i}{4} H_0^{(1)}(k_0 r) \]
A computational example: radiating line source

\[ \frac{\partial^2}{\partial x^2} u + \frac{\partial^2}{\partial z^2} u + k_0^2 u = -\delta \]

solution with standard RCWA (periodic BCs)
Domain width \( \Lambda = 5 \)
A computational example: radiating line source

\[ \frac{\partial^2}{\partial x^2} u + \frac{\partial^2}{\partial z^2} u + k_0^2 u = -\delta \]

solution with standard RCWA (periodic BCs)
Domain width \( \Lambda = 10 \)
A computational example: radiating line source

\[ \frac{\partial^2}{\partial x^2} u + \frac{\partial^2}{\partial z^2} u + k_0^2 u = -\delta \]

solution with standard RCWA (periodic BCs)
Domain width \( \Lambda = 20 \)
A computational example: radiating line source

\[ \frac{\partial^2}{\partial x^2} u + \frac{\partial^2}{\partial z^2} u + k_0^2 u = -\delta \]

solution with RCWA with PMLS
Domain width \( \Lambda = 5 \)
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Computations and results
Transformation of the incident field

Incoming field in old coordinates

\[ E^{inc}(x, z) = e^{-i(k_x x + k_z z)} \]

PML introduces a coordinate transformation. \( \tilde{E}^{inc} \) becomes

\[ \tilde{E}^{inc}(x, z) = e^{-i(k_x \tilde{x} + k_z z)} = e^{-i(k_x(x + i\beta(x)) + k_z z)} = e^{k_x \beta(x)} e^{-i(k_x x + k_z z)} \]

- Generally, not periodic. Only periodic for \( k_x = 0 \).
- RCWA cannot deal with non-periodic solutions.
Contrast/background decomposition

\[
\frac{1}{f'(x)} \frac{\partial}{\partial x} \left( \frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y + \epsilon(x, z) \tilde{E}_y = 0 \quad (1)
\]

total field = periodic part + non-periodic part

\[
\tilde{E}_y = \tilde{E}_y^c + \tilde{E}_y^b
\]

\(\tilde{E}_y^b\) satisfies

\[
\frac{1}{f'(x)} \frac{\partial}{\partial x} \left( \frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y^b \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y^b + \epsilon^b(z) \tilde{E}_y^b = 0 \quad (2)
\]

Subtract (2) from (1)

\[
\frac{1}{f'(x)} \frac{\partial}{\partial x} \left( \frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y^c \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y^c + \epsilon(x, z) \tilde{E}_y^c = -(\epsilon(x, z) - \epsilon^b(z)) \tilde{E}_y^b
\]
\[
\frac{1}{f'(x)} \frac{\partial}{\partial x} \left( \frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y^c \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y^c + \epsilon(x, z) \tilde{E}_y^c = -(\epsilon(x, z) - \epsilon^b(z))\tilde{E}_y^b
\]

Background field

\[
E_1^b = E^{inc} + E^r = e^{-q_1 z} e^{-ik_{x_0}x} + r e^{q_1 z} e^{-ik_{x_0}x}
\]
The contrast field satisfies

\[
\frac{1}{f'(x)} \frac{\partial}{\partial x} \left( \frac{1}{f'(x)} \frac{\partial}{\partial x} \tilde{E}_y^c \right) + \frac{\partial^2}{\partial z^2} \tilde{E}_y^c + \epsilon(x, z) \tilde{E}_y^c = -\left(\epsilon(x, z) - \epsilon^b(x, z)\right) E_y^b
\]

- Divide into layers, s.t. \( \epsilon \) is \( z \)-independent
- Expand \( x \)-dependent quantities in Fourier modes

\[
s''_1(z) = A_1 s_1(z)
\]

\[
s''_2(z) = A_2 s_2(z) + (E_1 - E_2) d_0 (e^{-q_1 z} + re^{q_1 z})
\]

\[
s''_3(z) = A_3 s_3(z)
\]

with \( A_i = (FK_x)^2 - E_i \), \( i = 1, 2, 3 \).

Note: eigenvalue problems are also solved in the top and bottom layers!
\[ \frac{\partial^2}{\partial z^2} s_2(z) = A_2 s_2(z) + (E_1 - E_2) d_0 (e^{-q_1 z} + re^{q_1 z}), \quad A_2 = (FK_x)^2 - E_2. \]

The solution vector is of the form

\[ s^c_2 = s^c_{2,\text{hom}} + s^c_{2,\text{part}} \]

Assume the following form for the particular solution (m. undet. coeff.)

\[ s^c_{2,\text{part}}(z) = p(e^{-q_1 z} + re^{q_1 z}) \]

Substitute this ansatz in the differential eqn. for \( s_2(z) \)

\[ (A_2 - q_1^2 I)p = -(E_1 - E_2)d_0 \]

The general solution

\[ s^c_2(z) = W_2(e^{-Q_2 z} c_2^+ + e^{Q_2 z} c_2^-) + p(e^{-q_1 z} + re^{q_1 z}) \]
<table>
<thead>
<tr>
<th>Classical RCWA</th>
<th>RCWA+PML+CFF</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta E + \epsilon(x, z)E = 0$</td>
<td>$\Delta E^c + \epsilon(x, z)E^c = (\epsilon^b - \epsilon)E^b$</td>
</tr>
<tr>
<td>$s''(z) = As(z)$</td>
<td>$s''(z) = As(z) + (\epsilon_1 I - E)d_0(e^{-q_1 z} + re^{q_1 z})$</td>
</tr>
<tr>
<td>$s(z) = W(e^{-Qz}c^+ + e^{Qz}c^-)$</td>
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Damping in the PML

Examine the contrast field $\tilde{E}_y^c$

The field is attenuated in the lateral PMLs

$$\tilde{E}_y^c(0, z) \approx \tilde{E}_y^c(5, z) \approx 0$$
Correctness of solution

RCWA+PML+CFF

Supercell RCWA
Error as a function of $N$ and $\sigma_0$

Supercell

$$\log_{10}(\|E(N, \Lambda) - E_{\text{ref}}\|_2)$$

CFF+PML

$$\log_{10}(\|E(N, \sigma) - E_{\text{ref}}\|_2)$$

$E_{\text{ref}} = E(N = 800, \Lambda = 15000)$

Accuracy $\approx 10^{-3}$, Supercell - 80 harm., CFF+PML - 10 harm.
Progress

- RCWA + PML
- RCWA + PML + CFF (TE)
- Extend to TM and conical
- Validate against an exact solution (radiating line)
- Stable recursion for RCWA + PML + CFF
- Full 3D code (finite in the $x$ and $y$ directions)
- Far-field
- Arbitrary illumination
- ...

M. Pisarencro et al. (2010), The aperiodic Fourier modal method in contrast-field formulation for simulation of scattering from finite structures, CASA Report 10-36
Thank You! Questions?
Shape reconstruction problem

Forward problem
Given the shape parameters $p$, compute the field intensity $I(p)$.

Inverse problem
Given the measured field intensity $I_{CCD}$, determine a set of shape parameters $p$; i.e. find $p$ which minimizes $\min_p ||I_{CCD} - I(p)||$.

Rest of the talk - solving the forward problem (Maxwell Eqns.).
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RCWA milestones

  RCWA (periodic structures)

- Jean-Pierre Berenger (1994)
  Perfectly Matched Layer for the Absorption of Electromagnetic Waves

  RCWA applied to waveguides (aperiodic structures, only normal incidence)