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# Correlations in A posteriori Error Trends for the Finite Element Method in the Presence of Changing Material Parameters

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***Abstract*—In this letter, we demonstrate that adjoint-based a posteriori elementwise error contribution estimates can be highly correlated in the presence of changing material parameters for finite element method scattering problems. Using a simple lossy dielectric sphere scattering problem set, we explore trends in elementwise a posteriori error contribution estimates as the real permittivity of the spherical scatterer is varied. We show that, not only do elementwise error contribution estimates for this problem remain highly correlated as material parameters vary, but that this correlation is stronger than that apparent for quantities of interest or gradients of such quantities across the same range of dielectric parameters. We also show correlation between the mean and standard deviation of elementwise error contribution estimate magnitudes.**

***Index Terms*—Computational electromagnetics, adjoint methods, error estimation, finite element method, material parameters.**

## I. Introduction

ERROR estimation, adaptive refinement, and uncertainty quantification are of growing interest in computational electromagnetics (CEM). Recently, adjoint-based techniques have been demonstrated as effective approaches to these three related research areas [1]. For error estimation problems, adjoint methods excel at producing accurate, signed error estimates for a quantity of interest (QoI), or many, stated as a linear or linearized functional on an approximate field solution obtained by finite element method (FEM), finite difference (FD) method, or method of moments (MoM). Such error estimates are typically more accurate than those produced by a priori means or application of a norm [2], [3]. Adjoint-based a posteriori error estimates can be applied effectively to adaptive discretization refinement to dramatically reduce solution error in few solves [4], [1].

Applied to uncertainty quantification, adjoint methods serve as an accurate approach to estimating QoI responses to uncertain model parameters. Higher-order parameter sampling (HOPS) [5] is the most notable approach. Recent research has demonstrated HOPS can approach the accuracy of Monte Carlo for FEM scattering problems while using two orders of magnitude fewer solves [6], making HOPS a compelling technique for accelerating uncertainty quantification computations in CEM. For complicated uncertainty quantification problems and low error tolerances, HOPS can still require tens or hundreds of solves, however, making HOPS a large, multi-solve problem.

We have recently speculated that adaptive refinement using adjoint-based a posteriori error estimates may be applicable to achieve efficiency gains for large, multi-solve problems like HOPS, Monte Carlo simulation, and radar cross section (RCS) computation [1], all of which require the solution of many similar problems. Naively, we could imagine performing adaptive refinement for each sub-problem separately, perhaps performing a handful of simulations on adapted discretizations to meet an error tolerance for each sub-problem, treating each sub-problem as [4] does. However, as the individual sub-problems composing most multi-solve problems relate closely, we contend that so too should their a posteriori elementwise error contribution estimates (EECEs). If this is true, then such refinement techniques could be iterated *across* sub-problems, rather than for each sub-problem, potentially yielding efficiency gains. Accordingly, this letter presents preliminary research exploring the relatedness (as measured by Pearson's correlation) between EECEs for a set of lossy dielectric sphere FEM scattering problems like those used for HOPS estimates in [6].

As the scope of this paper is rather narrow and adjoint methods are relatively rarely applied in CEM, especially for error estimation, there is little related research other than literature that has laid the theoretical background for development and application of such methods to CEM. Most existing goal-oriented error estimation methods in CEM have relied on bounding error in a norm or forming a priori estimates [7], [8], although we note [9] and [10] which leverage the adjoint, with [10], demonstrating that adjoint-based approaches can far outperform those using an energy norm. In general, much prior work concerning uncertainty quantification in CEM has applied polynomial chaos, rather than adjoint-based methods [11].

Manuscript received July 13, 2021, revised August 23, 2021. This work was supported by the US Air Force Research Laboratory, RF Analysis and Validation Engineering Software (RAVEnS), Applied Research Associates, under contract FA8650-20-C-1132.

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## II. Theory and Example Problems

The theory and derivations for applying the adjoint methodology to CEM, including the application of adjoint analysis to 3-D FEM scattering problems for a posteriori error estimation and adaptive refinement, are described in [4]. The details of the double higher order FEM discretization methodology can be found in [12]. We use a conformal perfectly matched layer (PML) for curvilinear meshes for FEM domain termination in scattering problems [13].

We simulated a set of 41 lossy dielectric sphere scattering sub-problems. Each sub-problem consisted of a lossy sphere 2 wavelengths in diameter encased in a spherical shell of air 0.3 wavelengths thick. The domain was truncated using a PML shell with 0.3 wavelength (λ) thickness surrounded by PEC. A single plane wave was used to excite each sub-problem, and double-higher-order frequency domain FEM was used to generate an approximate field solution for each, as in [6]. All discretizations were topologically identical, containing 256 geometrically quadratic ($K_u=K_v=K_w=2$ in the notation of [12]) hexahedral elements, and used the same second order ($N_u=N_v=N_w=2$ in the notation of [12]) Legendre basis described in [12]. Sub-problems varied only in the real component of the complex relative permittivity, with values ranging from 4.0 to 8.0 and the imaginary component fixed at -2.0j. Figure 1 shows the basic geometry of the domain.


**Fig. 1.** Lossy dielectric sphere problem geometry. Using the QoI from [6], a posteriori EECEs were computed using higher-order adjoint solutions, as in as in [4], for all sub-problems. The double higher order finite element was used to solve each problem. These adjoint solutions were also applied to compute a QoI value and QoI gradient for each sub-problem using the methods of [6]. Note that all QoI values, QoI gradients, and element-wise error contribution estimates are complex-valued.

## III. Results and Discussion

Solving and computing error estimates for all 41 sub-problems produced 41 complex valued EECEs for each element: one per sub-problem. To perform a meaningful analysis of EECE correlation with respect to changing relative permittivity, we first ordered these 41 EECE values for each element by the real relative permittivity of their associated sub-problem. For each of the first 33 (out of 41) EECE values per element, we cut a continuous subset of length 9, consisting of the chosen (1 out of 33) EECE value and the next 8 in the list. Performing this for all 256 elements, we had a total of 8,448 9-dimensional observations, the dimensions corresponding to relative indices between a given sub-problem and the 8 next sub problems (ordered by real relative permittivity). We similarly sampled 9-dimensional observations for real QoI values and QoI gradients. We computed correlation coefficients between all 9 dimensions for EECEs, QoI values, and QoI gradients, summarized in Fig. 2.

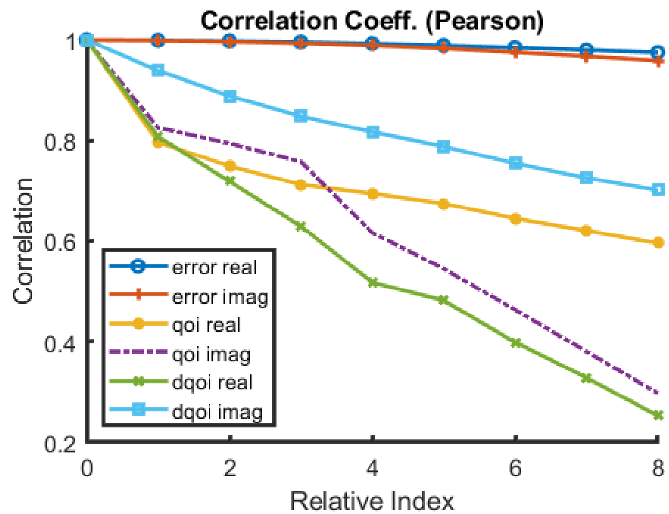


**Fig. 2.** Correlation coefficients for EECEs (error), QoI values, and QoI gradients (dqoi) with respect to relative sub-problem (or equivalently, real relative permittivity) index. Error contribution estimates are substantially more correlated between related sub-problems than QoI values or QoI gradients.

As evident in Fig. 2, correlation coefficients for EECEs decay slowly with respect to increased separation between sub-problems (relative index), and therefore with respect to increasing relative permittivity difference. Correlation coefficients for QoI values and QoI gradients decay far more quickly, for reference. However, for applications like adaptive refinement, we care about values of some refinement indicator derived from EECEs, rather than EECE values themselves (complex values cannot be ordered consistently). For a simple example refinement indicator, we use the magnitude of each EECE.

EECE magnitude has often been used as a simple benchmark for adaptive refinement using adjoint-based a posteriori error contribution estimates, for instance in [1] or [4]. Figure 3 shows EECE magnitudes for all 41 sub-problems and all 256 elements, ordered by the mean EECE magnitude over all sub-problems for each element. Qualitatively, the vertical banding of Fig. 3 suggests how slowly EECE magnitudes, and therefore our example refinement heuristic, vary over the range of real relative permittivity values tested.

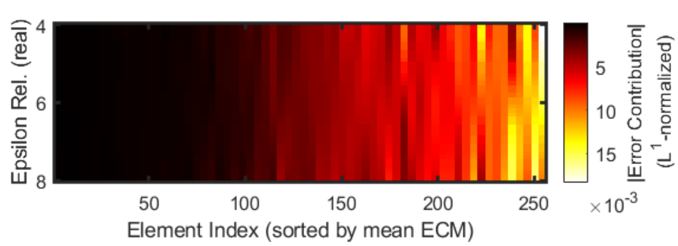


**Fig. 3.** EECE magnitudes normalized by L1-norm of EECE vector for each sub-problem. Vertical axis corresponds to sub-problems ordered by real relative permittivity. Horizontal axis corresponds to element index sorted by mean normalized EECE magnitude (ECM). Mean was evaluated for each element over all sub-problems. Note that several elements have nearly identical error trends due to symmetry of the problem.

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However, Fig. 3 also qualitatively suggests something potentially troubling: elements with higher mean EECE magnitude cover a wider range of EECE magnitude values with varying real relative permittivity. Figure 4 presents this trend quantitatively, showing EECE magnitude standard deviation with respect to EECE magnitude mean. We find the two are correlated with Pearson correlation 0.73.

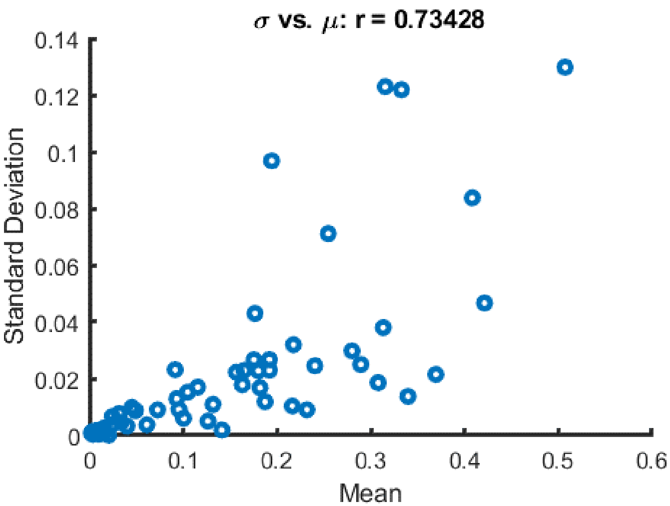


**Fig. 4.** EECE magnitude standard deviation with respect to mean. Standard deviation and mean are correlated.

This suggests that EECE correlation for such elements with high refinement indicator values may decay more quickly. If EECE correlation decays too quickly between related sub-problems, adaptive refinement methods like those presented in [4] may not satisfy desired error tolerances across all sub-problems. However, in Fig. 5, we suggest this may not be the case for existing adaptive refinement schemes. Figure 5, like Fig. 2, shows correlation coefficients between EECE values for neighboring sub-problems. Unlike Fig. 2, Fig. 5 also shows correlation coefficients for the top and bottom 25% of elements (as ordered by mean EECE magnitude). Even for elements with EECE mean magnitude values within the highest 25%, EECE values remain highly correlated over the relative index range tested.

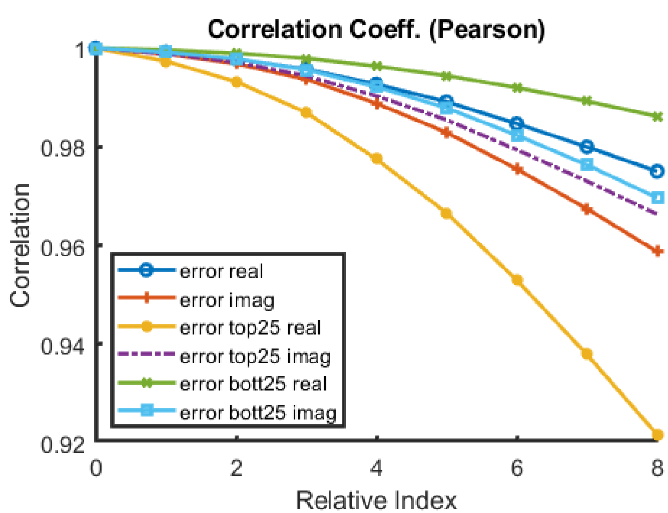


**Fig. 5.** Correlation coefficients for EECE (error) for all problems, problems in the top 25% of EECE magnitude, and problems in the bottom 25% of EECE magnitude. Note the difference in vertical axis scale from Fig. 1. Top 25% and bottom 25% have similar correlation between related sub-problems.

As demonstrated in [4], adaptive refinement approaches can reach low tolerances within a few iterations, so the mild correlation coefficient decay shown in Fig. 5 is likely tolerable, even given increased adaptive refinement convergence time due to application across sub-problems.

## IV. Conclusion

Correlation statistics were presented for elementwise error contribution estimate values for 41 lossy dielectric sphere scattering problems with varying relative permittivity. We found that EECE values, in contrast to the QoI values themselves, were highly correlated between related sub-problems, and their correlation coefficients decayed slowly with increasing difference in relative permittivity between problems. These results suggest that a single adjoint-based a posteriori EECE-informed adaptive refinement operation may yield a high-quality discretization across sub-problems and therefore achieve efficiency gains for multi-solve applications.

## References

[1] C. Key, A. Smull, D. Estep, T. Butler, and B. Notaroš, "A Posteriori Error Estimation and Adaptive Discretization Refinement Using Adjoint Methods in CEM: A Study with a One-Dimensional Higher-Order FEM Scattering Example," *IEEE Transactions on Antennas and Propagation*, vol. 68, no. 5, pp. 3791-3806, 2020.

[2] D. Estep. "A posteriori error bounds and global error control for approximations of ordinary differential equations," *SIAM J. Numer. Anal.*, vol. 32, no. pp. 1–48, 1995.

[3] K. Eriksson, D. Estep, P. Hansbo, and C. Johnson, "Introduction to adaptive methods for differential equations," *Acta Numerica*, pp. 105–158, 1995.

[4] J. J. Harmon, C. Key, D. Estep, T. Butler and B. M. Notaroš, "Adjoint-Based Accelerated Adaptive Refinement in Frequency Domain 3-D Finite Element Method Scattering Problems," *IEEE Transactions on Antennas and Propagation*, vol. 69, no. 2, pp. 940-949, 2021.

[5] D. Estep and D. Neckels, "Fast and Reliable Methods for Determining the Evolution of Uncertain Parameters in Differential Equations," *J. Comp. Physics*, vol. 213, pp. 530-556, 2006.

[6] J. J. Harmon, C. Key, D. Estep, T. Butler, B. M. Notaros, "Adjoint Sensitivity Analysis for Uncertain Material Parameters in Frequency Domain 3-D FEM," *IEEE Transactions on Antennas and Propagation*, Published in Early Access, doi: 10.1109/TAP.2021.3070059. 2021.

[7] M. M. Botha and D. B. Davidson, "An Explicit A Posteriori Error Indicator for Electromagnetic, Finite Element-Boundary Integral Analysis," *IEEE Transactions on Antennas and Propagation*, vol. 53, no. 11, pp. 3717-3725, 2005.

[8] K. C. Chellamuthu and N. Ida, "'A Posteriori' Element by Element Local Error Estimation Technique and 2D & 3D Adaptive Finite Element Mesh Refinement," *IEEE Transactions on Magnetics*, vol. 30, no. 5, pp. 3527- 3530, 1994.

[9] D. Pardo, L. E. Garcia-Castillo, L. F. Demkowicz, and C. Torres-Verdın, "A two-dimensional self-adaptive hp finite element method for the characterization of waveguide discontinuities. Part II: Goal-oriented hp adaptivity," *Computer Methods in Applied Mechanics and Engineering*, vol. 196, no. 49, pp. 4811 – 4822, 2007.

[10] L. E. Garcia-Castillo, D. Pardo, and L. F. Demkowicz, "Energy-Norm Based and Goal-Oriented Automatic hp Adaptivity for Electromagnetics: Application to Waveguide Discontinuities," *IEEE Transactions on Microwave Theory and Tech.*, vol. 56, no. 12, pp. 3039–3049, 2008.

This article has been accepted for publication in IEEE Antennas and Wireless Propagation Letters. This is the author's version which has not been fully edited and content may change prior to final publication. Citation information: DOI 10.1109/LAWP.2021.3116167



[11] G. K. Tomy and K. Vinoy, “A Fast Polynomial Expansion for Uncertainty Quantification in Stochastic Electromagnetic Problems,” *IEEE Antennas and Wireless Propagation Letters*, vol. 18, no. 10, pp. 2120-2124, 2019.

[12] M. M. Ilic and B. M. Notaros, “Higher Order Large-Domain Hierarchical FEM Technique for Electromagnetic Modeling Using Legendre Basis Functions on Generalized Hexahedra,” *Electromagnetics*, vol. 26, no. 7, pp. 517-529, 2006.

[13] A. P. Smull, A. B. Manic, S. B. Manic, and B. M. Notaros, “Anisotropic Locally-Conformal Perfectly Matched Layer for Higher Order Curvilinear Finite-Element Modeling,” *IEEE Transactions on Antennas and Propagation*, vol. 65, no. 12, pp. 7157–7165, 2017.