High-Order Electromagnetic Field Sensitivity Analysis with FDTD and the Complex-Step Derivative Approximation

Kae-An Liu, *Student Member, IEEE* and Costas D. Sarris, *Senior Member, IEEE*

***Abstract*—This research is focused on a new approach to compute electromagnetic field derivatives with respect to multiple design parameters in a single FDTD simulation. The field derivatives, up to any order, with respect to material and geometric parameters of a given geometry are found accurately on-the-fly in FDTD. This proposed computational framework offers the versatility of standard methods, e.g., finite-differences, while its accuracy significantly surpasses that of finite-differences. With accurate, first and high-order derivatives available, parametric expressions of electromagnetic fields and field-based functions, such as scattering parameters, are derived via Taylor expansions, demonstrating an important application of this proposed method to full-wave analysis based parametric modeling for electromagnetic design.**

I. Introduction

As the complexity of modern electromagnetic design increases, so does the importance of numerical techniques for sensitivity analysis [1], parametric modeling and uncertainty quantification [2]. Such methods aim at determining not just the field solution to a given problem, but also its variation under fabrication tolerances and other statistical uncertainties in the geometry and the materials comprising the structure under consideration.

Notably, sensitivity analysis with respect to any output function of interest can be performed if the corresponding derivatives of the electromagnetic field components are available. A standard approach for this analysis is offered by the finite-difference method. Consider an objective function $F(\xi)$. Its first-order derivative with respect to parameter ξ at nomial value ξ_0 is approximated by the centered finite difference (CFD) as follows:

$$\frac{F(\xi_0+h)-F(\xi_0-h)}{2h} = \frac{\partial F}{\partial \xi}(\xi_0) + \frac{h^2}{6}\frac{\partial^3 F}{\partial \xi^3}(\xi_0) + \mathcal{O}(h^4) \tag{1}$$

However, the CFD method is subject to subtractive cancellation errors. This issue becomes even more important in the context of the Finite-Difference Time-Domain (FDTD) method, where small geometric and material perturbations are desired, to limit associated numerical dispersion errors. Moreover, CFDs require two simulations per parameter, accumulating computational overhead when sensitivities with respect to multiple parameters are considered.

The authors are with the Edward S. Rogers Sr. Department of Electrical and Computer Engineering, University of Toronto, Toronto, ON M5S 3G4, Canada.

To overcome the subtractive cancellation errors in finite-difference methods, the complex-step derivative (CSD) approximation method is proposed [3]. For an analytic function f, its first-order derivative is found as:

$$\frac{\partial f}{\partial \xi} = \frac{\operatorname{Im}\{f(\xi+jh)\}}{h} + \mathcal{O}(h^2) \tag{2}$$

The CSD method has been applied to a standard FDTD simulation for the computation of first-order field derivatives with promising results [4]. In this research, a generalized form of (2), known as the multi-complex step derivative (MCSD) approximation is introduced to FDTD for the evaluation of first and higher order derivatives with respect to multiple design parameters [5].

With high-order derivatives available, parameteric expressions of electromagnetic fields and field-based functions, such as scattering parameters, are derived via Taylor expansions, demonstrating an important application of the proposed method to full-wave analysis based parametric modeling for electromagnetic design.

II. The Multi-Complex Step FDTD Method

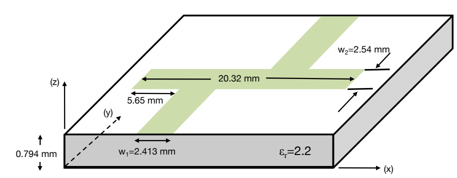

Fig. 1. The geometry of a microstrip filter from [6].

In a MCSD-based FDTD, the field derivatives with respect to material parameter ε_r and geometric parameters can be computed by assigning imaginary perturbations to standard FDTD update equations. For example, the perturbation of geometric parameter l is mapped to the corresponding cell size Δy, and $\Delta y' \equiv \Delta y + j_1 h + j_2 h$. On the other hand, ε_r is set to $\varepsilon_r + j_3 h + j_4 h$ for material sensitivity. The FDTD update equation with multi-complex steps is written as:

$$E^{x,n+1}_{i+\frac{1}{2},m,k} = E^{x,n}_{i+\frac{1}{2},m,k} + \frac{\Delta t}{\varepsilon_0\left(\varepsilon_r + j_3 h + j_4 h\right)}\Bigg(\frac{H^{z,n+\frac{1}{2}}_{i+\frac{1}{2},m+\frac{1}{2},k} - H^{z,n+\frac{1}{2}}_{i+\frac{1}{2},m-\frac{1}{2},k}}{(\Delta y + j_1 h + j_2 h)} - \frac{H^{y,n+\frac{1}{2}}_{i+\frac{1}{2},m,k+\frac{1}{2}} + H^{y,n+\frac{1}{2}}_{i+\frac{1}{2},m,k-\frac{1}{2}}}{\Delta z}\Bigg) \tag{3}$$

Then, the FDTD simulation produces (where $\tilde{\mathbf{E}}$, $\mathbf{E}$ are the electric fields of the complex step perturbed and the unperturbed problem, respectively) :

$$
\begin{aligned}
&\mathrm{Re}\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\} \approx \mathbf{E}^n_{i,m,k} \\
&\mathrm{Im}_1\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h \approx \mathrm{Im}_2\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h \approx \partial \mathbf{E}^n_{i,m,k}/\partial l \\
&\mathrm{Im}_3\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h \approx \mathrm{Im}_4\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h \approx \partial \mathbf{E}^n_{i,m,k}/\partial \varepsilon_r \\
&\mathrm{Im}_{12}\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h^2 \approx \partial^2 \mathbf{E}^n_{i,m,k}/\partial l^2 \\
&\mathrm{Im}_{13}\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h^2 \approx \partial^2 \mathbf{E}^n_{i,m,k}/\partial l \partial \varepsilon_r \\
&\mathrm{Im}_{34}\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h^2 \approx \partial^2 \mathbf{E}^n_{i,m,k}/\partial \varepsilon_r^2 \\
&\mathrm{Im}_{123}\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h^3 \approx \partial^3 \mathbf{E}^n_{i,m,k}/\partial l^2 \partial \varepsilon_r \\
&\mathrm{Im}_{134}\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h^3 \approx \partial^3 \mathbf{E}^n_{i,m,k}/\partial l \partial \varepsilon_r^2 \\
&\mathrm{Im}_{1234}\left\{\tilde{\mathbf{E}}^n_{i,m,k}\right\}/h^4 \approx \partial^4 \mathbf{E}^n_{i,m,k}/\partial \varepsilon_r^2 \partial l^2
\end{aligned}
\tag{4}
$$

The real part of the field arrays contains the solution to the problem and the imaginary dimensions contain derivatives from first to fourth order, including all entries to the Hessian matrix and all derivatives needed for a second-order Taylor series expansion of the fields with respect to $(l,\, \varepsilon_r)$.

III. Numerical Results

The advantages of MCSD-FDTD method are demonstrated through a three-dimensional FDTD simulation of a microstrip filter originally studied in [6] and reproduced here in Fig. 1 [7]. In particular, we focus on sensitivities of the S-parameters of the filter, with respect to the widths $w_{1,2}$, shown in Fig. 1. The derivatives of the S-parameters, are expressed in terms of the derivatives of the scattered and transmitted fields at the ports of the filter with respect to the design parameters.

For the MCSD-FDTD based computation of the sensitivities with respect to $w_{1,2}$, The cell modeling the segment of width w_1 are perturbed by $j_1 h_1 \Delta x$. Likewise, the Δy of the cells modeling the segment of width w_2 are perturbed by $j_2 h_2 \Delta y$.

Fig. 2 shows second order derivatives of S_{21}, computed via MCSD-FDTD and CFD-FDTD, for values of h_1, h_2 that vary between 10^{-7} and 10^{-3}. These results indicate the significant convergence problem of CFD and the robustness of MCSD.

IV. Conclusions

This research proposed and developed an accurate method to compute high-order field derivatives with respect to design parameters in a single FDTD simulation. The accuracy and robustness of the MCSD approximation and the relative simplicity of its implementation in FDTD are the most significant advantages of this method. With these accurate high-order field derivatives available, sensitivity analysis, parametric modelling, as well as uncertainty quantifications, can be performed efficiently, realizing a comprehensive framework for design optimization in electromagnetic simulations.

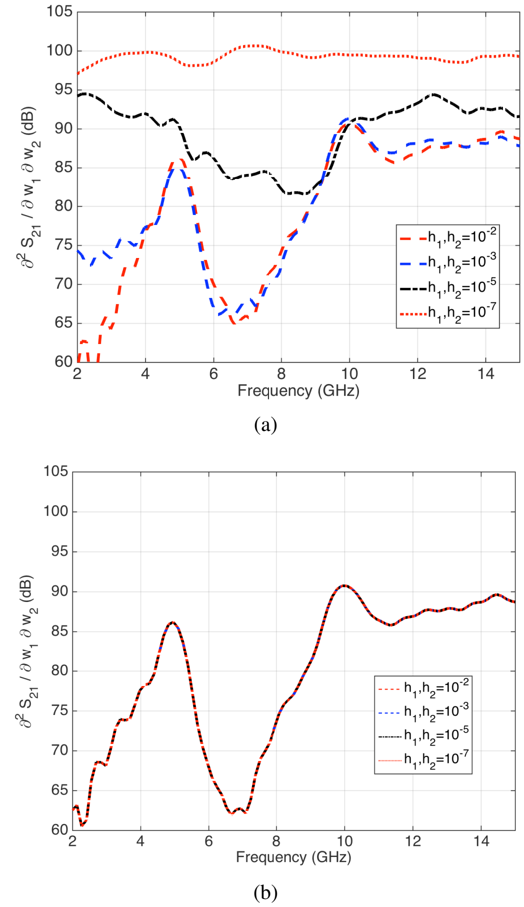

Fig. 2. Numerical sensitivities of the microstrip low-pass filter: $\partial^2 S_{21}/\partial w_1 \partial w_2$ computed via FDTD with (a) CFD and (b) MCSD methods.

V. Future Plans

I would like to thank MTT Pre-Graduate Scholarship for providing me with the valuable opportunity to participate in the 2018 IMS. This experience greatly motivated me to explore the industry. After graduation, I plan to join the EMC team of Intel Corporation, focusing on enhancing wireless communication quality of mobile platforms by reducing RF noise. I expect to turn this industrial experience as a platform for future academic research.

References

[1] J. W. Bandler and R. E. Seviora, “Computation of sensitivities for optimal design of microwave networks,” in *IEEE International Microwave Symposium Digest*, 1970, pp. 134–137.

[2] C. Chauvière, J. S. Hesthaven, and L. Lurati, “Computational modeling of uncertainty in time-domain electromagnetics,” *SIAM Journal on Scientific Computing*, vol. 28, pp. 751–775, February 2006.

[3] J. R. R. A. Martins, P. Sturdza, and J. J. Alonso, “The complex-step derivative approximation,” *ACM Transactions on Mathematical Software*, vol. 29, no. 3, pp. 245–262, September 2003.

[4] C. D. Sarris and H. Lang, “Broadband sensitivity analysis in a single FDTD simulation with the complex step derivative approximation,” in *IEEE MTT-S International Microwave Symposium*, May 2015, pp. 1–3.

[5] K. A. Liu and C. D. Sarris, “High-order sensitivity analysis with FDTD and the multi-complex step derivative approximation,” in *IEEE International Microwave Symposium*, June 2017, pp. 691–693.

[6] D. M. Sheen, S. M. Ali, M. D. Abouzahra, and J. A. Kong, “Application of the three-dimensional finite-difference time-domain method to the analysis of planar microstrip circuits,” *IEEE Transactions on Microwave Theory and Techniques*, vol. 38, pp. 849–857, July 1990.

[7] K. A. Liu, H. Lang, and C. D. Sarris, “Computation of high-order electromagnetic field sensitivity analysis with FDTD and the complex-step derivative approximation,” *Submitted*, 2019.