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Susan C. Hagness, Barry D. Van Veen

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14. ABSTRACT

The predictive power of computational electromagnetics (CEM) techniques has improved such that numerical artifacts are no longer the limiting factor in the accuracy of the simulation. Rather, simulation accuracy is limited by the inherent uncertainty in the input parameters. Device performance is subject to statistical uncertainty that is not accounted for by deterministic CEM modeling techniques. We conducted a comprehensive study and review of the state of the art in emerging stochastic CEM techniques for uncertainty quantification (UQ). Our review of existing techniques motivated 1) the creation of a classification framework for UQ techniques in CEM, 2) the

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Report Title

Final Report: STIR: Advances in Stochastic Computational Electromagnetics Modeling Techniques

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The predictive power of computational electromagnetics (CEM) techniques has improved such that numerical artifacts are no longer the limiting factor in the accuracy of the simulation. Rather, simulation accuracy is limited by the inherent uncertainty in the input parameters. Device performance is subject to statistical uncertainty that is not accounted for by deterministic CEM modeling techniques. We conducted a comprehensive study and review of the state of the art in emerging stochastic CEM techniques for uncertainty quantification (UQ). Our review of existing techniques motivated 1) the creation of a classification framework for UQ techniques in CEM, 2) the analysis of accuracy limitations of a particular class of techniques within this framework – namely polynomial basis-function-expansion techniques, 3) the development of a new sensitivity analysis technique based on an electric-field-integral-equation approach, and 4) the development of a new sampling-based UQ method that is suitable for problems with modest to large variability in the CEM simulated field values. Our project culminated with the development of a set of research recommendations that outlines the key challenges and research questions as well as the potential impact of future breakthroughs. Development of robust CEM techniques for quantifying uncertainty in electromagnetic device design would be truly transformative.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
05/21/2017	1	Sathya Ganta, Barry Van Veen, Susan Hagness. On the Accuracy of Polynomial Models in Stochastic Computational Electromagnetics Simulations, IEEE Antennas and Wireless Propagation Letters, ( ): . doi: 1,041,597.00
TOTAL:		**1**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received	Paper
TOTAL:	

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Three conference presentations were entered into the Report Entry app. All three conferences publish abstracts in conference proceedings; however, since they involve abstracts only, they may not qualify as formal conference proceedings here. Both the abstracts and the presentation slides were uploaded for completeness.

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received		Paper
05/21/2017	2	Sathya Ganta, Barry Van Veen, Susan Hagness. On the Computational Complexity of Polynomial Chaos Expansion for FDTD-Based Uncertainty Analyses, IEEE International Symposium on Antennas and Propagation and North American Radio Science Meeting. 24-JUL-15, Vancouver, BC Canada. : ,
05/21/2017	3	Sathya Ganta, Barry Van Veen, Susan Hagness. A Classification Framework for Methods of Uncertainty Quantification in Computational Electromagnetics (Invited Paper), National Radio Science Meeting. 06-JAN-16, Boulder, CO. : ,
05/21/2017	4	Sathya Ganta, Barry Van Veen, Susan Hagness. Efficient Uncertainty Quantification in Computational Electromagnetics using an Adaptive Metropolis-Hastings Method with Importance Sampling, 32nd URSI General Assembly and Scientific Symposium. 23-AUG-17, Montreal, Quebec CANADA. : ,
TOTAL:		**3**

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper
TOTAL:	

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received	Paper
TOTAL:	

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED	DISCIPLINE
Sathya Ganta	50	
FTE Equivalent:	**0.50**	
Total Number:	**1**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Susan Hagness	0.05	
Barry Van Veen	0.05	
FTE Equivalent:	**0.10**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

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Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See attachment

Technology Transfer

None to date.

Final Progress Report

“Advances in Stochastic Computational Electromagnetics Modeling Techniques”

Susan C. Hagness (PI) and Barry D. Van Veen
University of Wisconsin-Madison

List of Appendices, Illustrations and Tables

Statement of the Problem Studied

Large- and small-scale computational electromagnetics (CEM) simulations are an integral part of the engineering design and optimization process and invaluable as a “virtual” lab bench in scientific inquiry and exploration. CEM simulations of electromagnetic wave interactions with structures that are arbitrarily complex in terms of both volumetric configuration and material composition are routinely conducted over large frequency ranges, spatial scales, and time scales. Dozens of commercial and open-source CEM software packages are currently available to support these design, optimization, inquiry, and exploration activities for applications that span the entire electromagnetic spectrum. Table 1 presents representative examples of software packages that are based on the finite-difference time-domain (FDTD) method – just one of several state-of-the-art full-wave CEM techniques. This non-exhaustive list of FDTD software highlights the widespread availability of state-of-the-art CEM tools for use in electromagnetics engineering.

The predictive power of CEM techniques has improved such that numerical artifacts are no longer the limiting factor in the accuracy of the simulation. Rather, simulation accuracy is limited by the inherent uncertainty in the input parameters. Uncertainty in structural dimensions and material properties of electromagnetic devices is pervasive, and as a result, device performance is subject to statistical uncertainty that is not accounted for by deterministic CEM modeling techniques.

Uncertainty quantification (UQ) – a core field in statistics – has begun to impact the field of CEM to address this fundamental limitation. There are two possible goals for UQ methods in CEM. The forward problem is to accurately predict statistics, such as mean and variance, of a particular electromagnetic characteristic (e.g., field intensity, input impedance, scattering parameter, radiation pattern, etc.) due to a known uncertainty in the dimensions and/or material properties of the electromagnetic environment. Conversely, the goal of the inverse problem is to determine the acceptable level of uncertainty in the dimensions and/or properties such that variability in device performance metrics lies within acceptable limits. A number of stochastic CEM techniques have emerged over the past decade as the CEM community has begun to recognize the critical need for stochastic CEM simulation tools.

Table 1: Representative examples of commercial and open-source FDTD software packages available for conducting deterministic CEM simulations.

Commercial	***Software Title***	***Company***
	AxFDTD	Acceleware
	Empire XPU	IMST GmbH
	FDTD Solutions	Lumerical
	FullWAVE	Synopsys
	HyperLynx Full-Wave Solver	Mentor Graphics
	GEMS	2COMU
	OptiFDTD	Optiwave Systems
	SEMCAD	Speag
	XFDTD	Remcom
Open-Source	***Software Title***	***Organization***
	Angora	Northwestern Univ.
	FDTD++	Washington State Univ.
	GSVIT	Czech Metrology Institute
	Meep	MIT
	openEMS	Univ. Duisberg-Essen

We conducted a comprehensive study and review of the state of the art in emerging stochastic CEM techniques for UQ. This review was complemented by efforts to inventory typical uncertainty levels in electromagnetic properties measurements for reference. Our review of existing techniques motivated 1) the creation of a classification framework for UQ techniques in CEM, 2) the analysis of accuracy limitations of a particular class of techniques within this framework – namely polynomial basis-function-expansion techniques, 3) the development of a new sensitivity analysis technique based on an electric-field-integral-equation approach, and 4) the development of a new sampling-based UQ method that is suitable for problems with modest to large variability in the CEM simulated field values. Our project culminated with the development of a set of research recommendations that outlines the key challenges and research questions as well as the potential impact of future breakthroughs.

Summary of the Most Important Results

1. *Inventory of typical uncertainty levels in electromagnetic properties of materials*

A review of commercial (e.g. [1]) and non-commercial advanced (e.g. [2]-[4]) dielectric characterization techniques as well as specification sheets from one of the largest substrate manufacturers [5] yielded the following insights about the range of uncertainty in the measured properties of materials:

- The typical upper bound on uncertainty is approximately ±5%. This corresponds to the measurement precision of commercially available coaxial dielectric probes for characterizing liquids and semi-solids [1]. Clamped stripline techniques employed by Rogers Corp. in the characterization of their dielectric substrates results in ±2.4% uncertainty in their reported values [5].
- The precision of more advanced capacitor-based techniques [2]-[3] is on the order of ±1%. Even lower uncertainty, on the order of ±0.3%, is achieved with a split-post resonator technique for characterizing dielectric substrates [4].

This range serves as a reference for understanding the necessary capabilities of UQ techniques in CEM.

2. Development of a classification framework

We developed a classification framework to systematically organize current UQ methods into well-defined categories based on the approach used to represent variation in the fields and the mathematical techniques employed to estimate the mean and variance integrals of stochastic functions [6]. The advantage of such a framework is that it standardizes terminology and elucidates the relationship between methods; in addition, it reveals gaps and new directions in UQ research. State-of-the-art methods for UQ in CEM fall into two primary categories: sampling methods and basis-function expansion methods, as illustrated by the highest-level categories in Figure 1. Techniques based on basis function representations are further differentiated by the types of basis functions employed and the method used to estimate the unknown coefficients in the expansions. Sampling techniques are further differentiated by the strategies used to evaluate functions at samples points drawn from the assumed distribution of the uncertain parameter(s).

Basis-function expansion (BFE) methods: BFE methods approximate the electromagnetic fields as a weighted sum of basis functions -- functions of the uncertain parameters in addition to space/time or space/frequency, and use statistical characterization of the weights to characterize the variability of the fields. The accuracy of BFE methods scales with the number of terms in the expansion, but a larger number of terms requires a larger number of deterministic simulations. BFE methods can be much more numerically efficient than sampling techniques, but their performance is highly dependent on the choice of basis functions. Unfortunately, basis functions that perform well for some problems and ranges of uncertain parameters may fail miserably for others.

Sampling methods: The most common sampling method is the Monte Carlo technique, a "one-time sampling" method whereby large numbers of deterministic simulations are run for densely sampled values of the uncertain parameters and data is post-processed to quantify uncertainty. The accuracy of Monte Carlo scales with the number of samples, as does the computational burden. Consequently, this brute-force approach is extremely time-consuming. Furthermore, as the number of uncertain parameters increases, the Monte Carlo method quickly becomes highly impractical or completely intractable in many cases, even with the advent of massive high-throughput computing platforms. Iterative or multi-level sampling methods offer promise of fewer simulations, but generally require implementing those simulations in series. A broadly applicable, computationally efficient sampling method for problems involving even modest numbers of uncertain parameters does not yet exist.

We are currently writing a comprehensive review paper that places published papers on UQ in CEM within this classification framework and describes the computational strengths and weaknesses of the reported techniques. We will upload the manuscript into the ARO Report Entry App at the time of submission.

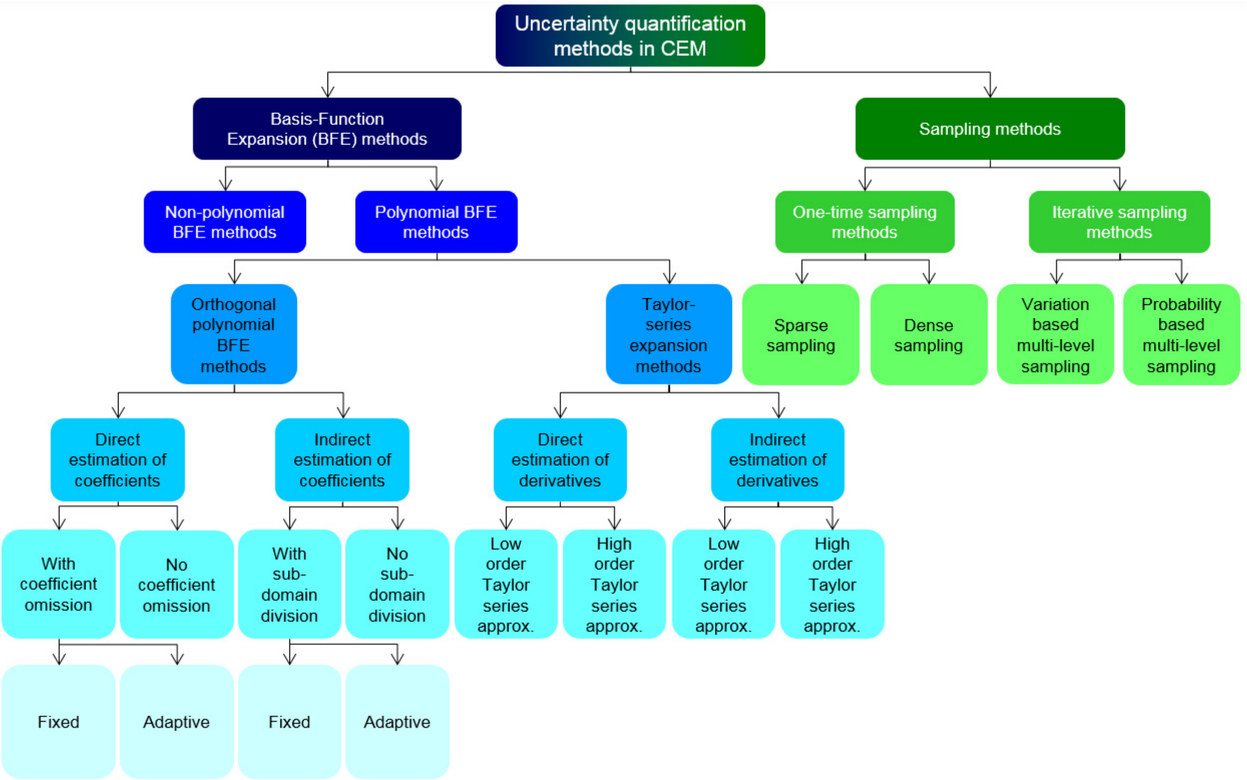

Figure 1. A classification framework for organizing current UQ methods into well-defined categories based on the approach used to represent variation in the fields and the mathematical techniques employed to estimate the mean and variance integrals of stochastic functions.

3. *Analysis of polynomial approximations in UQ*

Many techniques describe the stochastic variations in fields due to with uncertainties in device properties using polynomial model expansions. The output fields are represented as polynomial functions of the uncertain properties [7]-[13]. The coefficients of the polynomials are obtained either using a single stochastic CEM simulation [7]-[10] or by using a small number of deterministic CEM simulations [9]-[13]. Once the coefficients are obtained, the polynomial expansion is used to evaluate the mean and variance of the field quantities of interest.

The polynomial order of the expansion directly impacts the computational complexity of the CEM simulation. For example, we demonstrated that the polynomial order required to obtain accurate field means and variances using the polynomial chaos expansion (PCE) technique with the finite-difference time-domain (FDTD) method can be very small for some problems but extremely large for others [14]. Thus the computational cost of PCE-FDTD is highly variable, and in some cases prohibitively high. Furthermore, the necessary polynomial order to achieve sufficient accuracy is not known a priori. While this investigation provides important specific insights about the computational complexity of PCE-FDTD, it does not yield broadly applicable insights about the accuracy of polynomial approximations in general.

An important question that has not been addressed in the literature published to date is whether polynomial functions are adequate approximations of the relationship between uncertain properties and field quantities. The published work relating to this approach considers very specific scenarios and does not indicate whether the approach is broadly applicable. We addressed this gap by investigating the order of polynomial required to accurately estimate the field mean and variance in three canonical scattering scenarios [15]. If the required polynomial order is low, then the method can be effective. However, if the order is high, then a polynomial approach becomes too inefficient to be practical. The accuracy of the polynomial approximations was shown to be strongly dependent on the mean dielectric properties of the scatterers. Extremely high-order expansions were necessary to achieve accurate approximations in some instances. These results point to a serious limitation of polynomial approximation methods: namely, it is impossible to know in advance with realistic, complex devices whether or not a polynomial approximation is appropriate. Validating that polynomial approximation is providing accurate results is also impractical for realistic devices. Thus the key finding of this part of the study is that polynomial approximations have limited utility as a general tool for characterizing variability in field quantities associated with uncertain device properties.

4. Development of new algorithms for UQ in CEM

Over the course of this project we identified and pursued two promising new research directions that led to the development of a new sensitivity analysis technique and a new sampling technique.

Sensitivity analysis: We developed a technique for estimating the derivative of field values with respect to relevant parameters (such as dielectric properties or dimensions) using a linearized electric-field integral equation. We evaluated the accuracy of this approach in analyzing sensitivity for a canonical scattering problem and a practical integrated optical waveguide problem involving a 2D photonic crystal waveguide branch. Our proposed approach offers higher accuracy than other derivative estimation techniques such as difference approximations. It is particularly well suited for applications involving a large number of sensitivity parameters and a small number of observation points where the sensitivity of the fields is being evaluated.

Sampling technique: Computed field values can be used to improve the efficiency of sampling on the fly where sampling of uncertain physical parameters and execution of corresponding CEM simulations are performed sequentially. The adaptive Metropolis-Hastings algorithm [16] is one such sequential sampling algorithm. The computed field values can be used to change the target distribution and more efficiently sample the distribution of the field values. This latter approach is denoted "importance sampling" [17]. We have combined these two techniques to achieve significant reduction in computational cost over traditional Monte Carlo techniques; for example, the new sampling method provides more than a 20-fold decrease in cost in simulations involving a 2D photonic crystal waveguide branch and channel drop filter [18].

We are currently preparing full-length journal papers that report these two advances; the target journal for both is the *IEEE Transactions on Antennas and Propagation*. We will upload the manuscripts into the ARO Report Entry App at the time of their submission.

5. Research recommendations

There is a critical need for breakthroughs to quantify the effects of uncertainty with CEM simulation tools that are computationally efficient, accurate, and applicable to wide problem classes. Development of robust CEM techniques for quantifying uncertainty in electromagnetic device design would be truly transformative, and enable reliable design of high-performance devices that are immune to inevitable uncertainties in microfabrication tolerances, material properties, inhomogeneity, and so on. A significant, sustained research effort is warranted to realize the potential benefits of stochastic CEM tools. Specific areas for critical research advances are outlined below.

Methodological advances

- Sampling methods: Development of adaptive or "smart" techniques for efficient sampling of the space of uncertain parameters.
- Basis function expansion methods: Development of systematic methods for choosing basis functions that are well suited for specific classes of uncertainties and electromagnetic simulation problems, and identification of robust basis functions that are universally or near-universally applicable to a wide range of UQ problems.
- Both classes of methods: Development of strategies to address the inverse problem, that is, the problem of determining acceptable ranges of uncertainty on properties and dimensions such that the device performance lies within predetermined limits.

Cross-cutting experimental advances

- Experimental characterization of the statistical properties of the uncertainty in dielectric and magnetic properties that is inherent in natural and engineered materials or that arises due to environmental influences, such as temperature and pressure.
- Experimental characterization of the statistical properties of the uncertainty in dimensions that arises as a result of various fabrication techniques.

Cross-cutting computational advances

- Establishment of a taxonomy for specific classes of UQ problems in CEM.
- Development of general strategies for determining the suitability of specific methods for different problem classes.
- Establishment of canonical test cases for benchmarking UQ methods in CEM.
- Development of high throughput computing and/or high performance computing strategies that leverage the features of the stochastic CEM techniques for optimum computational efficiency.

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