Inverse Design of Photonic Structures Using Automatic Differentiable Rigorous Diffraction Interface Theory

Yi Huang,[1] Hong Tang,[1] Bowen Zheng,[1] Yunxi Dong,[1] Mohammad Haerinia,[1] Viktor A. Podolskiy,[2] and Hualiang Zhang,[1,*]

[1] *Department of Electrical and Computer Engineering, University of Massachusetts Lowell, Lowell, Massachusetts 01854, USA*

[2] *Department of Physics and Applied Physics, University of Massachusetts–Lowell, Lowell, Massachusetts 01854, USA*

[*] *Hualiang_Zhang@uml.edu*

Abstract: We present an automatic differentiable R-DIT for the fast inverse design of photonic structures. We demonstrated that the proposed method could achieve a 30% speedup per optimization on GPUs compared with the differentiable RCWA.

Automatic differentiation (AD) has become a powerful tool for different inverse design applications where AD provides an alternative to the adjoint methods, avoiding the need to derive derivative formulas. Rigorous coupled-wave analysis (RCWA) [1] is a widely-used technique capable of predicting the electromagnetic response of spatially-periodic composites. For meta-optics applications, Colburn and Majumdar [2] have successfully implemented rigorous coupled-wave analysis (RCWA) on AD frameworks by generalizing complex eigenproblems with the Lorentzian broadening technique. However, the performance of this AD-RCWA, as well as the performance of all RCWA algorithms, are significantly constrained by the requirement of the eigen decomposition, the time-consuming task that decelerates the computing on both central processing unit (CPU) and graphics processing unit (GPU) platforms, when solving for large, complicated models with many spatial modes.

Rigorous diffraction interface theory (R-DIT) [3] formalism has been proposed to speed up the optics analysis of thin periodic composites. Here we present an extension of the R-DIT framework based on automatic differentiation. As an example, we applied the developed automatic differentiable R-DIT to optimize a guided mode resonance filter (GMRF), demonstrating significant speedup over AD-RCWA. Furthermore, the proposed approach could accelerate the numerical calculation and optimization of other complex metasurfaces.

One of the key features of R-DIT is solving Maxwell's equations in the Fourier domain without solving eigenvalue problems, which is briefly explained in the following. Maxwell's equation in the Fourier domain can be expressed below (the negative sign convention e^{-jkz} is used in this text):

$$\frac{\mathrm{d}}{\mathrm{d}\tilde{z}}\begin{bmatrix}\vec{\mathscr{E}}\\ \vec{\mathscr{H}}\end{bmatrix}=\begin{bmatrix}0 & \hat{\mathbb{P}}\\ \hat{\mathbb{Q}} & 0\end{bmatrix}\begin{bmatrix}\vec{\mathscr{E}}\\ \vec{\mathscr{H}}\end{bmatrix} \tag{1}$$

where $\vec{\mathscr{E}}$ and $\vec{\mathscr{H}}$ are the tangential Fourier coefficients of the electrical field $\vec{E}$ and the normalized magnetic field $\vec{\tilde{H}}=-j\sqrt{\mu_0/\varepsilon_0}\vec{H}$, $\tilde{z}=k_0 z$ is the normalized coordinate, and $\hat{\mathbb{P}}$ and $\hat{\mathbb{Q}}$ are block matrices containing the information of the permittivity/permeability distributions of the specific layer. Instead of solving the eigenvalue problem for Eq. (1), R-DIT relies on Taylor expansion of electromagnetic fields and reduces the optics of diffractive metasurface layer to the generalized boundary condition relating the fields at the interfaces surrounding the metasurface:

$$\begin{bmatrix}\mathbb{I}+\frac{h^2}{8}\hat{\mathbb{P}}\hat{\mathbb{Q}}+\cdots & \frac{h}{2}\hat{\mathbb{P}}+\frac{h^3}{48}\hat{\mathbb{P}}\hat{\mathbb{Q}}\hat{\mathbb{P}}+\cdots\\ \frac{h}{2}\hat{\mathbb{Q}}+\frac{h^3}{48}\hat{\mathbb{Q}}\hat{\mathbb{P}}\hat{\mathbb{Q}}+\cdots & \mathbb{I}+\frac{h^2}{8}\hat{\mathbb{Q}}\hat{\mathbb{P}}\end{bmatrix}\begin{bmatrix}\vec{\mathscr{E}}\\ \vec{\mathscr{H}}\end{bmatrix}\Bigg|_{\tilde{z}=-k_0\frac{h}{2}}$$
$$=\begin{bmatrix}\mathbb{I}+\frac{h^2}{8}\hat{\mathbb{P}}\hat{\mathbb{Q}}+\cdots & -\frac{h}{2}\hat{\mathbb{P}}-\frac{h^3}{48}\hat{\mathbb{P}}\hat{\mathbb{Q}}\hat{\mathbb{P}}+\cdots\\ -\frac{h}{2}\hat{\mathbb{Q}}-\frac{h^3}{48}\hat{\mathbb{Q}}\hat{\mathbb{P}}\hat{\mathbb{Q}}+\cdots & \mathbb{I}+\frac{h^2}{8}\hat{\mathbb{Q}}\hat{\mathbb{P}}\end{bmatrix}\begin{bmatrix}\vec{\mathscr{E}}\\ \vec{\mathscr{H}}\end{bmatrix}\Bigg|_{\tilde{z}=+k_0\frac{h}{2}} \tag{2}$$

where h is the thickness of the metasurface layer, $z=0$ is its center,and $\mathbb{I}$ is the identity matrix. It is also worth mentioning that since only matrix multiplications are included in the derivation, there is no need to rewrite the backward computations on AD frameworks explicitly.

To demonstrate the efficacy of the proposed method, a guided mode resonance filter (GMRF) [4] operating at the free-space wavelength of around $\lambda_0 = 1540$ nm high-frequency selectivity was designed [Fig. 1 (a,b)]. We started

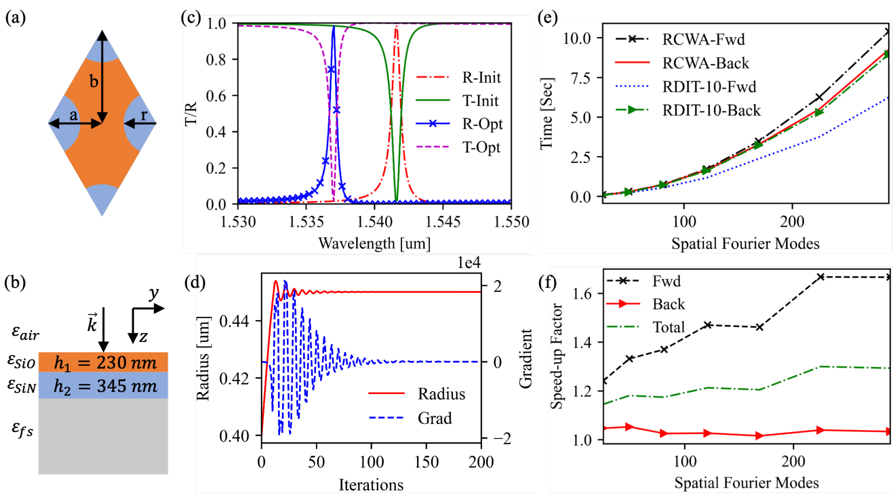

Fig. 1. (a) Geometry of the hexagonal unit cell of the proposed GMRF: $a = 575$ nm, $b = 995.9$ nm, r is the radius of the holes to be optimized; (b) Cross-section of the GMRF under investigation: top SiO grating ($\varepsilon_{\mathrm{SiO}} = 2.101$, $h_1 = 230$ nm), SiN waveguide ($\varepsilon_{\mathrm{SiN}} = 3.748$, $h_2 = 345$ nm) and fused silica substrate (semi-infinite layer with $\varepsilon_{\mathrm{fs}} = 2.280$), the TE-mode plane wave is normally incident from the air; (c) Spectrum with the initial radius $r = 400$ nm and it with the optimized radius $r = 450$ nm; (d) Radius and gradient of the transmission efficiency with respect to the radius over the iterations; (e, f) Forward and backward simulation times and speedup of RCWA and the 10th order of proposed R-DIT.

from an initial value $r = 400$ nm, with a reflection peak at $\lambda = 1541$ nm [Fig. 1 (c)]. The goal of the inverse design is to move the resonance to 1537 nm by changing the radius r. Based on the gradient descent method, the loss function was reduced by either maximizing the reflection or minimizing the transmission at 1537 nm according to the gradient information from the 10th order of R-DIT (10th order of Taylor expansion). The optimized response is shown in Fig. 1 (c). The derivative of the transmission efficiency with respect to the radius converges to 0 over iterations, and the optimal radius converges at $r = 450$ nm [Fig. 1 (d)].

To better understand how the proposed R-DIT performs during inverse design, we used a batch of GMRF models (batch size 100 and 10 frequencies) to go through the same optimization process as presented above with different spatial modes on the GPU platform (NVIDIA Tesla T4 offered by Google Colab). As a reference, we also developed a differentiable RCWA based on [2]. Fig. 1 (e) and (f) show the performance comparison between these two approaches. It is observed that, compared with RCWA, the developed R-DIT (10th order) has sped up the forward simulation time for about 20% to 70% (increased with the spatial modes since larger matrices perform much better with pure matrix multiplications than the complicated eigendecomposition). On the other hand, the backward simulation time is very similar because the back-propagation computation within AD frameworks relies on the chain rule, in which only generated computing graphs are used. Overall, the developed R-DIT achieved a 10% to 30% speedup for an optimization iteration compared to RCWA.

In summary, we presented an automatic differentiable R-DIT platform, which can perform fast gradient-based inverse design. To validate the proposed approach, a GRMF was designed and optimized. It is demonstrated that the proposed R-DIT can accelerate the computational process compared to existing methods (i.e., RCWA). It is expected that the proposed platform can be combined with machine learning techniques for fast inverse design of non-intuitive photonic structures.

This research was supported by the National Science Foundation (NSF) (awards No. 2132929 and 2118787).

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