Fast and efficient modeling of metallic gratings diffraction with metric sources

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Outline

• Grating diffraction: Fourier space methods
• Curvilinear space
• Generalized Source Method (GSM)
• Generalized Metric Sources concept
• Method capabilities
• Conclusions

Linear diffraction on a periodic corrugation interface
Grating diffraction: Fourier space methods

Cartesian space:

- Fourier-Modal Method (RCWA)
- Differential Method
- Generalized Source Method

Curvilinear space:

- Chandezon Method
- FMM with coordinate transform

Most suitable problems:

- dielectric, vertical walls or index gratings
- dielectric complex shape gratings
- metallic, smooth profile
- metallic, vertical walls
Grating diffraction: Fourier space methods

Cartesian space:
• Fourier-Modal Method (RCWA) \( O(N^3) \)
• Differential Method \( O(N^3) \)
• Generalized Source Method \( O(N\log N) \)

Curvilinear space:
• Chandezon Method \( O(N^3) \)
• FMM with coordinate transform \( O(N^3) \)

\( O(N\log N) \) method for complex corrugated metallic gratings?
Curvilinear space

Periodic corrugation treatment:

Fourier harmonics

GSM, FMM: slicing approximation in Cartesian coordinates

C-method: slicing approximation in curvilinear coordinates
  - only single-valued profile functions;
  - similar transformation in the whole 2D/3D space.

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Curvilinear space

KEY IDEA: transform only in a bounded region

Cartesian space region →

Curvilinear space region →

Cartesian space region →

Curvilinear coordinates continuously become Cartesian at interfaces of the grating region.

Slicing in curvilinear coordinates in a bounded region

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Generalized Source Method

Diffraction or scattering problem

Basis medium + basis analytic solution

Difference between initial and basis media gives rise to the generalized sources

\[ \mathbf{E}(\mathbf{r}) \]
\[ \nabla \times \mathbf{E} = i \omega \mu_0 \mathbf{H} \]
\[ \nabla \times \mathbf{H} = \mathbf{j} - i \omega \varepsilon \mathbf{E} \]
\[ \mathbf{E}_b(\mathbf{r}) \]
\[ \nabla \times \mathbf{E} = i \omega \mu_0 \mathbf{H} \]
\[ \nabla \times \mathbf{H} = -i \omega \varepsilon_b \mathbf{E} \]
\[ \mathbf{j}_{gen} = -i \omega (\varepsilon - \varepsilon_b) \mathbf{E} \]

• Implicit linear equation: \[ \mathbf{E} = \mathbf{E}_{inc} + \chi (\mathbf{E} - \varepsilon B) \]
• Discretization: Fourier space + Slicing
• GMRES+FFT assisted solution of the resulting algebraic system in \(O(N\log N)\) time and \(O(N)\) memory resort.

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Maxwell’s equations
\[ \nabla \times \vec{E} = -\vec{M} + i\omega \mu_0 \vec{H} \]
\[ \nabla \times \vec{H} = \vec{J} - i\omega \varepsilon \vec{E} \]
in a curvilinear space become
\[ \xi^{\alpha\beta\gamma} \partial_\beta E_\gamma = -M^\alpha + i\omega \mu_0 \sqrt{g} g^{\alpha\beta} H_\beta \]
\[ \xi^{\alpha\beta\gamma} \partial_\beta H_\gamma = J^\alpha - i\omega \varepsilon \sqrt{g} g^{\alpha\beta} E_\beta \]

In accordance with the GSM rationale we split equations into a basis part
\[ \xi^{\alpha\beta\gamma} \partial_\beta E_\gamma = i\omega \mu_0 \delta^{\alpha\beta} H_\beta \]
\[ \xi^{\alpha\beta\gamma} \partial_\beta H_\gamma = -i\omega \varepsilon_b \delta^{\alpha\beta} E_\beta \]
and Generalized Metric Sources
\[ M^\alpha = -i\omega \mu_0 (\sqrt{g} g^{\alpha\beta} - \delta^{\alpha\beta}) H_\beta \]
\[ J^\alpha = -i\omega \varepsilon_b (\sqrt{g} g^{\alpha\beta} - \delta^{\alpha\beta}) E_\beta \]

Coordinate transformation in a grating region
\[ q^i = q^i(x_1, x_2, x_3) \]
Fields are transformed via metric tensor:
\[ g^{\alpha\beta} = \sum_\gamma \frac{\partial q^\alpha}{\partial x_\gamma} \frac{\partial q^\beta}{\partial x_\gamma}, g = \det(g_{\alpha\beta}) \]
Generalized Metric Sources concept

Basis part:

\[ \zeta^{\alpha\beta\gamma} \partial_\beta E_\gamma = i\omega \mu_0 \delta^{\alpha\beta} H_\beta, \quad \nabla \times \vec{E} = i\omega \mu_0 \vec{H} \]
\[ \zeta^{\alpha\beta\gamma} \partial_\beta H_\gamma = -i\omega \varepsilon_b \delta^{\alpha\beta} E_\beta, \quad \nabla \times \vec{H} = -i\omega \varepsilon_b \vec{E} \]

is similar to the Maxwell’s equations in Cartesian metric, and continuously become the Maxwell’s equations at grating region boundaries

Generalized Metric Sources

\[ M^\alpha = -i\omega \mu_0 (\sqrt{g} g^{\alpha\beta} - \delta^{\alpha\beta}) H_\beta \]
\[ J^\alpha = -i\omega \varepsilon_b (\sqrt{g} g^{\alpha\beta} - \delta^{\alpha\beta}) E_\beta \]
Method capabilities

✓ Smooth profile gratings;
✓ Vertical wall gratings;
✓ “Overhanging” gratings;
✓ Multilayer periodic structures with different layer shapes;
✓ ...

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Method capabilities

Convergence example:

- convergence is similar for both metallic and dielectric gratings;
- convergence over slice number is polynomial and can be significantly increased by use of the second order Richardson extrapolation;
- convergence over diffraction order number is obtained by taking the best solutions from the convergence over slice number.

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Method capabilities

Convergence example:

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- Convergence over diffraction order number is obtained by taking the best solutions from the convergence over slice number.
0-th order reflection and transmission efficiencies depending on two grating periods for diffraction of a plane wave at wavelength $0.6328 \, \mu m$ under $10^\circ$ incidence on a gold sinusoidal grating of depth $0.05 \, \mu m$.

Conclusions

✓ Computationally and memory efficient (linear time complexity and memory requirements) volume integral curvilinear coordinate Fourier space method for grating diffraction simulation.

✓ Both metallic and dielectric gratings: similar convergence.

✓ High accuracy achievable

✓ No implicit use of the Rayleigh hypothesis: no restrictions for grating shapes and depths.

✓ Possible to use parallel GPU-enabled computations: about 50 times faster diffraction simulation.
Thank you

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