Adjoint Sensitivity Analysis for Uncertain Material Parameters in Frequency Domain 3-D FEM

Jake J. Harmon, *Graduate Student Member, IEEE*, Cam Key, *Graduate Student Member, IEEE*, Don Estep, Troy Butler, and Branislav M. Notaroš, *Fellow, IEEE*

***Abstract*—We present an application of adjoint analysis for efficient sensitivity analysis and estimation of quantities of interest in the presence of uncertain model parameters in 3-D finite element method scattering problems. We demonstrate that the adjoint solution may be leveraged to expedite quantification of uncertainty in the scattering model with extremely high accuracy and vast efficiency improvements in comparison to classic gradient approximation techniques and Monte Carlo methods. The proposed method is demonstrated for low- and high-dimensional parameter spaces for scattered electric field quantities of interest. The results indicate strong agreement with equivalent Monte Carlo simulations for quantity of interest responses and probability densities.**

***Index Terms*—adjoint methods, computational electromagnetics, finite element method, higher-order parameter sampling, sensitivity analysis, uncertain parameters, uncertainty quantification.**

I. Introduction

With traditional uncertainty propagation and gradient approximation techniques, analysis of variation among many parameters involves substantial computation times. Direct evaluation of gradients, for example, presents significant challenges to computational efficiency and feasibility, especially for high dimensional parameter spaces. Likewise, classical Monte Carlo (MC) methods are unsuitable for problems with many unknowns (e.g., complex geometries or high frequency), requiring many solutions of the forward problem.

Through the solution of a dual (or adjoint) problem, however, gradient approximation can be greatly expedited. The adjoint approach links the forward problem to the quantity of interest (QoI), permitting efficient analysis of changes in QoIs due to perturbations in model parameters, including estimation of the sensitivity of the output QoI to random variation. Leveraging the adjoint information, the higher-order parameter sampling (HOPS) technique enables a highly efficient method to generate accurate gradients and updated QoIs, relying only on the original forward solve and its corresponding adjoint solution [1]–[4]. Avoiding the need to directly evaluate gradients with respect to each parameter, this updated approach therefore yields vast improvements in computational efficiency. For uncertain parameters, e.g., describing the spatial heterogeneity of material properties in a scatterer, HOPS drastically reduces the computation time required to quantify uncertainties, achieving the accuracy of lengthy MC simulations with just a handful of solves. Since most practical problems require optimization and analysis of many parameters, this adjoint informed approach yields significant computational efficiency improvements over traditional methods.

In computational electromagnetics (CEM), adjoint analysis has been studied primarily for optimization in finite-difference time-domain (FDTD) methods, as in [5]–[16], rather than the simultaneous sensitivity and uncertainty quantification for the frequency domain finite element method (FEM) as in this work.

Adjoint analysis in CEM has also been successfully applied to inverse problems [17], [18]. The paper [19], in particular, leverages empirical interpolation methods assisted by duality for model reduction to expedite the analysis of uncertain conductivity in low frequency electromagnetics. Earlier works have also demonstrated the advantage of adjoint analysis for goal-oriented refinement, such as in [20]–[22].

Overall, however, adjoint analysis has remained relatively uncommon in CEM, while in other fields like computational fluid dynamics, such methods have seen significant research and development, such as for error estimation [23]–[29]. Additionally, previous work outside CEM has shown the viability of adjoint analysis for improving the analysis of unlikely events [30], dimensionality reduction [31], and accelerating optimization [32].

For determining the impact of uncertainty, traditional gradient estimation techniques have been applied to radar cross-section measurements for rough surfaces [33]. The use of automatic differentiation for studying small perturbations has also provided an efficient means to analyze parameter uncertainty in CEM [34].

Aside from standard MC methods as in [35]–[37] for rough surfaces, much of the remaining existing work in CEM regarding uncertainty quantification and uncertain parameters relies on solving stochastic partial differential equations (PDEs), typically using finite difference methods, such as for low-dimensional material parameter uncertainty [38], [39] or geometric variation [40]. Notably, polynomial chaos expansion (PCE) methods were applied in FDTD for analyzing variation

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Jake J. Harmon, Cam Key, and Branislav M. Notaroš are with the department of Electrical and Computer Engineering, Colorado State University, Fort Collins, CO 80523-1373 USA (e-mail: j.harmon@colostate.edu, camkey@rams.colostate.edu, branislav.notaros@colostate.edu).

Donald Estep is with the Department of Statistics, Colorado State University, Fort Collins, CO, USA (e-mail: donald.estep@colostate.edu).

Troy Butler is with the Department of Mathematical and Statistical Sciences, University of Colorado Denver, Denver, CO, USA (email: troy.butler@ucdenver.edu).

in the scattered electric field for a dielectric sphere scatterer with an uncertain relative permittivity and radius [41].

In FEM, similar stochastic PDE methods were applied to analyze surface roughness effects in 2-D for scattered field quantities [42], and transmission coefficient variation due to material uncertainty [43], [44]. While highly efficient for low-dimensional uncertainty, these stochastic methods, in addition to requiring significant modifications to a deterministic solver, are unsuitable for moderate and high dimensional uncertainty. Typically, variants of the stochastic spectral Galerkin approach (including intrusive PCE) require sophisticated preconditioners and computationally intensive model reduction to render the problem tractable [45]. Our approach, however, requires only the solution of deterministic PDEs, with the uncertainty introduced externally to the core solver, and naturally excels for high dimensional uncertainty.

On the other hand, nonintrusive uncertainty quantification methods for FEM, such as those based on stochastic collocation, seek to address the computational difficulties of solving stochastic PDEs. Stochastic collocation, which enables computing the coefficients for nonintrusive PCE, inherits a significant limitation in the dimension of the uncertainty due to the rapid growth in collocation points, particularly with standard tensor-product evaluations; however, sparse grid sampling (e.g., Smolyak sparse grids) alleviates, but does not eliminate, this difficulty [46], [47]. In [48], for example, nonintrusive PCE assisted by an adaptive Smolyak sparse grid algorithm provided a significant reduction in the computational load for analyzing dosimetry with uncertain tissue material parameters in 2-D FEM. A similar approach for 3-D FEM combined with basis reduction was applied for dosimetry applications in [49]. Moreover, Smolyak sparse grids and PCE were applied to construct stochastic impedance matrices for accurate analysis of composite cylindrical scatterers with geometric uncertainty in 2-D FEM [50]. Recently, a stochastic testing method with Smolyak sparse grids for nonintrusive PCE was studied for analysis of uniform waveguide dispersion with uncertain material parameters [51]. However, the approach in [51] requires Gaussian random variables, whereas our approach has no such limitation. Additionally, stochastic collocation techniques were applied to a variety of problems in FEM, as well as the method of moments (MoM) and hybrid methods, for low dimensional geometric and material uncertainty [52].

In contrast to these methods, our approach provides a distinct emphasis on the effect of uncertainty on the scattering QoI computed from the finite element solution. As an analog to goal-oriented error estimation and adaptive refinement, in which we address the particular regions contributing most significantly to the QoI, the proposed approach emphasizes the effect of uncertainty on the QoI specifically, permitting a substantial enhancement of efficiency, even when compared to sparse grid techniques, while retaining the convenience of other nonintrusive methods.

Recently, adjoint analysis applied to 1-D FEM demonstrated accurate QoI response estimation using the adjoint solution for univariate and deterministic scattering problems for dielectric slabs [53]. This work, in contrast, extends the findings of [54]–[58] to 3-D FEM uncertainty quantification and outcome prediction, and provides an efficient and effective methodology for propagating uncertainty in the solution of PDEs in CEM, with application to high dimensional parameter spaces.

Lastly, we provide derivations and explicit constructions for accelerating the analysis of uncertain parameters for a customizable and practical scattered electric field QoI through adjoint sensitivity and HOPS, showing vast improvements over traditional MC methods.

The rest of this paper is organized as follows. Section II outlines the formulation of the adjoint problem and develops the HOPS methodology for 3-D FEM. Section III provides numerical examples, illustrating rapid HOPS QoI prediction and probability density estimation for low- to high-dimensional parameter spaces in scattering problems. The examples demonstrate extremely significant computational savings for QoI estimation compared to the MC method with nearly identical accuracy.

II. The Adjoint: Derivations and Estimators

A. The Adjoint Problem

We first summarize the components of the standard forward problem, referred to as the double-curl wave equation:

$$\nabla\times\mu_r^{-1}\nabla\times\mathbf{E}^{sc}-k_0^2\varepsilon_r\mathbf{E}^{sc}=-\nabla\times\mu_r^{-1}\nabla\times\mathbf{E}^{inc}+k_0^2\varepsilon_r\mathbf{E}^{inc}, \tag{1}$$

with μ_r and ε_r representing the relative permeability and permittivity tensors, respectively, and k_0 denoting the free space wave number, and which we denote as

$$\mathcal{L}\mathbf{E}^{sc}=\mathbf{G}. \tag{2}$$

The domain is truncated by introducing an air layer and a perfectly matched layer (PML) [59], where the entire domain is surrounded by perfect electrical conductor (PEC). The solution is found using the double higher-order FEM [60]–[62]; however, the procedure is unchanged for low-order methods.

The adjoint operator $\mathcal{L}^*$ is defined by the Lagrange identity [3]:

$$\langle\mathcal{L}\mathbf{u},\mathbf{v}\rangle=\langle\mathbf{u},\mathcal{L}^*\mathbf{v}\rangle, \tag{3}$$

where $\langle\cdot,\cdot\rangle$ denotes the standard L^2 inner-product. As in [58], the adjoint operator satisfies

$$\mathcal{L}^*\mathbf{v}=\nabla\times(\mu_r^{-1})^*\nabla\times\mathbf{v}-k_0^2\varepsilon_r^*\mathbf{v}. \tag{4}$$

The adjoint operator therefore has the form of the forward operator, with the complex conjugate or conjugate transpose (in the case of tensor materials) of the model parameters.

Analogously to choosing different excitations for the forward problem, we select a suitable adjoint problem to relate the forward problem to a specific QoI. We therefore consider an arbitrary linear (or linearized) functional J of the forward solution $\mathbf{E}^{sc}$ of $\mathcal{L}\mathbf{E}^{sc}=\mathbf{G}$, such that for all $\mathbf{E}^{sc}$ the QoI is

$$J[\mathbf{E}^{sc}]=\langle\mathbf{E}^{sc},\mathbf{p}\rangle, \tag{5}$$

where the Riesz representation theorem [63] guarantees the existence of $\mathbf{p}$, and (5) determines the choice for the adjoint excitation:

$$\mathcal{L}^*\mathbf{v}=\mathbf{p}. \tag{6}$$

Solving for additional QoIs simply requires solving the adjoint problem with new right-hand sides. Conveniently, the Galerkin approximate adjoint solution does not require an explicit form for $\mathbf{p}$. Rather, only the ability to evaluate (5) is necessary [58].

For a practical choice of a QoI, we examine scattered electric field quantities as in [58]. Starting from the Kirchhoff integral and isolating the $\mathbf{w}$-component of the electric field to produce a scalar QoI, we have the following functional of the finite element solution,

$$J[\mathbf{E}^{sc}] = \oint_S \mathbf{w} \cdot [\hat{\mathbf{n}} \times (\nabla \times \mathbf{E}^{sc}) + jk_0(\hat{\mathbf{n}} \times \mathbf{E}^{sc} \times \mathbf{i}_r)] e^{jk_0 \mathbf{i}_r \cdot \mathbf{r}'} \, dS. \tag{7}$$

B. Handling Parameter Uncertainty with HOPS

Consider, for example, a model problem with ideal parameters (i.e., a perfectly smooth surface, exact conductivity and permittivity, etc.). For this reference problem, we would like to understand the impact of variations in the construction and the constituent parameters on the output QoI. Classically, the estimation of uncertain effects applies the MC method, in which each sample of the uncertain parameters incurs the additional cost of solving the perturbed forward problem. While MC simulations are simple to implement and can produce accurate results, the computation time demanded by the method is simply not sustainable for a moderate number of samples or for problems with many unknowns.

In the presence of parameter uncertainty, however, we can also exploit the utility of the adjoint solution to expedite sensitivity analysis, rapidly generating approximate gradient information for any number of uncertain parameters which perturb a deterministic PDE. HOPS requires just the solutions to the adjoint and forward problems at the deterministic references to generate gradient information for any number of uncertain parameters which perturb the construction of the model. This enables efficient generation of sensitivity information for many parameters, especially compared to classical gradient approximation approaches (e.g., first-order finite difference) which require numerous solutions of the forward problem.

By leveraging the adjoint solution with HOPS, we can construct an accurate QoI response from a small set of deterministic reference solutions, thereby addressing the efficiency problem which hampers the utility of traditional approaches. Random samples of parameters are propagated through the piecewise-linear response built using HOPS, avoiding full model solves. Additionally, considering that the adjoint solution might already be available from adaptive mesh refinement, HOPS provides significant potential for computational savings in uncertainty quantification.

To derive the form of the HOPS estimate, we proceed analogously to [1], [3]:

We begin with the deterministic reference forward problem (2)

$$\mathcal{L}\mathbf{E}^{ref} = \mathbf{G}, \tag{8}$$

and the corresponding reference adjoint problem,

$$\mathcal{L}^*\mathbf{v} = \mathbf{p}. \tag{9}$$

Perturbing some component κ of the reference problem with the random variable η produces the adjusted equation

$$\tilde{\mathcal{L}}\tilde{\mathbf{E}}^{sc} = \tilde{\mathbf{G}}, \tag{10}$$

noting that

$$\tilde{\mathcal{L}} = \mathcal{L} + \delta_{\eta-\kappa}\mathcal{L}, \tag{11}$$

$$\tilde{\mathbf{G}} = \mathbf{G} + \delta_{\eta-\kappa}\mathbf{G}, \tag{12}$$

and

$$\tilde{\mathbf{E}}^{sc} = \mathbf{E}^{ref} + \delta_{\eta-\kappa}\mathbf{E}^{ref}, \tag{13}$$

where $\delta_{\eta-\kappa}$ signifies the effects of the perturbation.

To reveal the dependence of the perturbed QoI on the reference QoI, we first expand (10) through substitution of (11) and (12) and take the inner-product with the adjoint solution $\mathbf{v}$, which shows:

$$\langle \mathcal{L}\tilde{\mathbf{E}}^{sc}, \mathbf{v}\rangle + \langle \delta_{\eta-\kappa}\mathcal{L}\tilde{\mathbf{E}}^{sc}, \mathbf{v}\rangle = \langle \mathbf{G}, \mathbf{v}\rangle + \langle \delta_{\eta-\kappa}\mathbf{G}, \mathbf{v}\rangle. \tag{14}$$

Applying the Lagrange identity to the first terms on the left- and right-hand sides and rearranging, we have

$$\langle \tilde{\mathbf{E}}^{sc}, \mathbf{p}\rangle = \langle \mathbf{E}^{ref}, \mathbf{p}\rangle + \langle \delta_{\eta-\kappa}\mathbf{G} - \delta_{\eta-\kappa}\mathcal{L}\tilde{\mathbf{E}}^{sc}, \mathbf{v}\rangle. \tag{15}$$

Under the assumption that the perturbations are relatively small (i.e., $\tilde{\mathbf{E}}^{sc} \approx \mathbf{E}^{ref}$),

$$\langle \tilde{\mathbf{E}}^{sc}, \mathbf{p}\rangle \approx \langle \mathbf{E}^{ref}, \mathbf{p}\rangle + \langle \delta_{\eta-\kappa}\mathbf{G} - \delta_{\eta-\kappa}\mathcal{L}\mathbf{E}^{ref}, \mathbf{v}\rangle. \tag{16}$$

Finally, applying the definition of the QoI, we have

$$J[\tilde{\mathbf{E}}^{sc}] \approx J[\mathbf{E}^{ref}] + \langle \delta_{\eta-\kappa}\mathbf{G} - \delta_{\eta-\kappa}\mathcal{L}\mathbf{E}^{ref}, \mathbf{v}\rangle, \tag{17}$$

which describes how, with the reference QoI and adjoint solution, we can compute an updated QoI for the perturbed problem.

For a specific realization of a HOPS-based estimate for an updated QoI, let κ denote the reference relative permittivity, and η the perturbed relative permittivity of a scatterer. To build the estimate (17), we have

$$D_{\varepsilon_r}\mathbf{G} = k_0^2\mathbf{E}^{inc}, \tag{18}$$

and

$$D_{\varepsilon_r}\mathcal{L}\mathbf{E}^{ref} = -k_0^2\mathbf{E}^{ref}. \tag{19}$$

Hence, we approximate the QoI for the perturbed model by

$$J[\tilde{\mathbf{E}}^{sc}] \approx J[\mathbf{E}^{ref}] + k_0^2\langle (\mathbf{E}^{inc} + \mathbf{E}^{ref})(\eta - \kappa), \mathbf{v}\rangle, \tag{20}$$

where η and κ denote, respectively, the perturbed and reference permittivities of the scatterer.

Substituting in the approximate Galerkin solution to the deterministic reference forward problem $\mathbf{E}^{ref} = \sum_i \alpha_i \mathbf{f}_i$ and the reference adjoint solution $\mathbf{v} = \sum_j \beta_j \mathbf{f}_j$ and expressing the inner-product in integral form, (20) becomes

$$\begin{aligned} J[\tilde{\mathbf{E}}^{sc}] \approx J[\mathbf{E}^{ref}] + \\ k_0^2 \sum_i \sum_j \alpha_i \beta_j^* \int_\Omega (\eta - \kappa)\mathbf{f}_i \cdot \mathbf{f}_j \, d\Omega \\ + k_0^2 \sum_j \beta_j^* \int_\Omega (\eta - \kappa)\mathbf{E}^{inc} \cdot \mathbf{f}_j \, d\Omega. \end{aligned} \tag{21}$$

We may analyze multiple parameters varied simultaneously, in which case $D_{\varepsilon_r}\mathbf{G}$ and $D_{\varepsilon_r}\mathcal{L}\mathbf{E}^{ref}$ are matrix quantities, and $(\eta-\kappa)$ is vector valued (with dimensions corresponding to the dimension of the parameter space). Such a treatment is relevant for varying material parameters independently throughout the volume, for instance if the permittivity of each element in the discretization is described by a random variable.

For example, we consider the 2-dimensional case where the perturbation is complex valued. Hence,

$$\boldsymbol{\eta} = \begin{bmatrix} \eta_r \\ \eta_r' \end{bmatrix}, \tag{22}$$

and likewise for $\boldsymbol{\kappa}$. The derivative matrix corresponding to the subtraction of (18) and (19) is then

$$\mathbf{D} = \begin{bmatrix} k_0^2\mathbf{E}^{inc} + k_0^2\mathbf{E}^{ref} & jk_0^2\mathbf{E}^{inc} + jk_0^2\mathbf{E}^{ref} \end{bmatrix}. \tag{23}$$

As a result, the updated form of (20) is

$$\langle \tilde{\mathbf{E}}^{sc}, \mathbf{p}\rangle \approx \langle \mathbf{E}^{ref}, \mathbf{p}\rangle + k_0^2\langle \mathbf{D}(\boldsymbol{\eta}-\boldsymbol{\kappa}), \mathbf{v}\rangle, \tag{24}$$

which is equivalent to simply treating η and κ as complex valued in the 1-dimensional parameter space estimate.

In addition to improved accuracy in general, for highly sensitive QoIs, or for large variance in the perturbed parameter, it is preferable to sample at multiple reference points. We can accomplish this by sampling at a uniform set of grid points or, for example, we can probabilistically tune the HOPS approximation efficiently with k-means clustering. In either case, samples of the perturbed parameter are associated with a reference point by proximity and the updated QoI is approximated as in (17).

III. Numerical Results

As discussed in Section II, the connection of the adjoint solution to the sensitivity of the QoI permits the effective estimation of changes in the QoI to parameters in the model. In each of the following numerical examples, we consider monostatic scattering from a sphere. While simple geometrically, the spherical scatterer, nevertheless, allows exploration of the prototypical problems in UQ. We note, however, several practical considerations for application to more complex problems and geometries. Chief in the value of the HOPS approach, not all parametric uncertainty drives equivalent effect in the QoI. In the case of multilinear dependence of the QoI on the uncertain parameters, the response may be constructed precisely for high dimensional uncertainty by a single HOPS point. Likewise, when sources of uncertainty induce limited effect in the QoI, significant resources may be saved without harm to the accuracy of the estimated probability densities. In the case of surface roughness, for example, the QoI may be insensitive to variation in a large portion of the surface, simplifying the computational procedure drastically. However, depending on the specific geometry and the scattering angle, a small degree of uncertainty may drive large variation in the QoI; in such cases, additional computational resources must be allocated to compensate, resulting in a denser distribution of HOPS points. Finally, the HOPS approach facilitates increasing computational effort where uncertainty dictates the largest change in the QoI. In the following examples, we illustrate the performance of the method for uniform sampling and probabilistically tuned sampling. In addition, the approach is conducive to adaptivity, which, in the case highly sensitive QoIs, simplifies the selection of HOPS points.

Consider a spherical scatterer with uncertain material parameters. We first impose that the conductivity of the entire sphere—considered as the imaginary component of the complex relative permittivity ε_d—is a random variable which varies according to some distribution $\pi(x)$ with a known mean ν and standard deviation σ. Therefore, according to the principle of maximum entropy, we let π denote a Gaussian distribution; however, any other distribution can be substituted (or treated simultaneously).

Furthermore, as the conductivity is a random variable, the solution itself is a random vector, and hence the QoI is a random variable. We therefore conduct a MC simulation of N samples to generate an approximate probability distribution which describes the behavior of the QoI.

In each of the N runs, the imaginary component of the sphere's relative permittivity is drawn from $\pi(x)$, and—after solving the forward problem on this discretization—the QoI from (7) is computed and stored, which we denote as q. For comparison, the results are demonstrated for three levels of HOPS resolution, with one, ten, and twenty HOPS reference points.

For a specific test case, let π be a Gaussian distribution of mean $\nu = -2.0$, and standard deviation $\sigma = 1/3$. The real component of the relative permittivity of the sphere is fixed at 6.0. For simplicity, the HOPS points were chosen uniformly within three standard deviations of the mean for the multi-point simulations, while the mean was selected for the single-point HOPS simulation.

As seen in Fig. 1, the adjoint-based method provides an accurate approximation of the QoI behavior and replication of the MC sampling. While the pure linear approximation about a single reference point diverges from the MC simulation near the extrema of the sample domain, the ten- and twenty-point HOPS simulations successfully capture the QoI response over the entire range.

We now apply HOPS to estimate the QoI probability densities using Gaussian kernel density estimation (GKDE) with bandwidths chosen according to Silverman's heuristic [64], as seen in Fig. 2. The probability density associated with variation in the conductivity is represented with acceptable accuracy by a single reference point. By ten or twenty reference points, however, the agreement with the 1000-point MC simulation is near-perfect.

We now quantify the performance of the three HOPS approximations by comparing the mean, variance, and total variation (TV) distance between the HOPS and MC densities. The TV distance provides a measure of the similarity of two probability distributions, where a value of zero indicates perfect agreement. As seen in Table I, HOPS converges to the 1000-point MC simulation by ten references points, producing an almost identical mean and variance for both the real and imaginary components. Lastly, the TV distances indicate extremely strong agreement with the MC densities for the

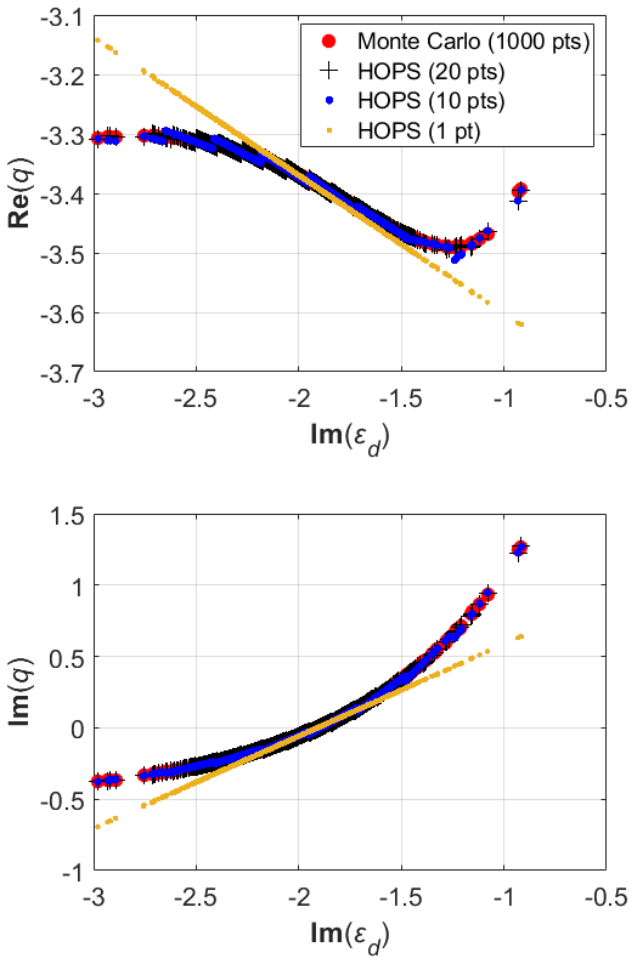

Fig. 1. Sampled real and imaginary monostatic scattering QoI responses for random variation in the imaginary component of the relative permittivity of the dielectric sphere.

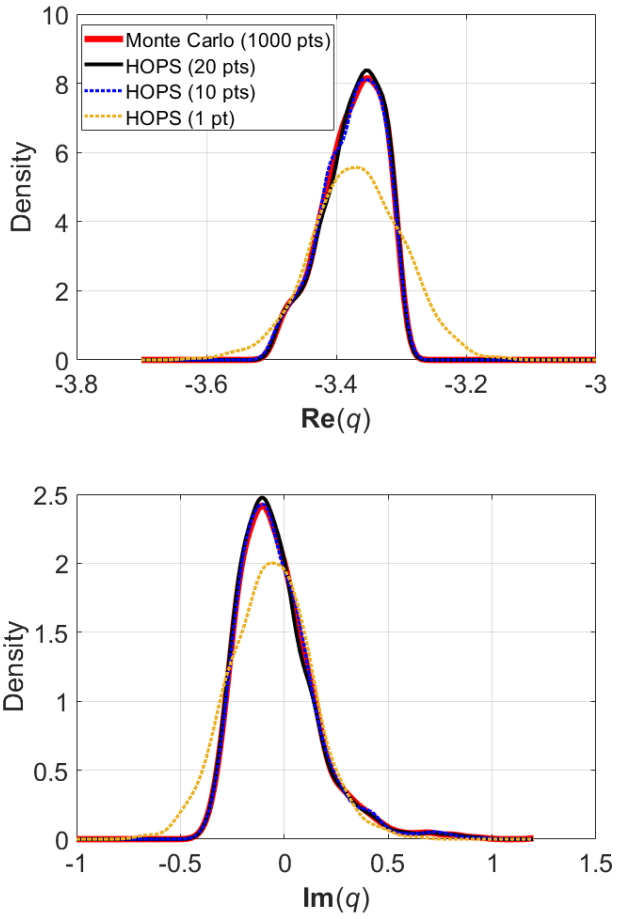

Fig. 2. Approximate real and imaginary monostatic scattering QoI probability densities due to random variation in the imaginary component of the relative permittivity of the dielectric sphere.

two higher resolution approximations. The ten-point HOPS approximation, however, indicates slightly better agreement than the twenty-point approximation according to this metric.

TABLE I
QUANTITATIVE COMPARISON OF HOPS AND MONTE CARLO FOR THE REAL AND IMAGINARY QOI PROBABILITY DENSITIES IN FIG. 2.

(a) Real QoI Density

	1 pt	10 pts	20 pts	MC
Mean	-3.3673	-3.3750	-3.3732	-3.3741
Variance	0.0053	0.0023	0.0022	0.0022
TV	0.4158	0.0293	0.0310	

(b) Imaginary QoI Density

	1 pt	10 pts	20 pts	MC
Mean	-0.0648	-0.0313	-0.0361	-0.0298
Variance	0.0407	0.0373	0.0374	0.0406
TV	0.2404	0.0264	0.0327	

To further validate the effectiveness of the HOPS methodology, we repeat an identical procedure for random variation in the real component of the relative permittivity. In contrast to the variation in the conductivity, random variation in this component of the relative permittivity induces a more complicated QoI response. Specifically, in this case the real component of the relative permittivity is described by a normal random variable of mean $\nu = 6.0$ with a standard deviation $\sigma = \sqrt{3}/3$, and the imaginary component is fixed at -2.0. As before, the HOPS reference points are chosen uniformly within three standard deviations of the mean.

For the first level of accuracy, as seen in Figs. 3 and 4, a single HOPS reference cannot adequately replicate the QoI response. Due to its more linear response, however, the real component of the QoI is much more reasonably modeled by the single HOPS point.

With ten reference points, and even more so with twenty reference points, the HOPS QoI response very closely matches that of the very computationally expensive MC simulation. As seen especially clearly in Fig. 3, the multi-point HOPS simulations very accurately capture the non-linear response of the QoI over the entire sample region.

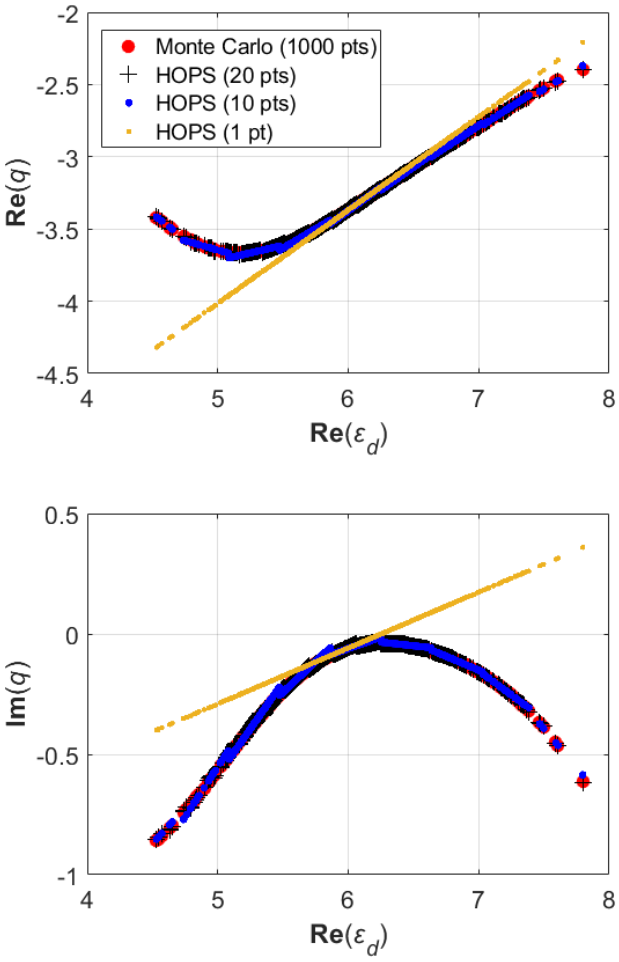

Fig. 3. Sampled real and imaginary monostatic scattering QoI responses for random variation in the real component of the relative permittivity of the dielectric sphere.

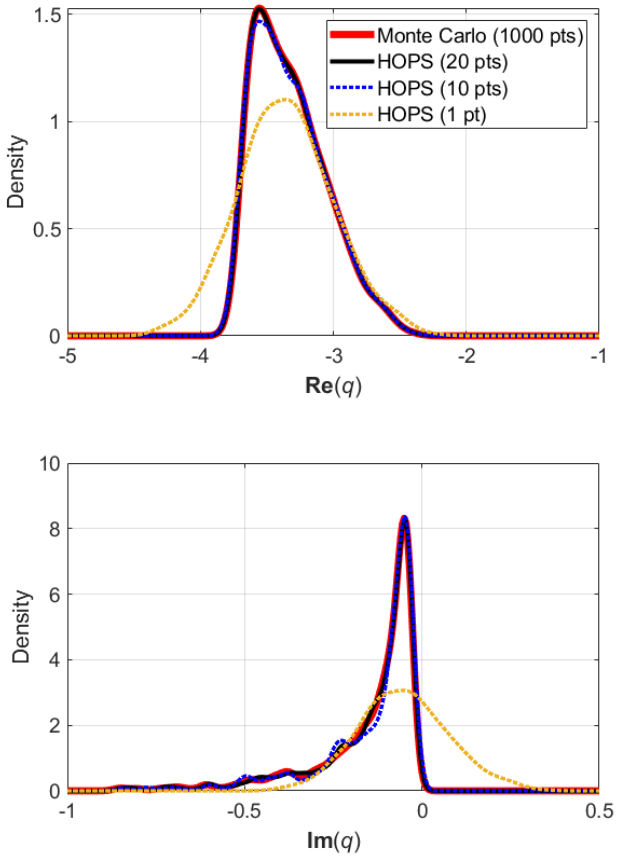

Fig. 4. Approximate real and imaginary QoI probability densities due to random variation in the real component of the relative permittivity.

TABLE II
QUANTITATIVE COMPARISON OF HOPS AND MONTE CARLO FOR THE REAL AND IMAGINARY QOI PROBABILITY DENSITIES IN FIG. 4.

(a) Real QoI Density

	1 pt	10 pt	20 pt	MC
Mean	-3.3546	-3.3215	-3.3201	-3.3197
Variance	0.1342	0.0793	0.0781	0.0779
TV	0.2982	0.0242	0.0039	

(b) Imaginary QoI Density

	1 pt	10 pts	20 pts	MC
Mean	-0.0533	-0.1442	-0.1472	-0.1482
Variance	0.0174	0.0226	0.0222	0.0222
TV	0.7379	0.1140	0.0522	

Moreover, the approximate densities for the real and imaginary components of the QoI demonstrate extremely close agreement with the MC simulation, as seen in Fig. 4 and Table II. In contrast to the variation in the imaginary component of the permittivity, in this case the twenty-point HOPS approximation provides a substantial boost in accuracy. While the ten- and twenty-point approximations provide close agreement with the mean and variance of the MC simulation, the twenty-point approximation produces very small TV distances of 0.0039 and 0.0522 for the real and imaginary components of the QoI, respectively.

As discussed in Section II, however, the adjoint approach excels when analyzing multiple parameters, and therefore many gradients at each reference. As a simple extension of the previous results, we demonstrate the combination of the two previous examples by assuming random variation of the real and imaginary components of the relative permittivity of the dielectric sphere. The real and imaginary components are described by separate random variables such that $\mathrm{Re}(\varepsilon_d)$ is Gaussian with a mean of 2.56 and a standard deviation of 0.2, and $\mathrm{Im}(\varepsilon_d)$ is pulled from a half-normal distribution of mean 0 and standard deviation 0.1.

In this case, the references are determined by k-means clustering of the set of sampled material parameters, which provides another simple and effective HOPS selection scheme. In contrast to PCE and similar methods, we can leverage

the parameter distribution to easily emphasize regions of the QoI response deemed statistically important by the probability distribution imposed on it. As such, selecting reference points by k-means clustering enables an efficient probabilistic tuning of the HOPS approximation, particularly for high dimensional uncertainty. We repeat this procedure, as before, for three levels of resolution, with one, ten, and twenty references.

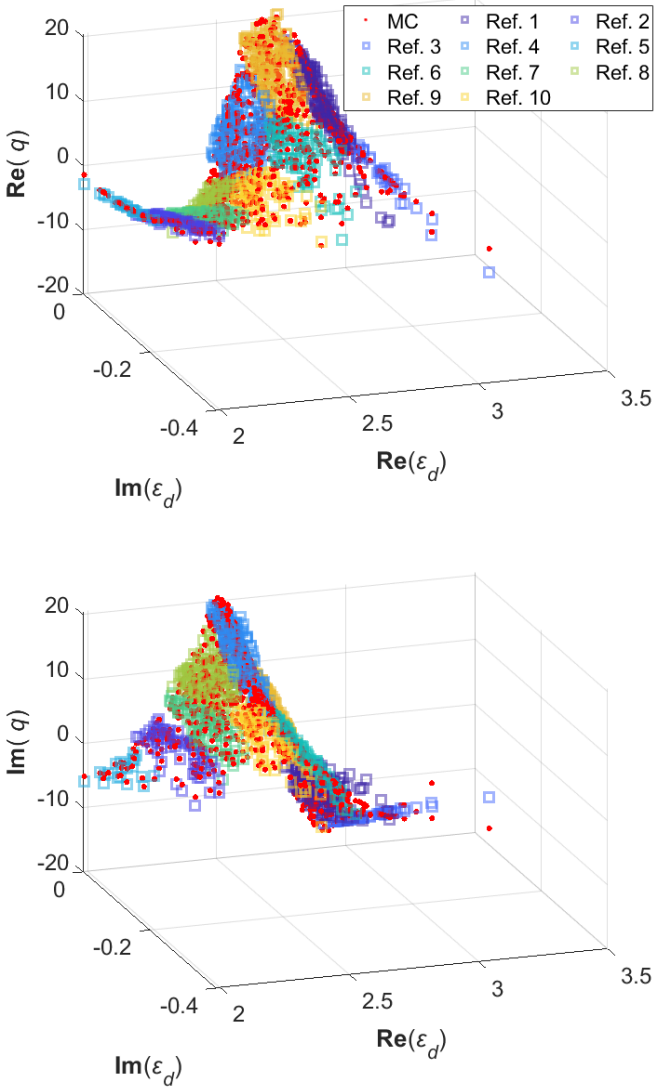

Fig. 5. Approximate real and imaginary monostatic scattering QoI responses due to simultaneous random variation in the real and imaginary components of the relative permittivity of the dielectric sphere for a HOPS simulation with ten reference points.

To illustrate the QoI reconstruction behavior for a two-dimensional parameter space, the approximate QoI responses are shown for the ten-point HOPS simulation in Fig. 5. Note that each estimate is associated with a single reference point as determined by Euclidean distance. The approximations, which are linear in both dimensions, demonstrate accurate replication of the QoI response generated through a 1000-point MC simulation. As implied by the QoI response in Fig. 5, the single-point HOPS simulation fails to capture the behavior of the problem to random variation of the dielectric, and

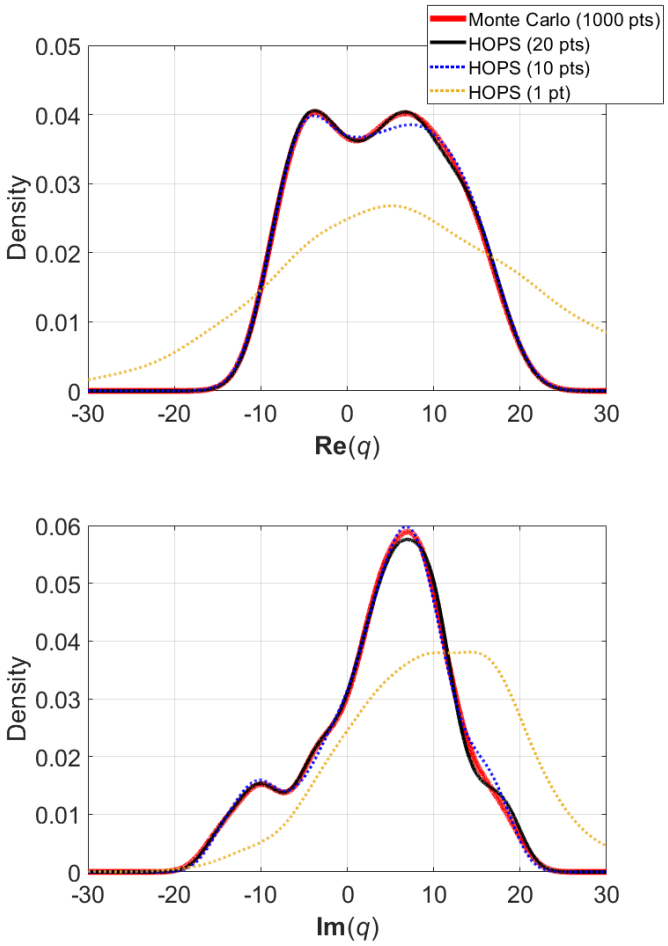

Fig. 6. Approximate real and imaginary monostatic scattering QoI probability densities due to simultaneous random variation in the real and imaginary components of the relative permittivity of the dielectric sphere.

therefore fails to match the probability density of the QoI in Fig. 6. However, using ten reference points, the HOPS density closely matches the MC density, with the twenty-point HOPS simulation providing even more accuracy in the response. The results in Table III further characterize the performance of the HOPS approximations. While the ten- and twenty-point approximations performed similarly, according to the TV distance metric, the twenty-point approximation achieved moderately better agreement with the MC simulation.

As a final demonstration, to further illustrate the advantage of the QoI-emphasis inherent to the HOPS approach, we consider a much higher dimensional example, in which every element of the spherical scatterer body is uncertain. This example corresponds to a 64-dimensional parameter space, where the material parameters of each element are purely real and independent and identically distributed such that $\varepsilon_{di} \sim N(2.56, 0.07^2)$ for the ith element.

We continue the approach in the previous examples, with a 1000-point MC simulation providing the benchmark for the HOPS based approximation. As seen in Fig. 7, given the relatively small variance of ε_{di} and the approximately multilinear local relationship between the uncertain parameters and the QoI, the probability density is closely replicated by

TABLE III
QUANTITATIVE COMPARISON OF HOPS AND MONTE CARLO FOR THE REAL AND IMAGINARY QOI PROBABILITY DENSITIES IN FIG. 6.

(a) Real QoI Density

	1 pt	10 pts	20 pts	MC
Mean	6.5878	3.6884	3.6321	3.6450
Variance	233.8040	66.7393	65.5116	65.3725
TV	0.6177	0.0196	0.0106	

(b) Imaginary QoI Density

	1 pt	10 pts	20 pts	MC
Mean	9.9566	4.1466	4.1130	4.0760
Variance	99.4212	65.5097	66.5074	65.8963
TV	0.5793	0.0369	0.0261	

a single HOPS point. For the real and imaginary components of the QoI, respectively, the HOPS approximation produced means of 11.63 and 18.04, and variances of 3.96 and 1.27. Likewise, the 1000-point MC simulation resulted in means of 11.39 and 17.84, and variances of 4.06 and 1.06. Lastly, the the HOPS approximation yielded TV distances of 0.075 and 0.14 with respect to the real and imaginary MC densities. While the previous examples illustrate the potential for high accuracy, this example fully demonstrates the significant computation time reduction that HOPS facilitates. A standard gradient estimation strategy to predict the distribution of the QoI under uncertainty as in this example would require 65 solves of the forward problem, whereas the HOPS simulation requires only one solution to the forward problem and one solution to the adjoint problem.

Overall, when analyzing the computational performance of HOPS compared to the MC simulations, we see a significant reduction in the computational cost. In the case of the MC simulations with 1000 samples, as the finite element discretizations have the same degrees of freedom for each approach, the single-point HOPS simulation yields an improvement in computation time by a factor of 500. Likewise, the ten- and twenty-point HOPS simulations reduce the computational cost by a factor of 50 and 20, respectively. Furthermore, as the HOPS reconstruction matches the full QoI response rapidly with increasing resolution, larger performance increases may be found when studying larger equivalent MC simulations. Finally, while the examples demonstrated apply uniform sampling and probabilistically tuned sampling, adaptive HOPS may yield additional performance increases and simplify application of the method to arbitrary uncertainty quantification problems in CEM.

IV. CONCLUSION

We have demonstrated the advantage of adjoint-based sensitivity analysis for expediting uncertain quantification in 3-D frequency domain CEM. Through application of the adjoint solution, the HOPS methodology in CEM facilitates rapid and accurate prediction of variation in practical quantities of interest in the presence of uncertainty and randomness in scattering models.

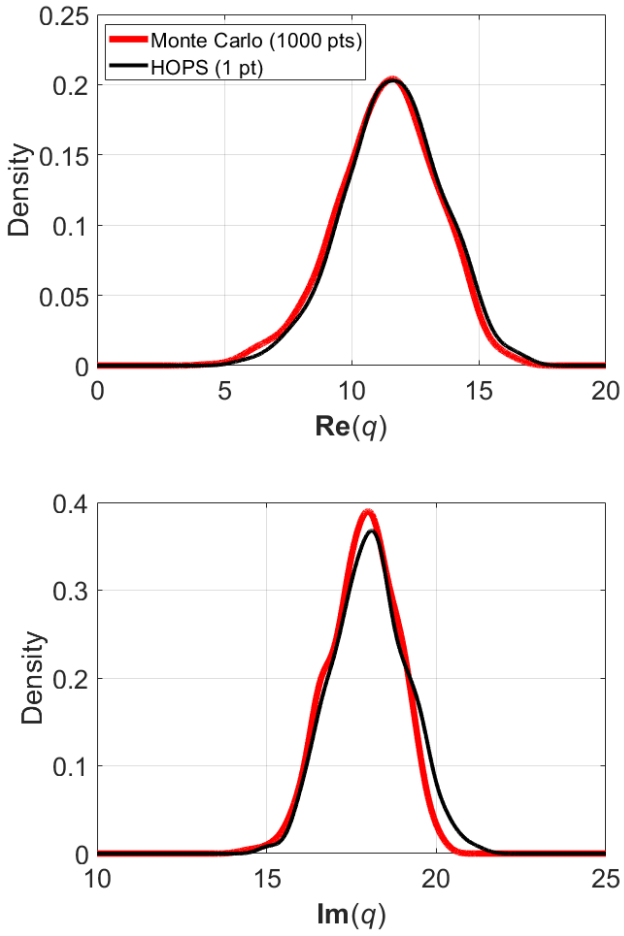

Fig. 7. Approximate real and imaginary monostatic scattering QoI probability densities due to random variation in the relative permittivity of each element of the dielectric sphere.

For outcome prediction of uncertain parameters, we contributed explicit constructions for evaluating random variation in the material parameters of a scatterer. And, finally, we showed how leveraging the adjoint solution and HOPS can replicate extremely computationally expensive Monte Carlo simulations at a small fraction of the cost and with similar accuracy, mandating just a handful of HOPS reference points for extremely close agreement.

For one-dimensional parameter spaces, the adjoint-based approach matches the efficiency of traditional methods, and in such cases where the original discretization is constructed through adjoint-based adaptive refinement, the readily available adjoint significantly boosts the effective performance of the HOPS method.

We further demonstrated application to higher dimensional parameter spaces, including a 2-dimensional problem, and a 64-dimensional problem with independent material uncertainty throughout the scatterer. In these cases, the independence of the computational complexity from the number of parameters results in substantial decreases in computation time while maintaining high accuracy.

We note several drawbacks of the proposed method in its current form for uncertainty quantification. Firstly, when

analyzing the effect of uncertainty on multiple quantities of interest, each QoI requires its own adjoint solution. Of course, when leveraging direct solvers, the added cost of solving multiple right-hand-sides for the adjoint problem may be significantly reduced. Secondly, while the HOPS methodology is extremely versatile and accurate results may be achieved efficiently even with uniform sampling, optimizing the selection of HOPS points requires either *a priori* knowledge or adaptivity. For broad applicability in analyzing uncertainty in CEM, we consider augmenting the proposed approach with adaptivity as the next key extension needed.

Adjoint-based methodologies, overall, provide significant value and potential to CEM applications, enabling the ability to accurately and efficiently refine models and eliminate discretization error fully automatically, while also significantly expediting the analysis of problems containing extensive random variation and uncertainty.

Future works will investigate automating sampling for improved efficiency and accuracy for high dimensional parameter spaces and highly sensitive QoI responses.

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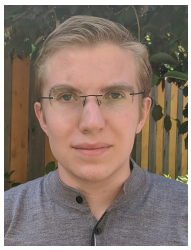


Jake J. Harmon (Graduate Student Member, IEEE) was born in Fort Collins, CO in 1996. He received the B.S. degree (*summa cum laude*) from Colorado State University, Fort Collins, in 2019, where he is currently pursuing the Ph.D. degree in electrical engineering.

His current research interests include adaptive numerical methods, uncertainty quantification, computational geometry, and higher order modeling in the finite element method and surface integral equation method of moments.

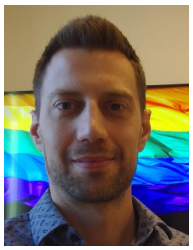
Cam Key (Graduate Student Member, IEEE) was born in Fort Collins, CO in 1996. He received his B.S. and Ph.D. in electrical and computer engineering from Colorado State University, Fort Collins, CO, USA, in 2018 and 2020, respectively.

His current research interests include uncertainty quantification, error prediction, and optimization for computational science and engineering; computational geometry, meshing, data science, machine learning, artificial intelligence, remote sensing and GIS, and novel applications of numerical methods across disciplines.

Donald Estep received the B.A. degree in mathematics from Columbia University, New York, NY, USA, in 1981, and the M.S. and Ph.D. degrees in applied mathematics from the University of Michigan, Ann Arbor, MI, USA, in 1987.

From 1987 to 2002, he was a Faculty Member with the School of Mathematics, Georgia Institute of Technology, Atlanta, GA, USA. He joined the Department of Mathematics, Colorado State University, in 2000, and moved to the Department of Statistics in 2006, where he was the Chair from 2017 to 2019. In 2019, he moved to the Department of Statistics and Actuarial Science, Simon Fraser University, to assume the position of Director of the Canadian Statistical Sciences Institute.

Dr. Estep was appointed as a fellow of the Society for Industrial and Applied Mathematics in 2014. He was appointed as a University Interdisciplinary Research Scholar in 2009 and a University Distinguished Professor in 2017 at Colorado State University. He served as a Co-Organizer and the first Chair of the SIAM Activity Group on Uncertainty Quantification from 2010 to 2012 and the Co-Editor-in-Chief (founding) of the SIAM/ASA Journal on Uncertainty Quantification from 2012 to 2017. He received the Computational and Mathematical Methods in Science and Engineering Prize in 2005. He held the Chalmers Jubilee Professorship at the Chalmers University of Technology from 2013 to 2014



Troy Butler received the B.S. degree in electrical engineering and the M.S. and Ph.D. degrees in mathematics from Colorado State University, Fort Collins, CO, USA, in 2003, 2005, and 2009, respectively.

From 2009 to 2012, he was a Post-Doctoral Research Fellow and a Research Associate with the Computational Hydraulics Group, Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX, USA, from 2009 to 2011 and from 2011 to 2012, respectively. From 2012 to 2013, he was a Research Scientist with the Department of Statistics, Colorado State University. In Fall 2013, he joined the University of Colorado at Denver (CU Denver), Denver, CO, as an Assistant Professor in mathematical and statistical sciences, where he was promoted with tenure to an Associate Professor in 2019. From 2014 to 2017, he was the Director of the Center for Computational Mathematics, CU Denver.

Branislav M. Notaroš (Fellow, IEEE) received the Dipl.Ing. (B.S.), M.S., and Ph.D. degrees in electrical engineering from the University of Belgrade, Belgrade, Yugoslavia, in 1988, 1992, and 1995, respectively.

From 1996 to 1999, he was an Assistant Professor with the School of Electrical Engineering, University of Belgrade. He was an Assistant Professor and an Associate Professor with the Department of Electrical and Computer Engineering, University of Massachusetts at Dartmouth, Dartmouth, MA, USA, from 1999 to 2006. He is currently a Professor of electrical and computer engineering, a University Distinguished Teaching Scholar, and the Director of the Electromagnetics Laboratory, Colorado State University, Fort Collins, CO, USA.

Dr. Notaroš was a recipient of the 2005 IEEE MTT-S Microwave Prize, the 1999 IEE Marconi Premium, the 2019 ACES Technical Achievement Award, the 2015 ASEE ECE Distinguished Educator Award, the 2015 IEEE Undergraduate Teaching Award, and many other research and teaching international and national awards. He serves as the General Chair for the 2022 IEEE International Symposium on Antennas and Propagation and the USNC-URSI Radio Science Meeting and a Track Editor for the IEEE TRANSACTIONS ON ANTENNAS AND PROPAGATION. He also serves as the President of the Applied Computational Electromagnetics Society (ACES), the Chair of the USNC-URSI Commission B, and the Meetings Committee Chair for the IEEE Antennas and Propagation Society.