Broadband Parametric Modeling of Electromagnetic Structures with the FDTD Method Coupled with the Multi-Complex Step Derivative Approximation

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The complex-step derivative approximation (CSDA) is a finite-difference-free method to approximate derivatives of analytic functions (J. R. R. A. Martins, P. Sturdza, J. J. Alonso, ACM Trans. on Math. Software, vol. 29, no. 3, Sept. 2003, pp. 245–262). For a function of one variable, CSDA assumes the form: $f'(x) \approx Im\left\{f(x+jh)\right\}/h$. Recently, CSDA was directly embedded into the Finite-Difference Time-Domain (FDTD) method to produce a broadband sensitivity analysis technique that requires a single FDTD simulation in total (C.D. Sarris, H.D. Lang, 2015 IEEE MTT-S Int. Microwave Symp. Digest). In that one simulation, both the output of interest and its sensitivity are derived at once over the simulated frequency bandwidth.

The CSDA formula for the first derivative of a function of one variable can be extended to higher order derivatives and multiple parameters, introducing multiple complex dimensions (G. Lantoine, R.P. Russell, T. Dargent, ACM Trans. on Math. Software, vol. 38, no. 3, Apr. 2012, pp. 1–21). For example, $f^{(n)}(x)$ (sticking for simplicity to the one variable case) can be approximated as: $f^{(n)}(x) \approx Im_{1\cdots n}\left\{f(x+j_1h+\cdots+j_nh)\right\}/h^n$, where the operator $Im_{1\cdots n}$ yields the $j_1\cdots j_n$-term of the expression inside the brackets (for example, $f^{(n)}(x)Im_{12}(x+j_1h+j_2h)^2 = h^2$, since the j_1j_2 term comes from the product $(j_1h)(j_2h)$ and is equal to h^2. Extending this expression to multiple variables, leads to the multi-complex step derivative approximation of Lantoine *et al.*, which can be still incorporated in standard FDTD. To that end, the regular FDTD equations are modified to embed the multiple complex dimensions present in the multi-complex step derivative approximation. It should be emphasized that all derivative approximations remain finite-difference free, hence not limited by subtractive cancellation errors.

In addition to introducing the multi-complex step derivative approximation FDTD method, this paper goes one step further to explore its application as a full-wave parametric analysis technique. Indeed, with high-order derivatives with respect to the design parameters at hand, one can readily express field-based functions of interest (e.g. scattering parameters, antenna gain and input impedance) in terms of the design parameters, by means of a Taylor expansion. Such full-wave (rather than circuit theory or other approximation based) models can dramatically speed-up optimization and uncertainty quantification studies of electromagnetic structures, while retaining the accuracy of a full-wave method. Three-dimensional examples of parametric models of microstrip patch antennas and planar microwave circuits will be presented.