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Numerical Solution for Scattering by Biperiodic Gratings Using FEM Coupled by Fourier-Mode Expansions

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Simulation of scattering by periodic surface structures is an important task in optical design. The corresponding boundary value problem for the time-harmonic Maxwell's equations over bounded computational domains includes a non-local boundary condition due to the radiation condition at infinity. Alternatively to the classical approach based on Dirichlet-to-Neumann maps, we follow Huber et al. [1] and replace the boundary condition by a coupling of the FEM with the Fourier-mode expansions in the upper and lower half space, respectively. In other words, the Galerkin method is modified coupling a, hopefully, small number of non-local trial functions through the boundary of the FEM domain via mortar techniques. Thus the Dirichlet-to-Neumann map is approximated by a stable low-rank operator adapted to the approximation properties of the Fourier-mode expansion. Modifying the coupling terms of Huber et al. [1] slightly, we can prove the unique solvability of the variational equation in the classical curl spaces. The FEM coupled with Fourier modes is stable and convergent.

Scattering by biperiodic grating - Mathematical model

Grating: surface structure in layer $b^- < x_3 < b^+$, periodic w.r.t. x_1 and x_2

Incoming wave: plane wave E^{inc} from above

Look for:
- quasi-periodic solution of time-harmonic Maxwell's equation in $H_{\text{qp}}(\text{curl},\mathbb{R}^3)$, i.e., solution of time-harmonic curl-curl equation for electric field
- solution with radiation condition on upper half space, i.e., admitting a Rayleigh series expansion for half space $b^+ < x_3$
- similar radiation condition on lower half space or classical boundary condition

FEM domain: $\vec{x} = (x', x_3)^\top \in \Omega := [0,\text{per}_1] \times [0,\text{per}_2] \times (b^-, b^+)$,
upper half space: $\Omega^+ := [0,\text{per}_1] \times [0,\text{per}_2] \times [b^+,\infty]$ with $k(\vec{x}) = k^+$ for $x \in \Omega^+$

$$\nabla \times \nabla \times E(\vec{x}) - k(\vec{x})^2 E(\vec{x}) = 0, \; \vec{x} \in \Omega \qquad E(\vec{x}) - E^{\text{inc}}(\vec{x}) = \sum_{n\in\mathbb{Z}^2} R_n e^{\mathbf{i}(\alpha_n \cdot x' + \beta_n x_3)}, \; \vec{x} \in \Omega^+$$

$$E^{\text{inc}} := R^{\text{inc}} e^{\mathbf{i}(\alpha^{(1)}x_1 + \alpha^{(2)}x_2 + \beta_n x_3)}, \quad \alpha_n := (\alpha_n^{(1)}, \alpha_n^{(2)})^\top = (\alpha^{(1)} + \frac{2\pi n_1}{\text{per}_1}, \alpha^{(2)} + \frac{2\pi n_2}{\text{per}_2})^\top,$$
$$\beta_n := \sqrt{(k^+)^2 - |\alpha_n|^2}, \quad R_n \perp (\alpha_n, \beta_n)^\top$$

Variational formulation including Dirichlet-to-Neumann map

Weak formulation for FEM in domain Ω bounded by upper boundary line $\Gamma_{b^+} := \{\vec{x} \in \overline{\Omega}: \; x_3 = b^+\}$
- Coupling with solution in half space Ω^+ via BEM technique: $\mathscr{R}$ - Dirichlet-to-Neumann map
- Troubles: If there is $n \in \mathbb{Z}^2$ such that $\beta_n = 0$, then there exists non-trivial solution $[e_3 e^{\mathbf{i}\alpha_n \cdot x'}]$ of homogeneous Dirichlet problem $(e_3 \times E)|_{\Gamma_{b^+}} = 0$ over half space Ω^+
- Modification (in red color): Simplifying assumptions
  - Small layer $\Omega_\varepsilon \subseteq \Omega$ beneath Γ_{b^+} filled with cover material of Ω^+
  - There is only one $n_0 \in \mathbb{Z}^2$ with $\beta_{n_0} = 0$.

Look for electric field $E \in H_{\text{qp}}(\text{curl},\Omega)$ and scalar $\lambda \in \mathbb{C}$ satisfying extended variational equation

$$\int_\Omega \left[\nabla \times E \cdot \nabla \times \overline{V} - k^2 E \cdot \overline{V}\right] d\vec{x} - \int_{\Gamma_{b^+}} \left\{\mathscr{R}(e_3 \times E) + \lambda \nabla \times \left[e_3 e^{\mathbf{i}\alpha_{n_0}\cdot x'}\right]\right\} \cdot (e_3 \times \overline{V}) dx' - \int_{\Gamma_{b^-}} \ldots$$
$$= \int_{\Gamma_{b^+}} \{(\nabla \times E^{in})_T - \mathscr{R}(e_3 \times E^{in})\} \cdot (e_3 \times \overline{V}) ds,$$
$$\int_{\Omega_\varepsilon} \left\{E - \lambda \left[e_3 e^{\mathbf{i}\alpha_{n_0}\cdot x'}\right]\right\} \cdot \overline{\left[e_3 e^{\mathbf{i}\alpha_{n_0}\cdot x'}\right]} d\vec{x} \; \overline{\eta} = 0, \qquad \forall V \in H_{\text{qp}}(\text{curl},\Omega), \; \forall \eta \in \mathbb{C}$$

$$(\mathscr{R}\widetilde{E})(x') := - \sum_{n_0 \neq n \in \mathbb{Z}^2} \frac{1}{i\beta_n} \left[(k^+)^2 \widetilde{E}_n - \left((\alpha_n, 0)^\top \cdot \widetilde{E}_n\right)(\alpha_n, 0)^\top\right] \exp(i\alpha_n \cdot x') \text{ if } \widetilde{E}(x') = \sum_{n\in\mathbb{Z}^2} \widetilde{E}_n e^{\mathbf{i}\alpha_\mathbf{n}\cdot\mathbf{x}'}$$
$$\Omega_\varepsilon := \{\vec{x} \in \Omega: \; b^+ - \varepsilon < x_3 < b^+\}, \quad \int_{\Gamma_{b^-}} \ldots \text{ boundary term for lower boundary}$$

Variational formulation using coupling with Fourier-mode expansion

- Idea of Huber et al. [1]: Direct coupling of Rayleigh-mode expansions in Ω^+ with solution over FEM domain Ω using the technique of Nitsche and Sternberg
- Analysis:
  - Modify, slightly, the variational formulation of Huber et al. [1] in particular change sign and approximate unbounded scalar product of traces by finite rank approximation
  - Split $H_{\text{qp}}(\text{curl},\Omega)$ according to the Hodge decomposition, split Rayleigh expansions into space spanned by TE modes $U_{n,0}$ and space spanned by TM modes $U_{n,0}$
  - Use well-known BEM techniques
  - Structure of operator of variational form: Sum of compact operator plus operator which is diagonal w.r.t. splitting, diagonal entries are positively or negatively coercive

Theorem [3]: *If there are no non-trivial solutions of homogeneous boundary value problem, then operator of variational form invertible*

$$a\Big((E,E^+,E^-),(V,V^+,V^-)\Big) = -a\Big((0,E^{\text{inc}},0),(V,V^+,V^-)\Big), \quad \forall (V,V^+,V^-) \in \mathbb{H}$$
$$a\Big((E,E^+,E^-),(V,V^+,V^-)\Big) := \int_\Omega \{\nabla \times E \cdot \nabla \times \overline{V} - k^2 E \cdot \overline{V}\} dx - \int_{\Gamma_{b^+}} \nabla \times E^+ \cdot e_3 \times \overline{V} ds$$
$$+ \int_{\Gamma_{b^+}} e_3 \times (E - E^+) \cdot \nabla \times \overline{V^+} ds$$
$$+ \sum_{n\in\Upsilon} \int_{\Gamma_{b^+}} e_3 \times (E - E^+) \cdot (e_3 \times \overline{U}_{n,0}) \, ds \, \overline{\int_{\Gamma_{b^+}} e_3 \times (V - V^+) \cdot (e_3 \times \overline{U}_{n,0}) ds} + \int_{\Gamma_{b^-}} \ldots$$

$$\mathbb{H} := H_{\text{qp}}(\text{curl},\Omega) \times Y^+ \times Y^-, \quad Y^+ := \text{span}\{U_{n,l}: \; n \in \mathbb{Z}^2, l = 0,1\}, \quad \|\cdot\|_{Y^+} := \|\cdot\|_{H(\text{curl},\Omega^+_{b^+})},$$
$$\Omega^+_{b^+} := \{\vec{x} \in \Omega^+: \; b^+ < x_3 < b^+ + 1\}, \quad U_{n,0} := (-\alpha_n^{(2)}, \alpha_n^{(1)}, 0)^\top e^{\mathbf{i}(\alpha_n \cdot x' + \beta_n x_3)}, \quad U_{n,1} := \nabla \times U_{n,0},$$
$$\int_{\Gamma_{b^-}} \ldots \text{ boundary terms for lower boundary}$$

Numerical analysis

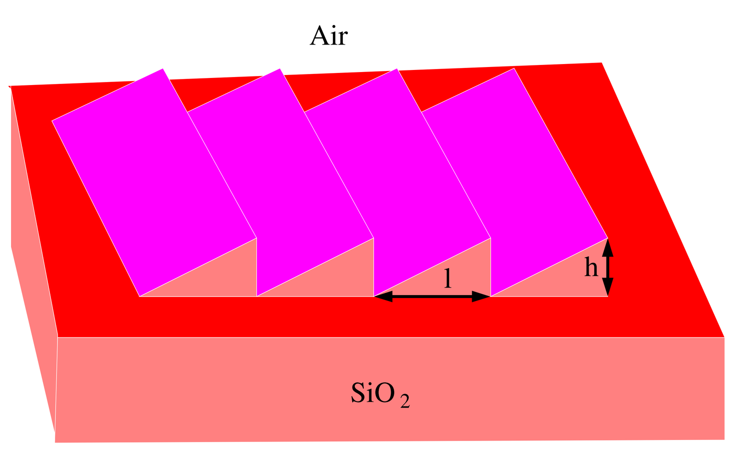
- Discretize field over Ω: Use finite element functions with collective compactness property, e.g., Nédélec's edge elements over regular FEM grids
- Truncate Rayleigh expansions: $\sum_{n\in\mathbb{Z}^2} \sum_{l=0}^1 c_{n,l} U_{n,l} \mapsto \sum_{n\in\mathbb{Z}^2: \, |n_i|<N} \sum_{l=0}^1 c_{n,l} U_{n,l}$
  - Experiments show that only small number of Rayleigh modes significant
  - Coefficients of Rayleigh modes decay exponentially for $|n| \to \infty$ if b^+ is chosen a bit larger.
  - Typically, number of modes much less than number of DOFs in FEM over Γ_{b^+}
- Analysis:
  - Use structure of operator in variational form
  - Show that discretized operators of non-compact off-diagonal operators tend to zero

Theorem [4]: *If there are no non-trivial solutions of homogeneous boundary value problem, then Galerkin method with FEM and truncated Rayleigh expansions is stable and convergent for meshsize $h \to 0$ and truncation threshold $N \to \infty$. Approximation error proportional to error of best approximation.*

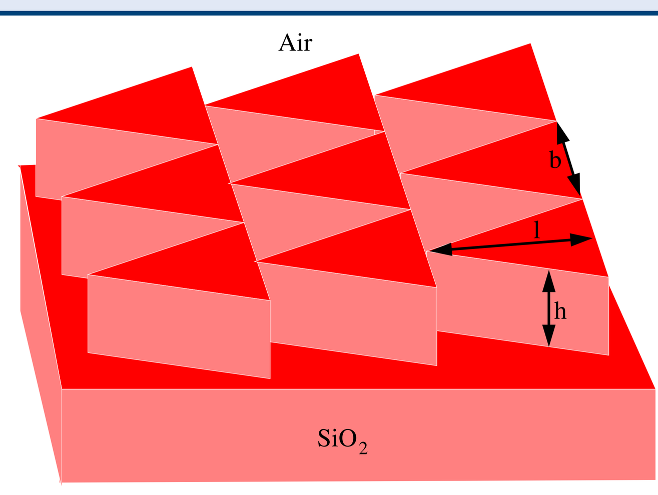
$$a\Big((E_h,E_N^+,E_N^-),(V_h,V_N^+,V_N^-)\Big) = -a\Big((0,E^{\text{inc}},0),(V_h,V_N^+,V_N^-)\Big) \quad \forall (V_h,V_N^+,V_N^-) \in \mathbb{H}_{h,N}$$

Simple example

- Echelle grating - designed to deflect line into the direction specular w.r.t. the faces
- Idea of Blaces - for b less and h larger than wavelength of light λ, similar effective medium distribution like echelle grating, Blaces are of higher stability (cf. Elfström et al. [2])
- We compare the new 3D coupling algorithm applied to the 2D echelle grating with the reliable results of the 2D FEM code solving the Helmholtz equation.
  $\lambda = 500\,$nm, period $l = 10\,\mu$m, height $h = 0.5\,\mu$m, illuminated exactly from above, TE polarization
- We compare the new 3D coupling algorithm applied to the blaces grating with the results of the algorithm by Huber et al. [1]
  period $\text{per}_1 = l = 10\,\mu$m, period $\text{per}_2 = b = \lambda/2$, other parameters like echelle



Echelle grating



Blaces

Echelle:
$N_1^+ = 22, N_2^+ = 2$
$N_1^- = 32, N_2^- = 2$
quadratic splines

meshsize	$e^+_{-2,0}$	$e^+_{0,0}$	$e^-_{1,0}$	$e^-_{2,0}$
125.0 nm	4.82	0.0027	43.23	3.78
62.5 nm	4.530	0.0022	45.0080	4.1289
31.2 nm	4.5039	0.0019	45.0559	4.1142
2D code	4.5025	0.0019	45.0630	4.1145

efficiencies (in %):

$$e_n^+ := \frac{\beta_n}{\beta_{(0,0)}} |R_n|^2$$
$$e_n^- := \frac{|k^+|^2 \sqrt{(k^-)^2 - |\alpha_n|^2}}{|k^-|^2 \beta_{(0,0)}} |R_n|^2$$

Blaces:
$N_1^+ = 22, N_2^+ = 2$
$N_1^- = 32, N_2^- = 2$
quadratic splines

meshsize	$e^+_{0,0}$	$e^+_{0,0}$	$e^+_{1,0}$	$e^+_{1,0}$	$e^-_{0,0}$	$e^-_{0,0}$	$e^-_{1,0}$	$e^-_{1,0}$
125.0 nm	2.8328	3.0985	0.1661	0.1661	75.2800	76.289	10.1503	10.1465
62.5 nm	2.8172	2.8333	0.1918	0.1918	75.5412	75.553	10.7248	10.7197
31.2 nm	2.8119	2.8136	0.1944	0.1944	75.4717	75.490	10.7787	10.7711

References:

[1] Huber, M., Schoeberl, J., Sinwel, A., and Zaglmayr, S., 2009, Simulation of diffraction in periodic media with a coupled finite element and plane wave approach, *SIAM J. Sci. Comput.* **31**, 1500–1517.
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