PROBABILISTIC FINITE-DIFFERENCE TIME-DOMAIN SIMULATIONS USING STOCHASTIC ELECTROMAGNETIC MACRO-MODELS

BY

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DISSERTATION

Submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Electrical and Computer Engineering in the Graduate College of the University of Illinois at Urbana-Champaign, 2011

Urbana, Illinois

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ABSTRACT

To enable an efficient stochastic-based design optimization methodology for multi-scale structures of electrical devices and systems, we propose the infusion of stochastic modeling with the electromagnetic macro-model in the finite-difference time-domain (FDTD) method. We provide a methodology for the efficient generation and utilization of the stochastic macro-model for the purpose of time-domain analysis in FDTD. The methodology quantifies the impact of uncertainty, manifested as random material and structural variations in the design and manufacturing process of the realized system, on the stochastic system’s electromagnetic performance.

In the current state of the art, and in absence of the stochastic macro-model, it is necessary to perform repeated discretization of the large deterministic domain for every random variation in the small fine-featured stochastic domain. The development of the stochastic macro-model eliminates the need for repeated discretization of the overall structure for every such random variation. Indeed, only a single FDTD grid needs to be developed for the deterministic portion of the overall structure irrespective of the realization generated by a specific choice of the random parameters in the domains exhibiting statistical variability; thus, the macro-model results in significant computational savings by eliminating operations pertaining to repeated discretization of the deterministic domain for each variation in the stochastic domain.

In essence, the macro-model is a state-space representation of the discretized Maxwell’s equations which encapsulates a certain fine-featured region of a multi-scale structure, in the FDTD grid. To enhance the computational efficiency of this state-space abstraction layer we apply a modified embodiment of the model order reduction (MOR) technique, known as enhanced nodal order reduction (ENOR), to minimize the internal degrees of freedom of the abstraction layer while maintaining sufficient engineering accuracy in
the system response. ENOR provides a passive reduced order admittance boundary condition model which expedites the efficient computation of field quantities in the fine-featured regions.

To enable cost-effective and high-accuracy FDTD simulations involving design and manufacturing variations of disparate spatial scales, the method of sub-gridding is utilized, with the stochastic macro-model implemented in the sub-gridded region. **To enable the insertion of the high spatial-resolution stochastic macro-model inside the FDTD grid**, a class of isotropic spatial filters is developed to suppress the spurious noise waves which are generated by the discrete wave-impedance mismatch at the boundary of the macro-model. To this end, we develop a class of spatial filter operators that: (a) are straightforward to design and implement within the existing Yee style FDTD explicit time-stepping scheme; (b) do not require complicated spatial/temporal interpolation in the field update equations; (c) are able to accommodate broadband electromagnetic sources; (d) exhibit spatial isotropy in their suppression of the spurious numerical reflections while preserving the pertinent portions of the signal’s power spectral density.
To Maryam
I would like to thank the following people who have helped me greatly during my stay at the University of Illinois at Urbana-Champaign:

My adviser, Professor Andreas C. Cangellaris, for his full support, encouragement, and patience, over the past five years; it was a tremendous privilege to work with him.

The members of my doctoral committee for their engagement, support, and constructive feedback.

All my present and former colleagues in the Center for Computational Electromagnetics for the many interesting technical and other discussions.

Dr. Alexandra Seceleanu of the Department of Mathematics for discussions and insight on the Smoljak algorithm.

Jamie Hutchinson, editor in the Publications Office of the Department of Electrical and Computer Engineering, for careful review and editing of this document.

My parents and my brothers for their love and faith in me over the years.

My kind and intelligent daughter, Diba, whose mere presence motivated me to never give up.

Most of all I thank my wife, Maryam, for her unfailing love and companionship and for her sacrifices during this often difficult journey.
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In order to engage in practical design of electronic devices and systems, one must contend with the presence of uncertainty in the design and manufacturing process which leads to material and structural variability in the final production of system. These random effects, which impact the manufactured system’s electrical performance and cause it to deviate away from the ideal design goal, are primarily rooted in material and geometric imprecisions in the manufacturing process. Although process improvement can go a long way to mitigate impact of uncertainty, it cannot completely eliminate it. As a result, one must contend with the presence of uncertainty and proceed to predict its impact.

A popular method to mitigate the effect of uncertainty is by allocation of parametric error tolerance; a practice commonly known as design guard-banding. While an effective method to address uncertainty, blanket placement of guard-bands on various design specification parameters can lead to substantial increase in cost of the final product and possibly make production infeasible; this is especially true in real-life practical systems where the number of design parameters can be in the hundreds or even thousands. As such, to optimize the design process, one must address the presence of random variability while avoiding over-design.

Given the uncertainty profile of individual random parameters in the system, the impact of uncertainty on the system response may be predicted in the early stages of the design process and provide significant cost savings in the design and manufacturing process of the final production. In order to enable an efficient stochastic-based design optimization methodology for electrical devices and systems, which comprehends random material and geometric variability, we propose to infuse the stochastic collocation method with the reduced-order state-space electromagnetic model into one of the methods used extensively for electromagnetic component/system analysis and design,
namely, the method of finite-difference time-domain (FDTD).

To this end, we propose to develop stochastic macro-modeling in FDTD through an abstraction layer that encapsulates those regions where, most often, uncertainty is present, namely, the fine-features of the structure. We name this abstraction layer the stochastic macro-model [1–3]. In essence, the macro-model is a reduced order state-space representation of the discretized Maxwell’s equations for a certain region of the grid. From the full-order state-space form, it is possible to obtain an admittance (or impedance) transfer function which serves to map the macro-model and the FDTD grid at the union of their common boundary. The input (excitation) to this admittance (or impedance) transfer function is the magnetic (or electric) field at the boundary of the macro-model. The output (response) of the admittance (or impedance) transfer function is the electric (or magnetic) field at the inner perimeter of the macro-model.

In order to enhance the computational efficiency of operations pertaining to the system transfer function, model order reduction (MOR) techniques [2–7] may be utilized to decrease the degrees of freedom of the full-order state-space model while maintaining sufficient accuracy. As such, we propose to apply the MOR technique known as ENOR [5] to the full-order state-space electromagnetic system transfer function, and use the resulting projection matrix to build the reduced order stochastic macro-model. At its heart, building the stochastic macro-model relies on highly accurate numerical integration over random space; for this, we utilize the sparse Smoljak grid [8] and the Clenshaw-Curtis quadrature [9] rules in single-dimensional random space, and extend these principles to cubature in multi-dimensional random space.

In comprehending the effects of random variability in material and geometric attributes on the electromagnetic response of multi-scale structures, the need arises to simulate electromagnetic behavior of structures with disparate spatial scales. The Courant stability condition, together with the fine nature of material and structural variability, dictates the need for very small temporal discretization in the stochastic domain; this leads to vastly more time iterations in a uniform FDTD grid, making it computationally costly. To enable cost-effective and high-accuracy FDTD simulations involving grids of disparate resolutions, the method of sub-gridding [10] is utilized, whereby the FDTD grid is divided into two regions: the coarse main grid, and the
The implementation of the sub-gridded macro-model inside the uniform FDTD grid requires the transition of fields from a coarser grid to a finer grid, which inevitably induces discrete wave impedance mismatch at the fine-coarse transition interface of the macro-model and injects spurious noise waves into the FDTD grid. Hence, a class of isotropic spatial filters is proposed to suppress spurious noise waves due to sub-gridded macro-modeling in FDTD simulations and to enable the insertion of the macro-model inside the uniform FDTD grid, in a general way and regardless of the choice of implementation for the fine-coarse transition. The proposed filters are suitable for both two-dimensional and three-dimensional applications. A simple procedure is introduced for the a-priori determination of the required filter order and the application frequency of the filter based on the maximum temporal frequency bandwidth of the electromagnetic source. The proposed filters are easy to implement in the context of the standard Yee algorithm and are applicable to computational domains that involve quite arbitrary material and geometric inhomogeneities.

It is our hope that the framework provided herein will be immediately useful in making a significant improvement in the existing state of the art, specifically, by eliminating the cost of repeated meshing of the deterministic domain for every variation in the fine-featured stochastic sub-domains.

In addition to being immediately applicable to solution of electromagnetic stochastic boundary value problems with methods rooted in finite differences (e.g., FDTD, finite element method, finite volume, etc.), the ideas herein may motivate extension to other classes of methods (e.g., semi-analytic) for solving stochastic boundary value problems involving various differential/integral equations. What makes this extension possible is the systems-based approach to solving boundary value problems. The work herein provides powerful examples of generation and utilization of mathematical abstraction layers of complex physical systems, which in turn enables the meticulous control and transformation of the systems into equivalent domains attributed with orders of magnitude higher computational efficiency. Through this systems-based approach, we are able to unleash the full power of the well-developed systems theory on the electromagnetic problems at hand.

Although throughout this development it is assumed that the material inside the stochastic macro-model belongs to the class of frequency-independent
media (i.e., non-dispersive), we note that the method may be extended to include dispersive media by appropriate modification of the pertinent formulations; this may be a topic for future research.

1.1 Main Contributions

We have two main contributions:

1. We developed a methodology for stochastic macro-modeling in FDTD, by infusing the macro-model with the stochastic collocation technique. This enables the quantification of the impact of parametric uncertainty in the fine-featured geometric and material properties of multi-scale structures, on the electromagnetic response of stochastic systems in FDTD.

2. We developed a general methodology to suppress noise waves in sub-gridded FDTD due to spurious reflections caused by the discrete wave impedance mismatch at fine-coarse grid interface. In particular, we introduced a class of spatial filters that: (a) are straightforward to design and implement within the existing Yee style FDTD explicit time-stepping scheme; (b) do not require complicated spatial/temporal interpolation in the field update equations; (c) are able to accommodate broadband electromagnetic sources; (d) exhibit spatial isotropy in their suppression of the spurious numerical reflections while preserving the pertinent portions of the true wave’s power spectral density. The derived formulations are applied to 2D and 3D sub-gridded FDTD simulations.

1.2 Organization

In Chapter 2 we develop a general methodology, based on isotropic spatial filter operators, to suppress noise waves in FDTD simulations caused by reflections due to discrete wave impedance mismatch at the fine-coarse grid interface. We discuss the characteristics of the sub-gridded FDTD and derive an analytic expression for the discrete wave impedance of the sub-gridded
FDTD, derive an analytic expression for late-time stability, introduce the theory of spatial filter operators, and provide numerical examples in 2D and 3D FDTD.

In Chapter 3 we introduce the basic formulation for the electrically lossy macro-model implemented as an admittance transfer function (ATF), and provide the pertinent reduced order state-space electromagnetic system representation, followed by several numerical examples. Additionally, the macro-model implemented as an impedance transfer function (ITF) is presented in Appendix C.

In Chapter 4, we develop the stochastic macro-model in FDTD and develop a methodology that captures the uncertainty in material and geometric attributes in fine-featured stochastic sub-domains, and quantifies the impact of such variability on the electromagnetic response of stochastic systems in FDTD. In Chapter 5, we provide several numerical examples which demonstrate the application of the stochastic macro-model. In Chapter 6 we conclude the dissertation with closing remarks.
2.1 Introduction

The finite-difference time-domain (FDTD) method with the standard Yee algorithm [11] has been one of the most popular methods in the electromagnetics community for the computer-aided analysis of field interaction in complex structures and media. Although the Yee algorithm can be applied to uniform grids accurately and efficiently, the Courant stability criterion places upper limits on the maximum temporal discretization based on the minimum spatial discretization. When the need arises to simulate structures with disparate spatial scales to obtain the steady-state field solutions, the very small temporal discretization dictates the need for vastly more iterations in the uniform FDTD grid, making it computationally costly. In such cases, and in order to overcome the computational cost imposed by the use of a uniform FDTD grid, various methods have been proposed, including sub-gridding, use of sub-cells, and macro-modeling.

In the case of the popular approach of sub-gridding, the grid is divided into fine and coarse spatial domains as necessary to capture the finer spatial variations of the structures to be modeled. This means that the spatial discretization varies in size as the grid transitions across regions that require higher spatial sampling, in order to resolve the finer structural details. In principle, sub-gridding should be quite robust, since it continues to use Yee’s simple update scheme in both fine and coarse grids; however, in practice, sub-gridding introduces various side effects that can impact solution accuracy. For example, any abrupt change in grid size gives rise to spurious reflections at the grid interface, due to the discrete wave impedance mismatch at the fine-coarse transition. This necessitates the use of proper schemes to mitigate such spurious effects in order to ensure solution accuracy [12–22]. While some
of these schemes consider direct changes to the standard Yee update equations or suggest new temporal/spatial interpolation techniques, a few others propose the application of filter operators to eliminate those spurious waves that dominate the spurious degradation in solution accuracy [16,18–20]. For example, the novel work [19, 20] uses 1D digital filters (1D convolution) for spatial decimation and interpolation of the fields at the fine-coarse interface to overcome aliasing, while resorting to phase compensation (scaling of space metric) to suppress the spurious reflections due to impedance-mismatch at the fine-coarse interface.

Our contribution here is to develop a general method to suppress noise waves in FDTD simulations due to spurious reflections caused by the numerical impedance mismatch at fine-coarse grid interface. Specifically, we propose a class of spatial filter operators that: (a) are straightforward to design and implement within the existing Yee style FDTD explicit time-stepping scheme [10]; (b) do not require complicated spatial/temporal interpolation in the field update equations; (c) are able to accommodate broadband electromagnetic sources; (d) exhibit spatial isotropy in their suppression of the spurious numerical reflections while preserving the pertinent portions of the signal's power spectral density. The derived formulations are applied to two-dimensional TM$^z$ and three-dimensional sub-gridded FDTD simulations. For this, we rely on ideas from digital image/signal processing [23–25] to develop a systematic method for the design of isotropic spatial filters in two and three dimensions via the McClellan transformation [26]. Furthermore, we provide a design procedure for a-priori determination of the required filter order and the required frequency of application of the filter based on the temporal frequency bandwidth of the electromagnetic source.

The chapter is organized as follows. In Section 2.2 we review the reflection properties of the interface between two finite difference grids of different discretization size. In Section 2.3, we derive the discrete wave impedance of the sub-gridded system. Using the results Section 2.2 and Section 2.3, in Section 2.4 we derive the criterion for late-time stability [22, 27–29] on the sub-gridded FDTD system. We use the results of stability and reflection analyses to inform the discussion that follows on the development of the proposed spatial filters. In Section 2.5, we present the isotropic spatial filter theory, followed by a series of numerical experiments in Section 2.6 that demonstrate the effectiveness of the proposed filters. Finally, Section 2.7
concludes with a brief summary and closing remarks.

2.2 Reflection Properties of the Grid Interface

In this section, we review the reflection properties of the interface between two uniform, finite-difference grids of different discretization size in the context of one-dimensional wave propagation [30, 31]. Our development follows the analysis in [22, 28]. In particular, the analysis is carried out for the interface between two grids of discretization size ratio of 1:3. This is the ratio used by several investigators for FDTD sub-gridding (e.g., [32]). The odd ratio is convenient, because it allows for convenient nesting of sub-grids within sub-grids. The finite difference grid interface is depicted in Figure 2.1.

![Diagram of one-dimensional, finite-difference grid interface between grids of discretization size ratio 1:3.](source)

Figure 2.1: One-dimensional, finite-difference grid interface between grids of discretization size ratio 1:3. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)

With $\Delta$ denoting the variable discretization size in the computational domain, $\Delta = h$ in the fine grid, while $\Delta = 3h$ in the coarse grid. For the one-dimensional plane wave propagation considered along the $x$ axis, the only electric and magnetic field components considered are, respectively, $E_z(x)$ and $H_y(x)$. Assuming normalized free-space permittivity ($\epsilon_0 = 1.0$) and permeability ($\mu_0 = 1.0$), the source-free Maxwell equations in this case simply become

$$\frac{d}{dt} E_z(x, t) = \frac{d}{dx} H_y(x, t) \quad (2.1)$$

$$\frac{d}{dt} H_y(x, t) = \frac{d}{dx} E_z(x, t) \quad (2.2)$$

For time-harmonic solutions of the form $\exp(jkx)\exp(j\omega t)$, where $j = \sqrt{-1}$, $\omega$ is the angular frequency, and $k$ is the propagation constant, the
phasor of each field component satisfies the Helmholtz scalar wave equation, shown below for the magnetic field.

\[ \frac{d^2}{dx^2} H_y + k_0^2 H_y = 0 \]  \hspace{1cm} (2.3)

Because normalized permittivity and permeability are used, it is \( k_0^2 = \omega^2 \) in (2.3). Using a central difference approximation of (2.3) on the fine and on the coarse grids, the respective numerical wave numbers \( k_F \) and \( k_C \) are readily obtained \[10\] and are given by

\[ k_F = \frac{1}{h} \cos^{-1} \left( 1 - \frac{(k_0 h)^2}{2} \right) \]  \hspace{1cm} (2.4)

\[ k_C = \frac{1}{3h} \cos^{-1} \left( 1 - \frac{(k_0 (3h))^2}{2} \right) \]  \hspace{1cm} (2.5)

Next, we examine the reflection and transmission properties of the grid interface. This is done by considering a plane wave propagating from left (fine grid) to right (coarse grid) on the grid shown in Figure 2.2. The total magnetic field phasor in the fine grid is of the form

\[ H_y[i] = H_0 \left( e^{-jk_F i h} + R_0 e^{+jk_F i h} \right) ; \quad i \leq 0 \]  \hspace{1cm} (2.6)

where \( R_0 \) is the reflection coefficient for the grid interface. The transmitted magnetic field phasor in the coarse grid is given by

\[ H_y[i] = H_0 T_0 e^{-jk_C i (3h)} ; \quad i \geq 0 \]  \hspace{1cm} (2.7)

In the above expressions the notation \( H_y[i] \) is used to denote the magnetic field value at position \( x = i\Delta \). Working with the phasor form of (2.1) and (2.2) discretized using central differences in the staggered Yee grid, the scheme in \[32\] is followed to derive a set of discrete equations from which expressions for \( R_0 \) and \( T_0 \) can be derived.

\[ j\omega H_y[1.5] = \frac{E_z[3] - E_z[0]}{3h} \]  \hspace{1cm} (2.8)

\[ j\omega H_y[-0.5] = \frac{E_z[0] - E_z[-1]}{h} \]  \hspace{1cm} (2.9)
Figure 2.2: Staggered electric and magnetic fields, with sub-gridding along one dimension. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)

\begin{align*}
\omega E_z[0] &= \frac{H_y[1.5] - H_y[-1.5]}{3h} \quad (2.10) \\
\omega E_z[-1] &= \frac{H_y[-0.5] - H_y[-1.5]}{h} \quad (2.11) \\
\omega E_z[3] &= \frac{H_y[4.5] - H_y[1.5]}{3h} \quad (2.12)
\end{align*}

Elimination of the electric field in the above equations yields two equations that involve only magnetic field values. Using (2.6) and (2.7) in these equations yields the linear system for the calculation of $R_0$ and $T_0$. The expressions obtained are

\begin{align*}
R_0 &= \frac{R_{num}}{denom} \quad (2.13) \\
T_0 &= -3e^{\frac{1}{2}j(h(k_F+9k_C)}(-1 + e^{2jhk_F})(-1 + h^2\omega^2)
\frac{denom}{(2.14)}
\end{align*}

where

\begin{align*}
R_{num} &= -e^{2jhk_F}(-3 + 2e^{jhk_F} + 3h^2\omega^2 \\
&\quad + e^{j(h(k_F+3k_C)}(-5 + 18h^2\omega^2) \\
&\quad + 3e^{3jhk_C}(2 - 11h^2\omega^2 + 9h^4\omega^4))
\end{align*}
The magnitude of the reflection coefficient $|R_0|$ vs. $h/\lambda$ is depicted in Figure 2.3. Also shown in the figure is the reflection coefficient obtained from the FDTD simulation of wave propagation across this grid interface. More specifically, the numerical reflection coefficient was obtained through the equation

$$R_{0m} = \frac{\mathcal{F}\{E^{ref}_z[0]\}}{\mathcal{F}\{E^{inc}_z[0]\}} \quad (2.15)$$

In the above equation $\mathcal{F}$ denotes the discrete Fourier transform (DFT) operator. The DFT of the incident electric field $\mathcal{F}\{E^{inc}_z[0]\}$ at the interface node $i = 0$ is computed using the recorded field at that node obtained from the FDTD simulation of a plane wave propagating on a uniform fine grid. The DFT of the reflected electric field is calculated as $\mathcal{F}\{E^{ref}_z[0]\} = \mathcal{F}\{E^{total}_z[0] - E^{inc}_z[0]\}$ at the interface node $i = 0$, where $E^{total}_z[0]$ is the recorded electric field at that node from the simulation of a plane wave propagation on the grid depicted in Figure 2.1.

As expected, and as clearly evident from the plot in Figure 2.3, wavelengths that are well resolved on both grids propagate through the grid interface with minimum reflection. The interval for which the reflection coefficient has magnitude 1.0 is $(2/3) \leq (k_0 h) \leq 2$ and is also depicted in Figure 2.3. The left end of the interval is at the cutoff wavelength for the coarse grid, $\lambda_C = \pi(3h)$, (see (2.5)), while the right end of the interval is at the cutoff wavelength on the fine grid, $\lambda_F = \pi h$ (see (2.4)). Unless suppressed, waves with wavelengths $\lambda < \pi(3h)$ will give rise to spurious reflections that may degrade the accuracy of the numerical wave response. In fact, as the figure suggests, the cutoff wavelength of any spatial filter used to suppress such wavelengths should be chosen even higher than $\lambda_C$ to ensure that the allowed wavelengths in the computational domain propagate through the grid interface with minimum reflection. Equation (2.13) provides a convenient means for the selection of...
the desired cutoff wavelength for the spatial filter. Clearly, this 1D reflection analysis may be repeated in 2D and 3D, as well.

![Figure 2.3: Magnitude of ideal ($R_0$) and computed ($R_{0m}$) reflection coefficient, and magnitude of transmission coefficient ($T_0$), vs. $h/\lambda$.](image)

Figure 2.3: Magnitude of ideal ($R_0$) and computed ($R_{0m}$) reflection coefficient, and magnitude of transmission coefficient ($T_0$), vs. $h/\lambda$. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)

2.3 Discrete Wave Impedance

In this section, we derive the analytic expression for the discrete wave-impedance. Consider the dispersion relation

$$\cos[\hat{k}\Delta] = 1 - \frac{(k\Delta)^2}{2}$$  \hspace{1cm} (2.16)

where $k = \omega \sqrt{\mu\epsilon}$ is the propagation constant of the medium, $\hat{k}$ is the discrete propagation constant, and $\Delta$ is the spatial discretization.

Using trigonometric identities, (2.16) can be written as
\[
\sin \left[ \frac{k\Delta}{2} \right] = \frac{k\Delta}{2} \tag{2.17}
\]

Let us assume the electric field has a plane wave form in the x-direction, given by

\[
E = E^+ e^{-jkx} \tag{2.18}
\]

From Maxwell’s equations in 1D and first order central difference, the H-field is obtained as

\[
H\mid_{x=(i+\frac{1}{2})\Delta} \approx (j\omega\mu)^{-1} E^+ e^{-j\hat{k}(i\Delta)} - E^+ e^{-j\hat{k}((i+1)\Delta)} \Delta \tag{2.19}
\]

The above can be re-written as

\[
H(x = (i + \frac{1}{2})\Delta) \approx \frac{E^+ e^{-jk(i+1/2)\Delta}}{j\omega\mu\Delta} (e^{+jk(\Delta/2)} - e^{-jk(\Delta/2)}) \tag{2.20}
\]

The E-field at index \( x = (i + 1/2)\Delta \) can be obtained from the average

\[
E(x = (i + \frac{1}{2})\Delta) = \frac{E^+ e^{-jk(i+1/2)\Delta}}{2} (e^{+jk(\Delta/2)} + e^{-jk(\Delta/2)}) \tag{2.21}
\]

Using (2.20) and (2.21), we obtain the complex discrete wave impedance

\[
Z_0 = \frac{E(x = (i + \frac{1}{2})\Delta)}{H(x = (i + \frac{1}{2})\Delta)} = \frac{j\omega\mu\Delta}{2} \frac{2\cos[k\Delta/2]}{2j\sin[k\Delta/2]} \tag{2.22}
\]

The expression (2.22) can be written as

\[
Z_0 = \frac{\omega\mu\Delta/2}{\tan[k\Delta/2]} = \eta_0 \frac{k\Delta/2}{\tan[k\Delta/2]} \tag{2.23}
\]

where \( \eta_0 = \sqrt{\frac{\mu}{\epsilon}} \) is the intrinsic wave impedance in the medium.

Using (2.17) in (2.23), further simplification is possible and we obtain

\[
Z_0 = \eta_0 \cos[\sin^{-1}[k\Delta/2]] \tag{2.24}
\]

Equation (2.24) is a general result. It is the discrete wave impedance on a uniform FDTD grid for one-dimensional wave propagation. It can be used to calculate the discrete wave impedance on the fine grid \( Z_{0_F} \), and the discrete wave impedance on the coarse grid \( Z_{0_C} \), as follows:
\[ Z_{0F} = \eta_F \cos[\sin^{-1}(k_F \Delta_F/2)] \]  
(2.25)

where \( \eta_F = \sqrt{\mu_F/\epsilon_F} \) is the intrinsic wave impedance in the fine grid, \( \Delta_F \) is the spatial discretization of the fine grid, and \( k_F = \omega \sqrt{\mu_F \epsilon_F} \) is the propagation constant in the fine medium. The quantities with subscript \( F \) reside in the fine grid (e.g., \( \mu_F \) is the material permeability in the fine grid).

\[ Z_{0C} = \eta_C \cos[\sin^{-1}(k_C \Delta_C/2)] \]  
(2.26)

where \( \eta_C = \sqrt{\mu_C/\epsilon_C} \) is the intrinsic wave impedance in the coarse grid, \( \Delta_C \) is the spatial discretization of the coarse grid, and \( k_C = \omega \sqrt{\mu_C \epsilon_C} \) is the propagation constant in the coarse medium. The quantities with subscript \( C \) reside in the coarse grid (e.g., \( \mu_C \) is the material permeability in the coarse grid).

We compute the numerical discrete wave impedance \( Z_{0M} \) in the fine grid according to

\[ Z_{0M} = \frac{\mathcal{F}\{E_{z}^{inc}\}[-2]}{\mathcal{F}\{H_{y}^{inc}\}[-2]} \]  
(2.27)

where the DFT of the incident electric field \( \mathcal{F}\{E_{z}^{inc}\}[-2] \) at the node \( i = -2 \) is computed while simulating a uniform fine-gridded FDTD, and the DFT of the incident magnetic field \( \mathcal{F}\{H_{y}^{inc}\}[-2] \) at the node \( i = -2 \) is computed by simulating the same uniform fine-grid. The magnetic field value at the index \( i = -2 \) is obtained by linear interpolation in time and space from the magnetic field values at \( i = -2.5 \) and \( i = -1.5 \).

We note that the discrete wave impedance \( Z_0 \) is not only a function of spatial discretization and wavelength, but also complex. This behavior is shown in Figure 2.4. The real part \( \Re\{.\} \) of \( Z_0 \) is approximately equal to the normalized free-space intrinsic wave impedance in the very well-resolved region (below \( h/\lambda < 0.05 \)) and the imaginary part \( \Im\{.\} \) of \( Z_0 \) is zero; however, as the wavelength moves into the less resolved domain, \( \Re\{Z_0\} \) approaches zero while \( \Im\{Z_0\} \) becomes non-zero.
Figure 2.4: Discrete wave impedance $Z_0$ in the fine grid; real part is $\text{Re}\{\cdot\}$, imaginary part is $\text{Im}\{\cdot\}$, analytic is $Z_{0,A}$, and computed is $Z_{0,M}$. 
2.4 Late-Time Stability of the Sub-Grid

Consider the transmission line (TL) equivalent model of the FDTD grid, shown in Figure 2.5. The figure depicts the region in the vicinity of a fine-coarse transition, with the fine region located on left and coarse region located on right.

![Diagram of FDTD grid and transmission line equivalent model](image)

Figure 2.5: Top: FDTD grid in fine-coarse transition. Bottom: Transmission line (TL) equivalent diagram. With wave propagation from fine grid to coarse grid, the coarse TL on right acts as load to fine TL on left. The fine TL has a discrete wave impedance $Z_{0F}$ (2.25). The coarse TL has a discrete wave impedance $Z_{0C}$ (2.26). The reflection coefficient at the fine-coarse interface is $R_0$ (2.13).

Based on time-average power considerations for such a transmission line system, the following passivity condition is derived in [33] and is given by

$$\left(1 - |R_0|^2 - 2\frac{\Im\{Z_{0F}\}}{\Re\{Z_{0F}\}} \Im\{R_0\}\right) \geq 0$$  \hspace{1cm} (2.28)

where, in reference to Figure 2.5, $Z_{0F}$ as given by (2.25) is the discrete wave impedance of the fine TL, $R_0$ as given by (2.13) is the reflection coefficient at the fine-coarse transition, the operator symbol $\Re\{\cdot\}$ denotes the real part,
and the operator symbol $\Im\{\cdot\}$ denotes the imaginary part.

The left-hand side of (2.28) is plotted in Figure 2.6. As can be seen, the stable region for the above sub-grid system is given by $h/\lambda \leq 1/\pi$. One way to ensure late-time stability, is to mitigate the occurrence (on the grids) of waves with wavelengths less than $\pi h$. To accomplish this, we resort to spatial filters discussed in the next section.

![Figure 2.6: Plot of $\chi$ vs. $h/\lambda$, where $\chi = 1 - |R_0|^2 - 2\Re\{Z_{oF}\} \Im\{R_0\}$. The passivity condition (2.28) requires that $\chi \geq 0$.](image)

### 2.5 Spatial Filter Theory

Given the results of the reflection analysis in Section 2.2 and results of the late-time stability analysis in Section 2.4, we declare two objectives: (a) mitigate waves with wavelengths that may cause late-time instability in the region $h/\lambda > 1/\pi$, and (b) mitigate waves with wavelengths that experience $|R_0| \geq \alpha$ on the grid and cause noise waves due to spurious reflections, where $\alpha \in (0, 1]$ is an arbitrarily specified level. In this section, the application of
isotropic spatial filters is proposed as a means to address both objectives. First, we develop the theory for 1D spatial filters, and then extend the 1D results to 2D and 3D.

2.5.1 1D spatial filter

If one follows the traditional finite impulse response (FIR) digital filter design procedure [23–25] which uses an ideal impulse response together with smoothing functions (such as Hamming or Kaiser windows to suppress the well-known Gibb’s phenomenon), one soon concludes that such an approach is not optimized to address our two stated objectives, discussed above. In light of this, use is made of the design criteria discussed in [34] to specify our spatial filter; these are repeated here for completeness of discussion. We note that these criteria may be changed as necessary to optimize filter performance for different applications.

We define the spatial frequency response of the filter

\[
F(z) = \sum_{n=0}^{N} \frac{1}{2} a_n (z^{-n} + z^n) = \sum_{n=0}^{N} a_n \cos (kh)
\]

(2.29)

where \(z = e^{kh}\), \(k\) is the propagation constant, \(a_n\) is the \(n^{th}\) Fourier coefficient, \(N\) is the integer maximum number of samples (also the filter order), and \(n\) is an integer. In the above equation, \(h\) is understood to represent the coarsest grid size relevant to the application of interest.

1. The filter must fully pass the zero frequency component of the signal entirely (i.e., \(F(z)\big|_{k=0} = 1\)).

2. The filter must fully eliminate all signal components with wavelength \(\lambda = 2h\) (i.e., \(F(z)\big|_{k=\pi/h} = 0\)).

3. The filter must have a frequency response as flat as possible near \(k = 0\) (i.e., \(\frac{d^r}{dk^r} F(z)\big|_{k=0} ; r = 1, 2, 3, ..., N\)).

As such, instead of the traditional FIR digital filter design procedure, we use the aforementioned design criteria to obtain a system of linear algebraic equations, the solution of which are the Fourier coefficients \(a_n\) in (2.29).
Once the unknown Fourier coefficients are found, to apply the filter to the FDTD grid at cell location $i$ with field value $\phi[i]$, we multiply the spatial frequency response (2.29) by the spatial frequency domain value of the field $\Phi[z]$, at that cell. The new filtered value of the cell is $\phi_F[i]$ and its Fourier series is $\Phi_F[z]$.

$$\Phi_F[z] = F(z)\Phi[z]$$

(2.30)

Given the frequency shifting property $\Phi[z]\xi_{\pm i_0} = \phi[i \mp i_0]$ of discrete LTI systems [35], and in light of (2.29) and (2.30), we obtain the inverse Fourier series of (2.30) which provides the filtered time-domain value at cell location $i$.

$$\phi_F[i] = a_0\phi[i] + \sum_{n=1}^{N} \frac{1}{2}a_n(\phi[i-n] + \phi[i+n])$$

(2.31)

The spatial frequency response of the 1st order 1D filter is shown in Figure 2.7.

2.5.2 2D spatial filter

Using the McClellan transformation technique [26], we expand the 1D filter (2.29) into a 2D filter. Since $n$ is an integer, we can express $\cos(knh)$ as an $n^{th}$ order Chebyshev polynomial with constant coefficients [25]

$$\cos(knh) = c_0 + c_1w + c_2w^2 + ... + c_nw^n$$

(2.32)

where $c_n$ is the constant coefficient and $w = \cos(kh)$.

Using (2.32), we rewrite (2.29)

$$F_{M1}(z) = \sum_{n=0}^{N} a_n \cos^n(kh)$$

(2.33)

For the 2D spatial filter, we use the McClellan transformation [26] to map a single spatial axis $\theta$ to two orthogonal spatial axes $\theta_1$ and $\theta_2$.

$$\cos(\theta) = A \cos(\theta_1) + B \cos(\theta_2) + C \cos(\theta_1) \cos(\theta_2) + D$$

(2.34)

where $A, B, C, D$ are real constants, and, for a circularly symmetric contour,
Figure 2.7: Magnitude of spatial frequency response for a 1D 1st order filter, where $\lambda = 2\pi/k$. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)
it is \( A = B = C = -D = 1/2 \).

Using transformation (2.34) in (2.33), we obtain

\[
F_{M2}(z_1, z_2) = \sum_{n=0}^{N} a_n (A \cos(k_1 h) + B \cos(k_2 h) + C \cos(k_1 h) \cos(k_2 h) + D)^n
\]  \hspace{1cm} (2.35)

where \( z_1 = e^{j k_1 h} \) and \( z_2 = e^{j k_2 h} \).

To obtain the 2D FDTD discrete implementation of the above, we reduce \( \cos^n(kh) \) to a linear combination of \( \cos(knh) \) terms, and replace \( a_n \) with the new constant coefficient \( a'_{n_1,n_2} \). Thus (2.35) can be written as

\[
F'_{M2}(z_1, z_2) = \sum_{n_1=0}^{N} \sum_{n_2=0}^{N} a'_{n_1,n_2} \cos(k_1 n_1 h) \cos(k_2 n_2 h)
\]  \hspace{1cm} (2.36)

Once the spatial filter is obtained, to apply it to the 2D FDTD grid at cell location \( \{i_1, i_2\} \) with field value \( \phi[i_1, i_2] \), we multiply the spatial frequency response (2.36) by the spatial frequency-domain value of the field \( \Phi[z_1, z_2] \), at that cell. The new filtered value of the cell is \( \phi_F[i_1, i_2] \) and its Fourier series is \( \Phi_F[z_1, z_2] \),

\[
\Phi_F[z_1, z_2] = F'_{M2}(z_1, z_2) \Phi[z_1, z_2]
\]  \hspace{1cm} (2.37)

The filtered discrete value may be obtained through the inverse Fourier series of (2.37), in a similar fashion as for the 1D case (2.31),

\[
\phi_F[i_1, i_2] = a'_{0,0} \phi[i_1, i_2] + \sum_{n_1=1}^{N} \sum_{n_2=1}^{N} \frac{1}{2} a'_{n_1,n_2} (\phi[i_1 - n_1, i_2 - n_2] + \phi[i_1 + n_1, i_2 + n_2])
\]  \hspace{1cm} (2.38)

The spatial frequency response of the 1st order 2D filter is shown in Figure 2.8.
Figure 2.8: Magnitude of spatial frequency response for a 2D 1st order filter, where $\lambda_1 = 2\pi/k_1$, $\lambda_2 = 2\pi/k_2$. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)
2.5.3 3D spatial filter

As in the 2D case, the development of the 3D spatial filter starts with the 1D design (2.29), but instead of applying the McClellan transformation [26] once, we apply it twice to map a single spatial axis $\theta$ to three orthogonal spatial axes $\theta_1$, $\theta_2$, and $\theta_3$.

\[
\cos(\theta) = (A + CD) \cos(\theta_1) + AB \cos(\theta_2) + B^2 \cos(\theta_3) + AC \cos(\theta_1) \cos(\theta_2) + BC \cos(\theta_1) \cos(\theta_3) + BC \cos(\theta_2) \cos(\theta_3) + C^2 \cos(\theta_1) \cos(\theta_2) \cos(\theta_3) + D + BD \tag{2.39}
\]

where $A, B, C, D$ are real constants, and for a spherically symmetric surface it is $A = B = C = -D = 1/2$.

The 3D frequency response is

\[
F'_{M3}(z_1, z_2, z_3) = \sum_{n_1=0}^{N} \sum_{n_2=0}^{N} \sum_{n_3=0}^{N} (a'_{n_1,n_2,n_3} \cos(k_1 n_1 h) \cos(k_2 n_2 h) \cos(k_3 n_3 h)) \tag{2.40}
\]

where $z_1 = e^{jk_1 h}$, $z_2 = e^{jk_2 h}$, $z_3 = e^{jk_3 h}$, and $a'_{n_1,n_2,n_3}$ is the 3D Fourier coefficient.

The 3D frequency-domain field value is

\[
\Phi_F[z_1, z_2, z_3] = F'_{M3}(z_1, z_2, z_3)\Phi[z_1, z_2, z_3] \tag{2.41}
\]

And finally, the 3D time-stepping formulation (convolution) is

\[
\phi_F[i_1, i_2, i_3] = a'_{0,0,0} \phi[i_1, i_2, i_3] + \sum_{n_1=1}^{N} \sum_{n_2=1}^{N} \sum_{n_3=1}^{N} \left( \frac{1}{2} a'_{n_1,n_2,n_3} (\phi[i_1 - n_1, i_2 - n_2, i_3 - n_3] + \phi[i_1 + n_1, i_2 + n_2, i_3 + n_3]) \right) \tag{2.42}
\]
The spatial frequency response of the 1st order 3D filter is shown in Figure 2.9 for surface contours plotted at five distinct magnitudes of $|F(z_1, z_2, z_3)| = \{0.05, 0.25, 0.5, 0.75, 0.95\}$.

A detailed geometric perspective of the 1st order 3D filter’s operation is presented in Appendix B.

Figure 2.9: Magnitude of spatial frequency response for a 3D 1st order filter. The surface contours are for $|F(z_1, z_2, z_3)| = \{0.05, 0.25, 0.5, 0.75, 0.95\}$, where $\lambda_1 = 2\pi/k_1, \lambda_2 = 2\pi/k_2, \lambda_3 = 2\pi/k_3$. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)

2.5.4 Filter order and frequency of its application

By using the expression for the 1D spatial frequency response (2.29) and given the circular symmetry in 2D and spherical symmetry in 3D, we can easily solve for the spatial wavelength $\lambda_{knee}$ of a given filter order. The corresponding temporal angular knee frequency is computed as $\omega_{knee} = v_{ph}(2\pi/\lambda_{knee})$, where $v_{ph}$ is the wave phase velocity in the medium. If a smaller $\lambda_{knee}$ is
desired, a higher order filter may be used.

Alternatively, we note that application of the filter \( p \) consecutive times during one update of the transient fields is equivalent to raising the magnitude of frequency response of the filter to the exponent \( p \). Thus, if a larger \( \lambda_{\text{knee}} \) is desired, we can select the smallest filter order with the closest \( \lambda_{\text{knee}} \) and raise its magnitude to the power \( p \), set the resulting expression equal to the desired magnitude at \( \lambda_{\text{knee}} \) and solve for \( p \). For example, for a 3 dB drop in magnitude at \( \lambda_{\text{knee}} \) we solve the following equation for \( p \):

\[
|\Phi_{F}(z)|^p = 10^{-3/20}|\Phi_{F}(z)|_{k=0}
\tag{2.43}
\]

Appendix A provides a sample table of \( h/\lambda_{\text{knee}} \) vs. \( p \) for 1\textsuperscript{st} through 5\textsuperscript{th} order spatial filters.

Once the order of the filter has been decided, the power \( p \) obtained using (2.43) serves as the maximum number of times the filter should be applied throughout the transient simulation without resulting in attenuation of the temporal frequency content of the response beyond acceptable levels. Clearly, application of the filter should start after wave transmissions through grid interfaces have commenced. Furthermore, given the finite stencil of the filter, its selective use at positions where such interfaces are encountered and at times appropriate for each position seems most appropriate.

### 2.6 Numerical Studies

To investigate the effectiveness of the proposed filters, we consider their application to the FDTD modeling of a two-dimensional (2D) and a three-dimensional (3D) cavity resonator. For the 2D case, a square box with perfectly conducting electric walls is excited by an infinitely long electric wire current source; hence, for the case of a \( z \)-directed line source, a TM\(^z \), 2D simulation is performed. For the 3D case, the resonator is a cube with perfectly conducting electric walls excited by a \( z \)-directed, half-wavelength electric dipole. In both cases, a non-uniform FDTD grid is used, resulting from the utilization of a 1:3 fine:coarse sub-gridding along \( x \) [32]. Information about the physical size of the resonators and the non-uniform grid used is provided below.
The excitation waveform is taken to be a Gaussian pulse. The Gaussian pulse is chosen to have a frequency bandwidth $f_{BW} \approx 3.0 \text{ GHz}$, and the fine grid is setup for a maximum frequency $f_{\text{max}} = 3.0 \text{ GHz}$ with spatial discretization $h = \lambda_{\text{min}}/20$, where $\lambda_{\text{min}} = v_{\text{ph}}/f_{\text{max}}$; we note that these choices for $h$, $f_{BW}$, and $f_{\text{max}}$ bring the $-3 \text{ dB}$ point of the Gaussian bandwidth to $h/\lambda \approx 0.05$ in the FDTD grid. This is to ensure good grid resolution to capture the signal’s power spectral density above the $-3 \text{ dB}$ point, while at the same time allowing sufficient energy in the low-resolution wavelength regime where the signal can still experience a spurious reflection value $|R_0| \neq 0$.

We define $\lambda_s$ as the wavelength at $f_{BW}$. The side of the 2D square resonator and the 3D cube resonator is $30\lambda_s$. The non-uniform grid along $x$ utilizes a grid of size $h$ over half of the resonator domain and a coarse grid of size $3h$ over the other half. Uniform grids of size $h$ are used along the remaining axes. For the 2D case the source is located in the fine grid at half-distance between PEC on left and fine-coarse transition on right, and the transient electric field is recorded at half-distance between source and fine-coarse transition on variable-length axis. For the 3D case, the half-wavelength dipole is placed along the $z$-axis in the fine grid, at half-distance along the uniform grid axes and half-distance between PEC and fine-coarse transition on variable-length axis, while the $z$-component of the electric field is recorded at half-distance between source and fine-coarse transition on variable-length axis.

The response is computed for the following three cases:

- Using a uniform grid of size $h$ along $x$. This is the reference solution and is referred to as $\text{Uniform}$ in the following.

- Using the non-uniform grid along $x$ as described above without any filtering of the response. This is referred to as $\text{SubUnFil}$.

- Using the non-uniform grid along $x$ as described above with filtering of the response. This is referred to as $\text{SubFil}$.

The idea is to let the signal from a source in the fine grid arrive at the fine-coarse interface, and then, as the spurious reflections propagate back into the fine grid, intercept this noise wave in a pre-defined region of the fine grid and eliminate it by application of spatial filters for a finite time and until noise is attenuated to an acceptable level. Given that in any FDTD simulation, the material properties of the grid are known in advance, we can
calculate the propagation velocity in the medium, and from it the flight time of signals. Using the signal flight times, and knowledge of location of the sub-grid interface, it is possible to develop a filter application schedule at specified regions of the fine grid. Alternatively, it is possible to use multi-resolution signal decomposition techniques based on wavelet transforms \cite{36, 37} to quickly identify locations within the grid that require filter application. Below, we implement the former technique and give a demonstration in 2D and 3D simulations.

The spurious reflections of \( R_0 \geq 1.0 \) begin to occur at \( k_0 h = 2/3 \). For this example, let us specify our attenuation requirement of the noise waves to be \(-3\) dB at \( h/\lambda \approx 0.015 \). Then, according to Table A.1, the first-order spatial filter is applied approximately 140 times along the fine-coarse grid interface (plus a 20-cell padding, equivalent to one \( \lambda_s \)) on the fine side, at increments of \( \tau = 1 \), at time steps \( \tau = 240 - 380 \). The filter is applied to both the E-field and H-field components, according to (2.38) for 2D simulation or (2.42) for 3D simulation.

We run both uniform and sub-gridded 2D \( \text{TM} \) FDTD simulations, and plot the electric field data at the fine-coarse interface from both simulations, in Figure 2.10. It can be seen that the electric field begins to experience spurious reflections starting at approximately \( \tau = 240 \) until \( \tau \approx 380 \), before the first reflection from left PEC arrives at the interface at \( \tau \approx 440 \); we would like to eliminate this noise. The 2D simulation results are shown in Figure 2.11. In the 3D case, we start filtering at \( \tau = 220 \) until \( \tau = 380 \). The 3D simulation results are shown in Figure 2.12.

2.7 Summary

For the standard Yee update algorithm with 1:3 sub-gridding, through a quantitative analysis of the update equations at the fine-coarse interface node, we derived an analytic expression for the reflection coefficient \( R_0 \) at the interface node, and correlated against computed results in 1D FDTD.

Here, the 1:3 sub-gridding ratio is chosen because 1:3 ratio (or 1:s ratio, where s is an odd integer) provides the means for sequential nesting of sub-grids within sub-grids quite efficiently; thereby, affecting transition from a coarse grid to a much finer grid.
Figure 2.10: Magnitude of z-component of the electric field $E_z (V/m)$ vs. time-step $\tau$ at the fine-coarse interface. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)
Figure 2.11: Magnitude of z-component of the electric field $E_z$ (V/m) vs. time-step $\tau$ for a 2D 1st order filter applied at increments of $\tau = 1$. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)
Figure 2.12: Magnitude of $z$-component of the electric field $E_z (V/m)$ vs. time-step $\tau$ for a 3D 1st order filter applied at increments of $\tau = 1$. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)
We developed the theory of spatial filter operators for 1D, 2D, and 3D by relying on signal/image processing concepts and utilizing spatial transformations to map from 1D to 2D and 3D. Along the way, we demonstrated a simple procedure for a-priori determination of the filter order and application time interval. The results showed that the methodology is effective in suppression of noise waves from fine-coarse grid interface for both 2D and 3D sub-gridded FDTD simulations.

It is clear that even at high spatial sampling resolution \( N_\lambda = 20 \) (with \( h = \lambda_{\text{min}}/N_\lambda \)) there exist spurious reflections which will not go away for a broad-band source, without significant increase of the grid resolution; thus, the 2D and 3D spatial filters offer a way to attenuate such noise waves at minimal cost. In this case, the cost associated with filtering is limited to a relatively small portion of the grid region (one \( \lambda_s \) wide) over a finite portion of the overall simulation time (140 filter operations in 2D and 160 filter operations in 3D, with each filter operation being near the same order as a cell update based on first order central difference), while requiring no additional computer memory. In contrast, a \( 3 \times \) increase in coarse grid sampling resolution with no sub-gridding and filtering would have increased the memory requirements by \( 9 \times \) in 2D and \( 27 \times \) in 3D, while tripling the number of required time-stepping updates in 2D and 3D for the same amount of simulated time.
3.1 Literature Review

As described in the novel work by [1–3] on model order reduction and system level electromagnetic simulations, the electromagnetic field solvers are not computationally optimized to address system level modeling. This is primarily due to the fact that the use of finite-methods based solvers (e.g., finite difference, finite elements, finite volume, etc.) results in a large number of degrees of freedom in the electromagnetic model, which hinders the computational cost of the simulation. As a result, electromagnetic modeling of realistic systems through finite methods often becomes impractical without some sort of domain decomposition or a divide-and-conquer approach that takes advantage of the success of such methods in modeling components of the system. Focusing on a discrete model for one of the components of a complex system, a state-space system of order in the tens or hundreds of thousands is quite common. This means the system transfer function matrix that operates on the input state variables (system excitation) to compute the values of the output state variables (system response) is of dimension $O(10^4 - 10^5)$. However, during any specific simulation only a few of the eigen-states of the system actually influence the system response, and as such, only these eigenstates are necessary to accurately model the system behavior with sufficient engineering accuracy. Therefore, by reducing the order of the system transfer function matrix about those frequencies of interest, we increase the computational efficiency while maintaining sufficient engineering accuracy. The basic idea behind the macro-model is the development of an abstraction layer that encapsulates the fine features of interest and represents its electromagnetic performance through a properly designed impedance (or admittance) transfer function that takes the tangential electric (or magnetic) field components
as input and produces tangential magnetic (or electric) field components as output.

In [38], the concept of model order reduction through use of Padé moment-
matching is utilized toward simulation of dispersive multi-conductor trans-
mission lines. In [39], model order reduction on S-domain methods for
time and frequency simulations is illustrated. In [40], a methodology for
fast broad-band simulation of passive wave-guiding structures is presented.
The methodology utilizes the FDTD method with a non-symmetric Lanczos
eigenvaule algorithm to obtain a reduced-order model of the electromagnetic
system response over the frequency range of interest. In [41] the idea of
macro-model is implemented in finite element method simulations. In [42]
the automatic generation of sub-domain FDTD models using model order
reduction is described, and subsequently in [43] implementation of MOR on
FDTD sub-cells is demonstrated. Additional discussions of various aspects
of MOR techniques are provided in [6,44–47].

There are various algorithms to obtain the reduced order model; one such
algorithm is ENOR [5], which gives a model order reduction procedure with
adaptive error control, for symmetric (reciprocal) RLC networks, using or-
thogonal projection, moment matching (expansion about the frequency of
interest), and Cholesky factorization (for computationally efficient solution
of matrix equations), to produce passive reciprocal reduced order models in
the form a symmetric positive definite (stable) system. This method for
MOR is used in [4] in FDTD simulations to reduce a full-order finite differ-
ence system transfer function (in the Laplace frequency domain) to a reduced
order approximate system.

The work in [48] is a formalization of the sub-gridding technique using
matrix notation, combined with MOR techniques of ENOR. The main goal
in [49] is to implement the macro-model into the difference operators without
introducing frequency dependence. This is so that the macro-model can be
applied to FDFD analysis of eigen-mode problems, such as calculation of
resonant frequencies of a cavity. This task is accomplished by applying the
orthogonal projection to the difference operators instead of to the matrix
transfer function.

The work in [50] outlines the algorithm for repeatedly nesting macro-
models and combining macro-models with the fast frequency sweep. The
main contribution here is that the matrices contain blocks of sub-matrices to
reflect the multiple transitions from main grid to multiple layers of fine grids. The work in [48] presents a simple way to reduce the spurious reflections due to sub-gridding to near -80 dB, about 40 dB lower than the method by [21], while not being as rigorous. The work in [51] is mainly a summary of previous work in [48–50] which are primarily demonstrated in two-dimensional space. In [51] the demonstrations are given in three-dimensional space. The work in [52] proposes that for the combined FDTD-macromodel scheme to be stable, the coupling between the fine-coarse grid has to be implemented properly; that is, by ensuring that the norm of the interpolation matrix satisfies certain conditions. Finally, the work in [53] provides an overview to the overall procedure for implementation of macro-models.

3.2 Formulation for Full Order Model

There are two possible ways to approach the development of the macro-model for a portion of a structure in an FDTD grid. One such way is to use the electric field as excitation at the boundary of the macro-model and input to the macro-model, then extract the magnetic field as response at the inner perimeter of the macro-model and output of the macro-model; this formulation leads to the impedance transfer function (ITF) matrix [48,48–53]. The disadvantage of this method is that electric loss cannot be modeled easily in the macro-model, due to the need to invert the non-square Curl-$E$ operator matrix; thus, the impedance transfer function is not ideal for capturing the most general case with lossy material.

Alternatively, we can use the magnetic field as excitation at the boundary of the macro-model and input to the macro-model, then extract the electric field as response at the inner perimeter of the macro-model and output of the macro-model; this leads to the admittance transfer function (ATF) matrix, which readily facilitates modeling of electrically lossy material in the macro-model.

The more general admittance transfer function which comprehends lossy material is the focus of our work; as such, it is used for numerical studies in this chapter, and provides the foundation for the stochastic macro-model in the next chapter. For completeness and to highlight the differences between ATF and ITF, the formulation for the impedance transfer function is provided
in Appendix C.

In order to generate a macro-model for a portion of the FDTD grid, we start with the time-harmonic frequency phasor form of source-free Maxwell equations, where the time-harmonic term $e^{j\omega t}$ is suppressed.

$$\nabla \times \mathbf{E} = -j\omega \mu \mathbf{H} \quad (3.1)$$

$$\nabla \times \mathbf{H} = j\omega \epsilon \mathbf{E} + \sigma \mathbf{E} \quad (3.2)$$

where $j = \sqrt{-1}$, $\omega$ is the angular frequency, $\mathbf{E}$ is the electric field intensity vector, $\mathbf{H}$ is the magnetic field intensity vector, $\sigma$ is the material conductivity tensor, $\mu$ is the material permeability tensor, and $\epsilon$ is the material permittivity tensor.

For the macro-model implemented as an admittance transfer function, equations (3.1)-(3.2) can be written as a finite-difference based semi-discretized system in the Laplace (s-domain) in matrix form as follows:

$$D_E \mathbf{e} = -s P_\mu \mathbf{h} \quad (3.3)$$

$$D_H \mathbf{h} + Q_h \mathbf{h}_b = s P_\epsilon \mathbf{e} + P_\sigma \mathbf{e} \quad (3.4)$$

where the Laplace variable $s$ is the complex frequency $s = \alpha + j\omega$, $\alpha$ is the real part of frequency, $\omega$ is the imaginary part of frequency, $D_E$ is the spatial Curl-$\mathbf{E}$ operator matrix, $D_H$ is the spatial Curl-$\mathbf{H}$ operator matrix, $\mathbf{e}$ is the electric field vector inside the macro-model, $\mathbf{h}_b$ is the magnetic field vector containing boundary conditions on the perimeter of the macro-model, $Q_h$ is the selector matrix for magnetic field at boundary, $\mathbf{h}$ is the magnetic field vector inside and on the perimeter of the macro-model, and the diagonal matrices $P_\epsilon$, $P_\mu$, and $P_\sigma$ represent material permittivity, permeability, and conductivity, respectively, as functions of position inside the macro-model.

With the above formulation, we have

$$D_E = D_H^T \quad (3.5)$$

where the symbol $^T$ denotes the matrix transpose operator.

And in state-space form it is
\[
\begin{bmatrix}
D_E & 0 \\
P_\sigma & -D_H
\end{bmatrix}
\begin{bmatrix}
e \\
h
\end{bmatrix}
+ \begin{bmatrix}
0 \\
Q_h
\end{bmatrix}
h_b + s \begin{bmatrix}
0 & P_\mu \\
P_\epsilon & 0
\end{bmatrix}
\begin{bmatrix}
e \\
h
\end{bmatrix}
= \begin{bmatrix}
0 \\
0
\end{bmatrix}
\] (3.6)

The dimensions for each tensor are as follows:

- \( h \): \( N \times 1 \)
- \( h_b \): \( n \times 1 \)
- \( Q_h \): \( M \times n \)
- \( e \): \( M \times 1 \)
- \( D_E \): \( N \times M \)
- \( D_H \): \( M \times N \)
- \( P_\epsilon \): \( M \times M \)
- \( P_\sigma \): \( M \times M \)
- \( P_\mu \): \( N \times N \)

where \( M, N, n \) are integers, determined by the size of the macro-model.

Solving (3.3) for \( h \), we obtain

\[
h = -\frac{1}{s}P_\mu^{-1}D_E e
\] (3.7)

Substitution of (3.7) in (3.4) gives the relation

\[
Ye = Q_h h_b
\] (3.8)

where the admittance transfer function matrix \( Y \) is

\[
Y = \frac{1}{s}D_H P_\mu^{-1}D_E + P_\sigma + sP_\epsilon
\] (3.9)

From (3.8) \( e \) is simply obtained by

\[
e = Y^{-1}Q_h h_b
\] (3.10)

### 3.2.1 Time-stepping formulation

The Laplace operator \( s \) can be written in time domain as

\[
s \Leftrightarrow \frac{d}{dt}
\] (3.11)

Similarly, the Laplace operator \( s^2 \) can be written in time domain as
We assume that the material constitutive parameters belong to the class of non-dispersive (frequency-independent) materials; thus the matrices \( \{P_\epsilon, P_\mu, P_\sigma\} \) are independent of the complex frequency \( s \), which implies they are also independent of time. Therefore, the only time-dependent quantities are \( h_\sigma \) and \( e \). Then, using (3.11),(3.12) we may transform (3.8) to its time-domain equivalent

\[
D_H P_\mu^{-1} D_E e + P_\sigma \frac{d}{dt} e + P_\epsilon \frac{d^2}{dt^2} e = Q_h \frac{d}{dt} h_\sigma
\]  

(3.13)

With a central-difference based time-derivative operator, operating on a generic function of time \( f[t] \), we have

\[
\frac{d}{dt} f[t] = \frac{f[t + \Delta t] - f[t - \Delta t]}{2\Delta t}
\]  

(3.14)

\[
\frac{d^2}{dt^2} f[t] = \frac{f[t + \Delta t] - 2f[t] + f[t - \Delta t]}{\Delta t^2}
\]  

(3.15)

where \( \Delta t \) is the temporal discretization.

Using (3.14),(3.15), we expand the time-derivatives in (3.13) to obtain the discrete time-domain relation

\[
D_H P_\mu^{-1} D_E e[n] + P_\sigma \frac{e[n + 1/2] - e[n - 1/2]}{\Delta t} + P_\epsilon \frac{e[n + 1] - 2e[n] + e[n - 1]}{\Delta t^2} = Q_h \frac{h_\sigma[n + 1/2] - h_\sigma[n - 1/2]}{\Delta t}
\]  

(3.16)

where \( n \) is the discrete time variable.

Solving for the electric field in the future time-step at \( n + 1 \), we obtain the following time-stepping formulation:
\[ e[n+1] = P_e^{-1}(-(\Delta t)^2 D_H P_\mu^{-1} D_E e[n] \\
- (\Delta t) P_\sigma (e[n + 1/2] - e[n - 1/2]) \\
+ P_e (2e[n] - e[n - 1]) \\
+ (\Delta t) Q_h (h_b[n + 1/2] - h_b[n - 1/2])) \] (3.17)

We note that the above time-stepping requires the value of \( e \) at time steps \( n + 1/2 \) and \( n - 1/2 \); however, since the electric field is not computed at these half-step increments, we approximate them by temporal interpolation as follows:

\[ e[n + 1/2] = \frac{e[n] + e[n + 1]}{2} \] (3.18)
\[ e[n - 1/2] = \frac{e[n] + e[n - 1]}{2} \] (3.19)

Finally, substitution of (3.18)-(3.19) into (3.17) gives

\[ e[n + 1] = \nu^{-1} \cdot \left( \frac{\Delta t}{2} P_\sigma e[n - 1] \\
- (\Delta t)^2 D_H P_\mu^{-1} D_E e[n] + P_e (2e[n] - e[n - 1]) \\
+ (\Delta t) Q_h (h_b[n + 1/2] - h_b[n - 1/2]) \right) \] (3.20)

where \( \nu = (P_e + \frac{\Delta t}{2} P_\sigma) \) is the sum of two diagonal matrices; thus, its inversion is trivial.

This completes the derivation of the full-order ATF system in terms of matrix equations. Next, we discuss an appropriate model order reduction scheme, to be applied to the above full-order system.

### 3.3 Model Order Reduction

In order to improve the computational efficiency of the sub-gridded model, we utilize model order reduction (MOR). In essence, MOR projects the column-space of the full-order system to a compact (i.e. reduced-order) sub-space; this is accomplished by finding the strong orthogonal axes inside the full-
order space and placing them in a sub-space projection matrix $V$.

Various MOR techniques may be used [2–7] to decrease the degrees of freedom of the full-order system while maintaining sufficient engineering accuracy. The MOR algorithm of ENOR [5] is convenient because it uses the fast Cholesky factorization for computationally efficient solution of matrix equations to produce a symmetric reduced order model while providing adaptive error control to derive the projection matrix. The orthogonal projection operation is essentially the Galerkin process, which takes a (differential or integral) system of equations with infinite degrees of freedom and transforms it to a system of equations with finite degrees of freedom. The projection matrix is obtained by moment matching which involves expansion about the frequency of interest, and it is applied to the full-order system to produce passive reciprocal reduced order models in the form of a symmetric positive semi-definite system transfer function matrix, so long as the original system transfer function matrix is also positive semi-definite. The positive semi-definite nature of the reduced order system ensures passivity, and therefore stability, of the reduced order model.

Both [5] and [6] used Cholesky factorization in the MOR algorithm for its utility in speeding up the solution of the projection matrix by providing upper and lower triangular matrices for use in back substitution; this choice eliminates the need for computationally costly row-echelon operations. The Cholesky factorization becomes especially important for reduction of very large matrices.

It is worth noting that Cholesky factorization works on positive definite matrices only. For the matrix equation to be Cholesky factorizable, an additional requirement is imposed on the choice of the expansion frequency $s_0$; that is, $s_0$ must be a real frequency if Cholesky factorization is indeed used.

Following a similar procedure to [5], we define the matrix quantities $C \in \mathbb{R}^{M \times M}$, $G \in \mathbb{R}^{M \times M}$, $B \in \mathbb{R}^{M \times n}$, $J \in \mathbb{R}^{n \times n}$, $X \in \mathbb{R}^{M \times n}$, and $\Gamma \in \mathbb{R}^{M \times M}$, where $M, n$ are integers, as follows:

$$C = P_c \quad (3.21)$$

$$G = P_\sigma \quad (3.22)$$
\[ \Gamma = D_H P_{\mu}^{-1} D_E \]  

(3.23)

\[ B = Q_h \]  

(3.24)

Using (3.21) - (3.23), we may re-write the admittance transfer function matrix (3.9) as

\[ Y = \left( C_s + G + \frac{1}{s} \Gamma \right) \]  

(3.25)

The total system in Laplace (s-domain) is given by

\[ \left( C_s + G + \frac{1}{s} \Gamma \right) X[s] = BJ[s] \]  

(3.26)

We set \( s = s_0(1 - z) \), where the complex variable \( z = \frac{-1}{s_0}(s - s_0) \). Also, we define the auxiliary variable

\[ Y'[z] = \frac{X[z]}{1 - z} \]  

(3.27)

The expansion frequency can be chosen along any path on the complex Laplace plane, and was chosen to be on the real axis in [5,6]; however, because ENOR requires Cholesky factorization, and Cholesky factorization requires a positive-definite matrix, which in turn must comprise all real components, we choose to expand about a real frequency \( s_0 = f_0 \) Hz. Further discussion on expansion about real vs. imaginary frequency may be found at [44–47].

Next, we expand \( X[z], Y'[z], J[z] \) in powers of \( z \) about the frequency \( s_0 \), and substitute these expansions into (3.26) and (3.27), equate coefficients of same powers of \( z \), and after some algebraic manipulations obtain the following recurrence relation:

\[ \left( C_{s_0} + G + \frac{1}{s_0} \Gamma \right) X_k = C_{s_0}X_{k-1} - \frac{1}{s_0} \Gamma Y'_{k-1} + Q_h J_k \]  

(3.28)

where the desired number of iterations (i.e., number of moments about \( s_0 \)) \( k \) is an integer, the relative tolerance \( tol_{rel} \) is a real number signifying the eigenvalue noise floor of the system, and it is
The yet unknown $X_k$ are proportional to the (block) moments of the electric field vector (i.e. system response) when expanded about the frequency $s_0$.

We set the $h$-field source (i.e. system excitation) as follows:

$$J_k = \begin{cases} 
I_{n \times n} & \text{if } k = 0, \\
0 & \text{if } k \neq 0,
\end{cases} \quad (3.29)$$

and solve (3.28) for as many $k$-terms as desired.

The choice of setting $J_{(k=0)} = I_{n \times n}$, where $I_{n \times n}$ is the $n \times n$ identity matrix, is equivalent to having a discrete impulse (magnetic) source at each excitation node in $Q_h h_b$, resulting in the discrete impulse response of the system.

Once the solutions to $X_k$ are obtained, we form $V = [X_0, X_1, ..., X_q]$, where the projection matrix $V \in \mathbb{R}^{M \times m}$ is comprised of the first $q$ block moments, and the integer $m \ll M$ is the order of reduction.

We propose that the model order reduction technique of ENOR produces an approximation of the full-order Maxwell’s state-space system, which yields sufficient accuracy in representing fields of a broad-band nature. What constitutes “sufficient accuracy” is decided by the specific application and its given criteria for accuracy. The previous work in the literature shows that a finite set of dominant eigenvectors obtains a good-enough approximation of transient response of various systems (e.g., waveguides). ENOR achieves this by moment-matching (about $s_0$) of the system transfer function, while employing an adaptive error control scheme to decide what minimal set of modes and moments is necessary to minimize the error between the time response of projected reduced-order and full-order models. ENOR provides the mechanism for this adaptive error control through parameters of relative tolerance $tol_{rel}$ and maximum number of iterations $k_{iter}$.

The argument $tol_{rel}$ is used to admit into the projection matrix only those eigenvectors associated with eigenvalues above the noise floor (a level be-
low which the associated eigenvector is deemed to have insignificant relative
correlation to the system response). The argument $k_{\text{iter}}$ is used to decide
the maximum number of moments about the expansion frequency $s_0$ that
are necessary to represent the system with sufficient accuracy. This iterative
process continues until the reduced-order and full-order system discrete
impulse responses are matched to desired specification. Thus, the ENOR
algorithm produces the necessary and sufficient vector basis for construction
of the eigen-space which is used to represent the dominant eigen-modes of
the original system transfer function, thereby leading to a projection matrix
whose column space spans the eigen-space of the full-order system.

In the following chapter, the stochastic domains are assumed to be relatively small fine-featured sub-domains of the much larger coarse deterministic
domains, in multi-scale structures. This implies that the stochastic macro-
model region is electrically small and thus the spatial distribution of fields in
the stochastic macro-model region exhibits small sensitivity over frequency.
Thus, a relatively small set of moments obtains sufficiently accurate represen-
tation of the transient field profile in the stochastic macro-model region.

Next, we apply the above MOR technique of ENOR to project the full-
order system to obtain a reduced order ATF.

3.4 Formulation for Reduced Order Model

In order to apply the MOR technique on the full-order ATF system, we
proceed as follows.

Using the projection matrix $V$, we obtain the following projected quantities

\[ C_p = V^T CV \]  \hspace{1cm} (3.30)  

\[ G_p = V^T GV \]  \hspace{1cm} (3.31)  

\[ \Gamma_p = V^T \Gamma V \]  \hspace{1cm} (3.32)  

\[ Q_{h_p} = V^T Q_h \]  \hspace{1cm} (3.33)
To obtain the reduced order admittance transfer function (about \( s_0 \)), we simply replace \( C \) by \( C_p \), replace \( G \) by \( G_p \), and replace \( \Gamma \) by \( \Gamma_p \) in (3.25), to obtain

\[
Y_p = \left( C_p s + G_p + \frac{1}{s} \Gamma_p \right) \tag{3.34}
\]

Then, to obtain the reduced order \( e \)-field, we replace \( Y \) with \( Y_p \) and replace \( Q_h \) with \( Q_{hp} \) in (3.10) to obtain

\[
e_p = Y_p^{-1} Q_{hp} h_b \tag{3.35}
\]

To demonstrate the effect of MOR on a system, we apply ENOR to a random system admittance transfer function of size 961 × 961. For comparison, we also apply direct eigen-decomposition by calculating the same system’s eigenvectors and eigenvalues, and keeping only those eigenvectors which are significant based on their associated normalized eigenvalues; the comparison is shown as density plots in Figure 3.1. The original full order system has its degrees of freedom dispersed smoothly on the entire matrix structure. The ENOR reduced system is computed with one \( k \) iteration. Clearly, the ENOR reduced system has a much smaller size, 56 × 56, and the system’s degrees of freedom are less smoothly distributed on the matrix structure. As expected, the direct eigenvector decomposition redistributes the original system’s degrees of freedom over the diagonal of a much smaller highly sparse diagonal matrix.

### 3.5 Time Stepping and Stability

Following the same procedure for the full-order system, and using (3.34),(3.35), we obtain the reduced order time-stepping formula

\[
e_p[n + 1] = \nu_p^{-1} \cdot \left( \frac{\Delta t}{2} G_p e_p[n - 1] \right.
- (\Delta t)^2 \Gamma_p e_p[n] + C_p \left( 2 e_p[n] - e_p[n - 1] \right)
+ (\Delta t) Q_{hp} \left( h_b[n + 1/2] - h_b[n - 1/2] \right)) \tag{3.36}
\]

where \( \nu_p = (C_p + \frac{\Delta t}{2} G_p) \).
Figure 3.1: Density plots of (a) the original system transfer function matrix, (b) the reduced order system transfer function matrix, based on ENOR, (c) the reduced order system transfer function matrix, based on direct Eigen-decomposition. The density plot represents the structure of the matrix, where each matrix element is represented by a color in the continuous spectrum of the standard temperature map. The maximum and minimum values are represented by red and blue, respectively.
The time-stepping formula (3.36) is based on 2nd order accurate central difference operator (3.15) in both time and space, as well as time-averaging (3.18),(3.19). The stability analysis for such a case is carried out in [54] based on the von Neumann [55] method and in [56] based on discrete system analysis [57], and reveals that the stability condition for lossy and lossless media are the same, with the stable region given by

$$\Delta t \leq \Delta t_{\text{max}} = \frac{\sqrt{\mu \epsilon}}{\sqrt{\frac{1}{(\Delta x)^2}} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}}$$

(3.37)

where $\mu$ and $\epsilon$ are the smallest values of the material permeability and permittivity in the grid, $\Delta t_{\text{max}}$ is the maximum allowed temporal discretization, and $\Delta x, \Delta y, \Delta z$ are the spatial discretization steps in the direction of orthogonal unit vectors $\hat{x}, \hat{y}, \hat{z}$, respectively.

It is worth noting that instead of the conditionally stable central difference operation, it is possible to implement the discrete difference operation as an unconditionally stable operator such as the Newmark-$\beta$ [56]. This choice yields greater flexibility in spatial-temporal discretizations; however, for the sake of simplicity in demonstrating the main ideas, we use central difference throughout this work.

Having obtained the time-stepping formulation (3.36), we modify the standard Yee time-stepping scheme through Algorithm 1.

3.6 Use of the Macro Model Inside an FDTD Grid

The diagram in Figure 3.2 shows the relative locations of electric and magnetic field vector components with respect to each other and the computational grid.

The fields are used in the time-stepping routine, as follows:

- The $h_b$-fields at the arrows are the macro-model input (excitation) at the perimeter of macro-model immediately outside the electric field boundary layer. These are updated using the electric field values at dashed circles and disks. The vector $h$ contains the state variables inside the macro-model and at the perimeter of the macro-model.

- The $e$-fields at disks are the macro-model output (response). These are
Figure 3.2: Diagram of field arrangement for the macro-model implemented as an admittance transfer function.
Algorithm 1 Modified Yee time-update algorithm (ATF).

1. Initialize the FDTD grid with boundary and initial conditions.
2. At time-step \( n \), update the \( \mathbf{H} \)-field in the coarse grid using the usual FDTD update scheme.
3. Update the electric field (response) \( \mathbf{e}_p \) using the magnetic field ( excitation) \( \mathbf{h}_b \) and (3.36).
4. Obtain \( \mathbf{e} = V.\mathbf{e}_p \), to be used in the next update of \( \mathbf{H} \)-field in the coarse-grid.
5. At time-step \( n + 1/2 \), update the \( \mathbf{E} \)-field in the coarse grid, including \( \mathbf{e}_b \) on boundary of the macro-model.
6. Update the source, located in the coarse grid.
7. Iterate to \( n + 1/2 \) and goto 2.

the boundary electric field state variables \( \mathbf{e}_b \). The \( \mathbf{e} \)-fields at disks are updated using the system transfer function matrix.

- The dotted circles (inside the macro-model) are the place-holders for \( \mathbf{e} \)-field, around which the \( \mathbf{h} \)-field is never updated, since they fall into the macro-model region. When MOR is applied, it reduces the degrees of freedom of the original model, as dictated by the dotted circle domain, to a desired level as specified by the relative tolerance \( tol_{rel} \) and maximum iteration number \( k_{iter} \) during computation of the projection vector.

3.7 Numerical Studies

To demonstrate the concepts discussed thus far, we perform 2D (with \( \frac{\partial}{\partial z} = 0 \)) TM\(^z\) simulations, in rectangular coordinates with unit vectors \{\( \hat{x}, \hat{y}, \hat{z} \}\}, with one electric field component along the z-axis (\( E_z \)), one magnetic field component along x-axis (\( H_x \)) and another magnetic field component along y-axis (\( H_y \)). Although the numerical examples in this chapter are 2D, the macro-model formulations derived above are just as valid for application towards 3D problems; the only required adjustment is that for the case of 3D
the tangential magnetic field excitation should be the fields around the outer
faces of a 3D volume (rather than around the contours of a 2D surface), and
the tangential electric field response should be the fields immediately beneath
the surface of a 3D volume (rather than the fields immediately beneath the
boundary of a 2D contour); see Appendix D.

The i-axis represents the spatial index along the x-axis, and the j-axis
represents the spatial index along the y-axis. A square cell is used for spatial
discretization, such that spatial discretization along the x-axis $\Delta x$ is equal to
the spatial discretization along the y-axis $\Delta y$. The spatial discretization in
the fine grid is designated as $\Delta x_F$, which is $1/3$ of the spatial discretization
of the coarse grid $\Delta x_C$.

The magnetic field has a component along the x-axis and a component
along the y-axis, and the electric field has a component along the z-axis,
transverse to x-y plane. We use the total field / scattered field (TF/SF)
method [10] to generate a plane wave source with a Gaussian distribution.
The TF/SF region is placed inside the computational domain, where the
relative location of each simulation region is identified in Figure 3.3. The
plane wave is depicted in Figure 3.4, where it is generated at $i_a$, propagates
in the +x direction, and leaves the TF region at $i_b$. Outside of the SF region,
the computational domain is bounded by a perfectly matched layer (PML)
region, and subsequently the entire FDTD domain is truncated with the
perfect electric conductor (PEC) walls.

We conduct three experiments. In the following experiments we simulate
inside a cavity resonator, which means the PML region is set to have a
thickness equal to zero.

In the first experiment, we place a single macro-model at the center of
a square shaped cavity resonator $\{i_c, j_c\}$, with free-space everywhere; see
Figure 3.4.

The second experiment is setup with two apertures inside a metal screen
along the y-z plane. Each aperture is modeled as a macro-model, where the
aperture is centered symmetrically inside the macro-model. The metal screen
is modeled as copper. In order to mimic an infinite-plane metal screen in the
y-z plane, we place two perfect magnetic conductor walls horizontally in the
FDTD domain just one cell inside the TF/SF boundary at $j = j_a + 1$ and
at $j = j_b - 1$, and truncate the metal screen at these PMC walls. This has
the effect of producing infinite non-inverted mirror images of the tangential
Figure 3.3: The total field / scattered field (TF/SF) region is placed inside the computational domain. The perfect electric conductor (PEC) truncates the entire FDTD domain. The perfectly matched layer (PML) pads the PEC. The scattered field (SF) region is inside the PML region. The total field (TF) region is inside the SF region. The scattering objects to be simulated are placed inside the TF region.
electric fields and normal magnetic fields between the PMC sheets, along +y and -y axis; see Figure 3.5. The second experiment is depicted in Figure 3.6.

The third experiment modifies the second experiment by adding one more aperture at the center of the grid. The apertures are placed at equal spacing from each other along the y-axis and modeled with a macro-model, as shown in Figure 3.7.

The ratio of coarse grid to fine grid (inside macro-model) resolution is 3:1. The plane wave emanates from the left \((i = i_a)\) in the coarse grid, propagates to the right towards the macro-model region at center, and leaves the TF region on the right \((i = i_b)\).

The metal screen is placed at the center of the grid along the x-axis at \(i = i_c\), and each aperture is centered with a square macro-model, with an aperture length equal to \(5\Delta x_C\) along the y-axis. The square macro-model edge is equal to \(7\Delta x_C\). The metal screen has a width equal to \(\Delta x_C\), equivalent to three fine cells in the fine grid. The metal screen is assumed to be copper with a conductivity \(\sigma = 5.7 \times 10^8\) S/m.

The electric field \(E_z(V/m)\) is computed in FDTD at point \(\{i_M, j_M\}\) located...
Figure 3.5: The PMC walls are inserted horizontally inside the FDTD domain, to generate mirror images of the metal screen with apertures. The metal screen is truncated at the PMC boundary.
Figure 3.6: Diagram of double apertures experiment.

Figure 3.7: Diagram of triple apertures experiment.
at the center of the grid along the y-axis and $\Delta x_C$ to the right of the macro-model’s right edge along the x-axis. The $E_z$ is computed for the following three cases:

- Using a uniform high resolution fine grid for the entire FDTD computational domain. This is the reference solution and is referred to as $UHF$ in the following.

- Using sub-gridding with 3:1 ratio, in place of macro-model region. This is referred to as $SUB$.

- Using macro-model. This is referred to as $MAC$.

The grid’s maximum frequency is $f_{max} = 3.0$ GHz, which gives $\lambda_{min} = c/f_{max} = 0.1$ m, where propagation velocity in free-space is $c = 1/\sqrt{\mu_0\epsilon_0} = 3 \times 10^8$ m/s, the permeability of free-space is $\mu_0 = 4\pi10^{-7}$ H/m, and the permittivity of free-space is $\epsilon_0 = \frac{10^{-9}}{36\pi}$ F/m. The Gaussian source has a frequency bandwidth $f_{sBW} = 0.5$ GHz, and we define the source wavelength $\lambda_s = c/f_{sBW} = 0.6$ m. The Gaussian source peak is set to occur at $t_p = 1.2$ ns. The spatial sampling resolution is $N_\lambda = 20$ in the coarse grid and $N_\lambda = 60$ in the fine grid; this makes the spatial discretization $\Delta x_F = \lambda_{min}/N_\lambda \approx 0.0016$ m in the fine grid, and $\Delta x_C = 0.005$ m in the coarse grid. The Courant factor [10] is set to 0.5, which makes the temporal discretization $\Delta t = 0.5\Delta x_F/c$. The TF region in the computational domain is set to be equal to one $\lambda_s$ on each side.

For the following experiments, we set $tol_{rel} = 10^{-3}$, $k_{iter} = 1$, and expand about $s_0 = 1.0$ GHz. This produces a projection matrix $V$ with dimensions $364 \times 52$, which means the reduced order system matrix ($C_p, G_p, \Gamma_p$) have dimensions $52 \times 52$.

The result of the first experiment, shown in Figure 3.8, demonstrates that a single macro-model in free-space correlates very well with the uniform high resolution simulation, which means the macro-model is working as expected. The signal starts propagation from left side of TF, passes through the macro-model filled with free-space, and leaves the TF on the right.

The result of the second simulation, shown in Figure 3.9, indicates that two macro-models each placed over an aperture correlate very well against the uniform high resolution simulation. The signal starts propagation from the
Figure 3.8: Magnitude of $E_z$ (V/m) vs. time-step $n$, with one macro-model in free-space.
left side of TF, arrives at the metal screen with two apertures, and begins to experience reflections from the metal screen as well as propagation through the apertures.

![Graph showing the magnitude of $E_z$ (V/m) vs. time-step $n$, with two macro-models, each covering an aperture.](image)

Figure 3.9: Magnitude of $E_z$ (V/m) vs. time-step $n$, with two macro-models, each covering an aperture.

The simulation result for the third experiment, shown in Figure 3.10, illustrates excellent agreement between the macro-model and the uniform high resolution simulations. Note the slightly increased magnitude compared with the second experiment; this is due to the presence of an additional aperture which allows more energy through the metal screen, where each aperture acts as a dipole antenna. The above results provide good evidence of the operational status and high accuracy of the macro-model system.

Next, we show $\vec{E}$-field density plots of the TF region in the uniform high resolution computational grid, as the plane-wave propagates through the double and triple apertures. For the following sets of plots (Figures 3.11-3.12), we set $f_{sBW} = 3.0$ GHz, $t_p = 0.2$ ns, each aperture length to $9\Delta x_C$ along the y-axis, and the computational domain to $5\lambda_s$ on each side.

Also, we show $\vec{E}$-field density plots of the TF region in the reduced order
Figure 3.10: Magnitude of $E_z$ (V/m) vs. time-step $n$, with three macro-models, each covering one aperture.
Figure 3.11: Density plot of $E_z$ (V/m) at time-step $n = 362$, with two apertures in metal screen. Uniform high resolution.
Figure 3.12: Density plot of $E_z$ (V/m) at time-step $n = 362$, with three aperture in metal screen. Uniform high resolution.
computational grid (Figures 3.13-3.14), as the plane-wave propagates through the double and triple apertures.

![Density plot of $E_z$ (V/m) at time-step $n = 420$, with two macro-models, each covering one aperture.](image)

Figure 3.13: Density plot of $E_z$ (V/m) at time-step $n = 420$, with two macro-models, each covering one aperture.

To validate the FDTD solutions, we correlate the uniform high resolution far-field radiation pattern of a single aperture vs. the approximate solution for radiation pattern. To obtain the approximate solution, we proceed as follows. First, we approximate the high conductivity metal screen as PEC. Then, we use the field equivalence principle \[58\] to replace the $\vec{E}$-field in the aperture with an equivalent magnetic surface current density $\vec{M}_s$, and replace the PEC screen with vacuum.

In this case, $\vec{E} = E_z \hat{z}$, which makes $\vec{M}_s = M_y \hat{y} = 2E_z \hat{y}$ (see Figure 3.15); then we compute the electric vector potential $\vec{F}$

$$\vec{F} = \frac{\epsilon}{4\pi} \int \oint_{S'} \frac{e^{-j\beta R} \vec{M}_s[x', y']}{R} \, dS'$$

\[3.38\]

where the propagation constant $\beta = \omega \sqrt{\mu_0 \epsilon_0}$, the vector $\vec{R} = \vec{r} - \vec{r}'$, the magnitude of $\vec{R} = R$, the source location is given by $\vec{r}'$, and the observation
Figure 3.14: Density plot of $E_z$ (V/m) at time-step $n = 420$, with three macro-models, each covering one aperture.

Figure 3.15: The field equivalence principle to model the aperture current. $S_x$ is the $x$-component of the Poynting vector $\vec{S}$, depicting power flow in $+x$-direction. Metal screen is placed at $x = x_{ms}$. 
field point location is given by $\vec{r}'$. Here, $\vec{r}, \vec{r}', \vec{R}$ are the radial vector components in the spherical coordinate system, where the spherical coordinate unit vectors are $\{\hat{r}, \hat{\phi}, \hat{\theta}\}$ shown in Figure 3.16.

Further simplifying the analysis, we assume the metal screen is infinitely thin in the x-direction; thus we have a 1D integral in (3.38). Also, due to analyzing a 2D domain with no variation along the z-direction, the observation point lies on the x-y plane at $\theta = \pi/2$. In addition, we assume to be in the far-field region, which allows us to simplify the integral by using parallel ray approximation to reduce the expansion of $R$ (based on the binomial expansion theorem) to be $R \approx r$ in the magnitude term, and $R \approx r - \hat{r} \cdot \vec{r}'$ in (the phase of) the exponential term, where the magnitude of vector from origin to the field point $|\vec{r}| = r$ and magnitude of vector from origin to the source point $|\vec{r}'| = r'$. Finally, using physical optics approximation [59] we assume the field in the aperture to be equal to the incident plane wave, and uniformly distributed across the aperture.

In this case, we set the broadside incident plane wave to have a Gaussian distribution in time

$$g[t] = E_0 e^{-\frac{(t-t_p)^2}{2t_{PW}^2}} (u[t] - u[t_{sim}]) \quad (3.39)$$

where $E_0$ is the peak magnitude of the incident electric field, $t_p$ is the time at which the peak occurs, $u$ is the unit-step function, $t_{PW}$ is the pulse-width, and $t_{sim}$ is the maximum simulation time.

The Fourier transform of $g[t]$ is
\[ G[\omega] = E_0 e^{-j\omega t_p - \frac{\omega^2 t_{PW}^2}{2}} \sqrt{\frac{\pi}{2} t_{PW}} \times \left( \vartheta \left( \frac{t_p - j\omega t_{PW}^2}{\sqrt{2} t_{PW}} \right) + \vartheta \left( \frac{-t_p + j\omega t_{PW}^2 + t_{sim}}{\sqrt{2} t_{PW}} \right) \right) \] (3.40)

where the function \( \vartheta[.] \) is the integral of the Gaussian distribution given by
\[ \vartheta[z] = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt. \]

Thus, the electric field in the aperture is expressed in the frequency domain as
\[ \vec{E}_a[\omega, x] = \hat{z} G[\omega] e^{-j\beta x} \] (3.41)

We set the aperture center to be the new coordinate origin, and obtain the electric field in the aperture at \( x = 0 \) as
\[ \vec{E}_a[\omega, x = 0] = \hat{z} G[\omega] \] (3.42)

Using the above simplifications, (3.38) only possesses a \( \hat{y} \) component in rectangular coordinates. Using spherical coordinate transformations, and neglecting the \( \hat{r} \) component due to being in far-field, the \( \hat{\phi} \) component of (3.38) is
\[ F_{\phi}[r, \phi, \omega] = \cos \phi \left( \frac{e^{-j\beta r}}{4\pi r} \int_{-L/2}^{L/2} 2G[\omega] e^{j\beta r'} r' \, dy' \right) \] (3.43)

where \( L \) is the length of the aperture in the y-direction, and for the y-directed magnetic current density we have \( \hat{r} \cdot \vec{r}' = y' \sin \phi \).

Thus, the electric field \( \vec{E} = \hat{\theta} E_\theta \) in frequency domain is obtained by [60]
\[ E_\theta[r, \phi, \omega] = -j\omega \eta F_{\phi} \] (3.44)

where the intrinsic impedance \( \eta = \sqrt{\mu/\epsilon} \). We note that at \( \theta = \pi/2 \), it is \( E_\theta = -E_z \).

To compare the frequency domain approximate expression with the time-domain computed data from FDTD, we apply the discrete inverse Fourier transform (DIFT) to (3.44).

For the next sets of plots, we set \( f_{sBW} = 3.0 \) GHz and keep the PML
thickness at zero while increasing the computational domain to $40\lambda_s$ on each side so as to avoid reflections from PEC walls and signals from image apertures (on the other side of the PMC walls). We plot the far-field radiation pattern of a single aperture placed at grid’s center, obtained from the UHF grid simulation. For this, we compute the E-field in the Fraunhofer (far-zone) region [60] at a far-field distance greater than $r_{ff} = 2D^2/\lambda_s$, where $D$ is the largest dimension of the radiator. In this case, we set the aperture to have a length of $D = 9\Delta x_F$, that makes $D = 0.0144$ m. Thus, the far-zone is located at a distance greater than approximately 0.00415 m, or less than $3\Delta x_F$. As such, we compute the E-field at a radial distance of $50\Delta x_F$ over $-\pi/2 \leq \phi \leq \pi/2$.

Let us also check the radiation pattern of three such apertures placed at equal distances from each other along the y-axis, in a collinear array [60]. In this case, the apertures have equal phase and amplitude. For this, we use the array factor

$$AF = \frac{\sin \frac{N}{2} \psi}{\sin \frac{1}{2} \psi}$$

(3.45)

where the progressive phase $\psi = \beta d \sin \phi$, $d$ is the distance between centers of two apertures, and the number of apertures $N = 3$.

To obtain the far-zone radiation pattern for the array, we multiply the radiation pattern for the single element (3.44) by the array factor (3.45), then apply the discrete inverse Fourier transform of the resulting expression to obtain the radiation pattern in time domain.

For the FDTD simulations, we set the computational domain length to $30\lambda_s$ and each aperture length to $7\Delta x_F$. We set the distance between each aperture to be equal to $11\Delta x_F$. These choices make the far-zone distance for the entire array approximately equal to $529\Delta x_F$, and we record data at radial distance of $650\Delta x_F$ from the center of the middle aperture.

The FDTD and approximate solutions shown in Figures 3.17-3.20 are quite close; however, they are not a perfect match. The discrepancies are in part due to the simplifying assumptions discussed earlier. In addition, for the approximate solution of the array we assume there is no coupling between the elements and that each element pattern is due to an aperture in an infinite PEC plane; whereas, in the FDTD simulation the apertures are placed in a copper screen relatively close to each other and there is coupling between
apertures. As such, this makes the element patterns non-ideal and reduces the accuracy of pattern multiplication in the approximate solution. Furthermore, we reduced the size of elements to keep the far-zone distance for the array relatively small; this reduces the uniformity of field distribution in the apertures and further impacts the accuracy of the approximate solution.

Figure 3.17: FDFD (solid black) vs. approximate (dotted red) radiation pattern of $E_\theta$ at radial distance of $50\Delta x_F$ from the aperture’s center. Computed in the Fraunhofer region at time step $n = 2450$ in the UHF grid.
Figure 3.18: FDTD (solid black) vs. approximate (dotted red) radiation pattern of $E_\theta$ at radial distance of $50\Delta x_F$ from the aperture’s center. Computed in the Fraunhofer region at time step $n = 2550$ in the UHF grid.
Figure 3.19: FDTD (solid black) vs. approximate (dotted red) radiation pattern of collinear array, with $E_\theta$ at radial distance of $650\Delta x_F$ from the aperture’s center. Computed in the Fraunhofer region at time step $n = 3111$ in the UHF grid.
Figure 3.20: FDTD (solid black) vs. approximate (dotted red) radiation pattern of collinear array, with $E_{\theta}$ at radial distance of $650\Delta x_F$ from the aperture’s center. Computed in the Fraunhofer region at time step $n = 3200$ in the UHF grid.
4.1 Motivation

In this chapter, we develop a methodology for stochastic macro-modeling in FDTD, by infusing the macro-model with the stochastic collocation technique. This expedites the quantification of the impact of parametric uncertainty in the fine-featured geometric and material properties of multi-scale structures, on the electromagnetic response of stochastic systems in FDTD.

To motivate this chapter, we induce a random geometric variation in the example of aperture array from the previous chapter, and observe the impact of such random variation on the magnitude of the electric field. For this, first we simulate three apertures in a metal screen, all having the same length along the y-axis equal to $19\Delta x_C$, where $\Delta x_C$ is the spatial discretization in the coarse grid; the resulting signal is designated by “Eq”. Then, we reduce the center aperture’s length by $5\Delta x_C$ (i.e. approximately 50%) and repeat the simulation; the resulting signal is designated by “UnEq”. The effect can be seen in Figure 4.1.

Assuming the specification level for minimum high-voltage is violated by the UnEq signal, it is evident that such random variations can have a detrimental effect. To remedy such variations due to uncertainty, typically the structure is over-designed by large margins to ensure that the performance specifications are met and even exceeded for mission critical tasks; however, usually over-design adds cost.

To comprehend the effects of uncertainty (e.g., [61, 62]) in fine-featured regions of multi-scale structures, and to efficiently quantify the impact of such uncertainty on the electromagnetic response of stochastic systems, we propose the stochastic macro-model in FDTD. This provides a computationally efficient method to mitigate the impact of random variations early in
Figure 4.1: Normalized electric field $E_z$ vs. time-step $n$. Three equal-length apertures (solid black designated as Eq) vs. three apertures with the center apertures’s length approximately equal to 50% length of the other two apertures (dashed blue designated as UnEq).
the design stage. The development of the stochastic macro-model eliminates
the need for repeated discretization of the overall structure. Indeed, only a
single grid needs to be developed for the deterministic portion of the overall
structure irrespective of the realization generated by a specific choice of the
random parameters in the domains exhibiting statistical variability, thus re-
sulting in significant computational savings by avoiding re-discretization of
the deterministic domain for each variation in the stochastic domain.

This chapter is organized as follows. In Section 4.2, we begin with the
deterministic macro-model. Then we introduce the method of stochastic col-
location in Section 4.3 as the method of choice for statistical analysis. In
Section 4.4 we introduce the stochastic macro-model, which relies on the
machinery of homogeneous chaos, described in Section 4.5, to expand each
random system parameter into a set of orthogonal polynomials in random
space. The computation of the coefficients in the expansions are discussed in
Section 4.6. The construction of the stochastic projection matrix is discussed
in Section 4.7, followed by the solution of the reduced order coefficients in
Section 4.8. In Section 4.9 we develop the solution to the stochastic field
quantities in the FDTD grid, followed by an algorithm for generation and
utilization of the stochastic macro-model in FDTD. The method of numerical
integration in random space over the sparse Smoljak grid is detailed
in Section 4.10. We conclude the chapter by application of the proposed
methodology in several numerical examples illustrated in Section 5.

4.2 Deterministic Reduced Order Model

As discussed in Chapter 3, a fine-featured region of interest in the FDTD grid
may be encapsulated by casting it as a deterministic 2nd order state-space
abstraction layer

\[ Ye = Q_h h_b \]  

(4.1)

where \( Y = (sC + G + \frac{1}{s} \Gamma) \) is in \( \mathbb{R}^{M \times M} \), and matrices \( C, G, \Gamma, Q_h \) are assumed
to be time-invariant (i.e. non-dispersive material is assumed).

To simplify the notation for the ensuing developments we insert the sub-
script \( \_F \) to designate the full-order system.
where $Y_F = (sC_F + G_F + \frac{1}{s}\Gamma_F)$ is in $\mathbb{R}^{M\times M}$, the input $u_F = Q_{h_F} h_{b_F}$ is in $\mathbb{R}^{M\times 1}$, and the electric field vector $e_F$ is in $\mathbb{R}^{M\times 1}$.

As was highlighted in Section 3.1, the reduction in degrees of freedom increases computational efficiency; thus, the system equations may be subject to model order reduction by using the sub-space projection matrix $V \in \mathbb{R}^{M\times m}$ (with $m \ll M$) obtained through a convenient MOR technique; in this case, we use ENOR to obtain $V$.

Hereafter, the reduced order deterministic model is given by

$$Y z = u$$

where

$$z = V^T e_F, \quad Y = V^T \left( sC_F + G_F + \frac{1}{s}\Gamma_F \right) V, \quad u = V^T Q_{h_F} h_{b_F}$$

The deterministic reduced order model is comprised of $Y \in \mathbb{R}^{m\times m}$, $u \in \mathbb{R}^{m\times 1}$, and $z \in \mathbb{R}^{m\times 1}$.

The system (4.3) provides a complete description of the deterministic model in the Laplace domain. In Chapter 3 we obtained the time-stepping formula (3.36) for this deterministic reduced order system.

4.3 Stochastic Collocation Method

To determine statistical measures (e.g., mean, variance, etc.) of the system response under input uncertainty, various sampling methods (e.g., Monte Carlo [63]), non-sampling methods (e.g., stochastic Galerkin), or perturbation methods [64–67] may be utilized. Among the non-sampling methods, the stochastic Galerkin method [68] has recently been used in the literature [69–71]. Although the stochastic Galerkin method has a fast (exponential) convergence rate under sufficient smoothness conditions in random
space, the numerical implementation becomes non-trivial [72,73] for systems with complicated governing differential equations and boundary conditions, with the complications mostly due to the coupled nature of the associated differential algebraic equations (DAE).

A popular and well-developed sampling method that uses deterministic experiments (using decoupled DAE) to deduce the statistical measures is the Monte Carlo method [63, 74–76]. The main advantage of the Monte Carlo method is its simplicity in numerical implementation. In its most basic form, a Monte Carlo algorithm is based on choosing a random value for each parameter of the system under uncertainty according to the parameter’s probability density functions (PDF), and performing simulations until convergence in the statistical indicators is reached.

At its core, the Monte Carlo method relies on the ability to generate random numbers [77]. Because a computer is a deterministic system, it cannot generate truly random numbers; however, with appropriate precautions, it is possible to generate pseudo-random numbers [78, 79]. The key is to ensure that no repetitive pattern emerges in the generated set of numbers. The pseudo-random numbers generated according to arbitrary probability distributions are then used to select the various deterministic experiments, from which the statistical measures of the system response are obtained. Although the rate of convergence is independent of the number of random variables, it is relatively slow; such that, for \( K \) sample experiments, the brute-force Monte Carlo converges asymptotically as \( 1/\sqrt{K} \). Thus, for large \( K \), Monte Carlo requires a large number of experiments to converge.

A method that combines the ease of numerical implementation of Monte Carlo with the speed of the stochastic Galerkin method is the stochastic collocation method [80,81]. For relatively small number of random variables, the stochastic collocation method is only weakly dependent on the number of random variables, and under sufficient smoothness conditions in random space, it can have an exponential rate of convergence, while requiring the solution to a set of deterministic problems only.

In the stochastic collocation method, the basic idea is to expand a random variable in terms of orthogonal polynomials. In essence, the polynomial chaos serves as an interpolation mechanism to describe the statistical solution in random space. The expansion of a random variable in terms of Hermite polynomials was introduced in the theory of homogeneous chaos [82] in context
of a Brownian motion process. The development of non-linear functionals in terms of Fourier-Hermite functionals [83] indicates that the expansion based on homogeneous chaos is extensible to any second order stochastic process, and paves the way to the expansion of random variables in terms of the polynomial chaos [84, 85]. This is quite convenient, given that a second order stochastic process is characterized by having random variables with finite variance; and since all real system parameters exhibit finite variance, then polynomial chaos may be used to expand random processes in any real system. Subsequently, other investigators [70] have mapped the choice of various classes of probability distribution functions to the convergent-optimal choice of the type of polynomial chaos.

Finally, it is important to note that the stochastic collocation method relies on accurate multi-dimensional numerical integration methods (cubature) to ensure solution accuracy. Various investigators have worked on this topic in context of Smoljak grid [9, 86–92].

In the next section, we apply the stochastic collocation method towards stochastic macro (reduced order) modeling in FDTD.

### 4.4 Stochastic Reduced Order Model

The idea of using stochastic modeling together with model order reduction, for assessment of random input variations on system output, has been studied by a number of different investigators, and its utility for various applications has been demonstrated in the past [65–67, 93–97]. Here, we develop the methodology to quantify uncertainty in fine-featured regions in the FDTD grid through the stochastic macro-model.

Let us assume that the input parameters (i.e. structural, material, and excitation tensors) in the full-order system exhibit uncertainty; these parameters are considered random variables and will be denoted by the superscript symbol. The uncertainty in system description may be represented as follows:

\[
\tilde{Y}_F \tilde{\epsilon}_F = \tilde{u}_F
\]

(4.4)

where
\[
\tilde{Y}_F = \left( s\tilde{\mathcal{C}}_F + \tilde{\mathcal{G}}_F + \frac{1}{s} \tilde{\mathcal{\Gamma}}_F \right), \quad \tilde{u}_F = \tilde{Q}_{h_F} \tilde{h}_{b_F}
\]

Let \(Y_{F_j}\) be the \(j^{th}\) admittance transfer function (ATF) for a certain combination of structural, material and excitation parameters based on each random variable’s probability density function; that is, any given \(Y_{F_j}\) may be regarded as a deterministic instance of the system state.

Let all the possible combinations of the full-order system parameters in \(d\)-dimensional continuous random space \(\Xi \in [-1, 1]^d\) be given in a set \(Y_{F_s}\). Because of the infinite dimension of \(Y_{F_s}\), its computationally feasible statistical analysis requires that we truncate the set \(Y_{F_s}\) by choosing a finite subset of parametric combinations in continuous random space. An important question is how should we select such a subset to minimize the number of elements in \(Y_{F_s}\) while maintaining sufficient accuracy in the resulting statistical analysis. One approach is through the use of the Smoljak grid, to be discussed in Section 4.10.

Once the elements in the finite set \(Y_{F_s}\) have been determined, we may apply MOR to each deterministic ATF \(Y_{F_j}\) and obtain a deterministic projection matrix \(V_j\). Having obtained \(V_j, \forall j \in 1, 2, \ldots, J\), we may use interpolation to obtain the random projection matrix \(\tilde{V}\) which may be used to compute a projection matrix for any possible parametric combination in continuous random space; the interpolated projection matrix is expressed in terms of orthogonal polynomials, to be discussed in Section 4.5. Thus, random variability in system parameters due to uncertainty may be represented through the random projection matrix \(\tilde{V}\). To generate \(\tilde{V}\) for stochastic macro-modeling of the fine-featured sub-grid region, the sub-grid region must be generated \(J\) times.

The approach described above offers the key computational advantage that, once the random projection matrix \(\tilde{V}\), and by extension, the stochastic macro-model of the smaller fine-featured region, has been generated, the larger deterministic region (i.e. the deterministic main FDTD grid) need not be discretized repeatedly for every random variation in the fine-featured stochastic region! This is in sharp contrast, in terms of computational cost, to the case where in the absence of the stochastic macro-model it would have been necessary to perform repeated discretization of the large deterministic domain for every random variation in the small fine-featured
stochastic domain.

Hence, we obtain the following stochastic reduced order system description:

\[ \dot{\tilde{Y}} \tilde{z} = \tilde{u} \quad (4.5) \]

where

\[ \tilde{z} = \tilde{V}^T \tilde{e}_F, \quad \tilde{Y} = \tilde{V}^T \left( s\tilde{C}_F + \tilde{G}_F + \frac{1}{s} \tilde{\Gamma}_F \right) \tilde{V}, \quad \tilde{u} = \tilde{V}^T \tilde{Q}_h \tilde{h}_b \]

The reduced-order stochastic model (4.5) comprehends structural, material, and excitation variability, due to presence of uncertainty in the system. It is clear that for each \( j \)th instance of system parameters in random space, we need to generate the projection matrix \( V_j \). We may obtain \( V_j \) using the random variables \( \tilde{C}_{Fj}, \tilde{G}_{Fj}, \tilde{\Gamma}_{Fj} \) and \( \tilde{Q}_{hFj}, \forall j \in 1, 2, \ldots J \) and their associated PDFs.

An overview of the stochastic macro-model generation is as follows: First we expand the full-order system’s random variables in terms of series of orthogonal polynomials [69–72, 80, 97–99] and unknown coefficients. Next, we perform multi-dimensional numerical integration (cubature) of the expanded stochastic variables in random space over the Smoljak grid, to solve for the unknown coefficients. For the cubature nodes and weights we utilize the Clenshaw-Curtis rule [100–102]. Finally, we substitute the solved coefficient solutions back into the polynomial equations, and perform truncated polynomial projection to obtain the approximate reduced order stochastic model.

The various steps in the stochastic model order reduction process are discussed in detail in the following.

4.5 Orthogonal Expansion

The optimal choice of orthogonal basis for several different kinds of probability distributions is discussed in [69–71]. Let us define the infinite-dimensional Hilbert space \( L^2 \) as the set of all square-integrable functions. For optimal (fastest) convergence in the \( L^2 \) sense we use the continuous Gaussian distri-
bution together with the class of Hermite polynomials \( \mathcal{H}_p \in [-\infty, \infty] \); this combination gives an exponential convergence rate.

The Gaussian distribution function is given by

\[
\alpha[\tilde{\xi}] = e^{-\frac{1}{2} \tilde{\xi}^T \tilde{\xi}}
\]

where \( \tilde{\xi} = \{\xi_1, \xi_2, \ldots, \xi_n\} \) is the set of independent random variables, and the symbol \( T \) denotes the transpose operator.

The \( n^{th} \) order Hermite polynomial \( \mathcal{H}_n \) is obtained by the relation [103], [84], [70]

\[
\mathcal{H}_n[\{\xi_1, \xi_2, \ldots, \xi_n\}] = e^{\frac{1}{2} \tilde{\xi}^T \tilde{\xi}} (-1^n) \frac{\partial^n}{\partial \xi_1 \partial \xi_2 \ldots \partial \xi_n} e^{-\frac{1}{2} \tilde{\xi}^T \tilde{\xi}} \tag{4.7}
\]

Hence, for the case of two random variables \( \tilde{\xi} = \{\xi_1, \xi_2\} \) we obtain the 0\(^{th}\), 1\(^{st}\), and 2\(^{nd}\) order polynomial chaos orthogonal basis, as follows:

\begin{align*}
\text{order 0 :} & \quad \mathcal{H}_0[\{\}] = 1 \\
\text{order 1 :} & \quad \mathcal{H}_1[\{\xi_1\}] = \xi_1, \quad \mathcal{H}_1[\{\xi_2\}] = \xi_2 \\
\text{order 2 :} & \quad \mathcal{H}_2[\{\xi_1, \xi_1\}] = \xi_1^2 - 1, \quad \mathcal{H}_2[\{\xi_1, \xi_2\}] = \xi_1 \xi_2 \\
& \quad \mathcal{H}_2[\{\xi_2, \xi_2\}] = \xi_2^2 - 1 \tag{4.8}
\end{align*}

The homogeneous chaos polynomial forms a complete basis in the space of Gaussian variables and satisfies the orthogonality relation

\[
\langle \mathcal{H}_i[\{\xi_1, \ldots, \xi_n\}] \mathcal{H}_j[\{\xi_1, \ldots, \xi_n\}] \rangle = \langle \mathcal{H}_i^2 \rangle \delta_{ij} \tag{4.9}
\]

where \( \delta_{ij} \) is the Kroneker delta, and it is

\[
\langle f(\tilde{\xi})g(\tilde{\xi}) \rangle = \int_{\mathbb{R}^n} f(\tilde{\xi})g(\tilde{\xi}) \frac{1}{\sqrt{(2\pi)^n}} e^{-\frac{1}{2} \tilde{\xi}^T \tilde{\xi}} d\tilde{\xi} \tag{4.10}
\]

Having obtained the orthogonal basis of polynomial chaos, we may proceed to expand the random variables in terms of such orthogonal basis. The higher the polynomial order, the more degrees of freedom are available in capturing the interactions of independent random variables and their collective impact on the stochastic response. It is important to note that using higher order
polynomials must be accompanied with sufficiently accurate cubature as controlled by the choice of level $k$ in the Smoljak grid. If the cubature is not of sufficient accuracy, the higher order polynomial can exacerbate the cubature errors and rapidly lead to large errors in the final results.

If we assume that uncertainty is present in the fine-featured region inside the macro-model only, and the exterior region to the macro-model is free of uncertainty, then this implies that the magnetic field excitation at the boundary of the macro-model as a total field quantity is comprised of a deterministic incident magnetic field $\tilde{h}_{bf}^i$ and a stochastic scattered magnetic field $\tilde{h}_{bf}^s$; that is, the total magnetic field excitation is stochastic. Thus, the magnetic field excitation at the boundary of the macro-model is $\tilde{h}_{bf} = \tilde{h}_{bf}^t = \tilde{h}_{bf}^i + \tilde{h}_{bf}^s$, and therefore it must be treated as a stochastic parameter and expanded in terms of polynomial chaos basis.

Additionally, if we assume that uncertainty is present in the fine-featured region inside the macro-model, as well as outside of macro-model due to presence of multiple stochastic macro-models, such that the exterior region to the macro-model exhibits uncertainty as well, then this implies that the magnetic field excitation at the boundary of the macro-model as a total field quantity is comprised of a stochastic incident magnetic field $\tilde{h}_{bf}^i$ and a stochastic scattered magnetic field $\tilde{h}_{bf}^s$; that is, the total magnetic field excitation is again stochastic. Thus, the magnetic field excitation at the boundary of the macro-model is $\tilde{h}_{bf} = \tilde{h}_{bf}^t = \tilde{h}_{bf}^i + \tilde{h}_{bf}^s$, and therefore it must be treated as a stochastic parameter and expanded in terms of polynomial chaos basis.

To keep a conceptual framework on the ensuing developments, we take the example case where there are two independent random variables and expand in terms of basis $\{1, \xi_1, \xi_2\}$ where the highest order polynomial is of 1st order.
\[ \tilde{e}_F = e_{F_0} + \xi_1 e_{F_1} + \xi_2 e_{F_2} \]
\[ \tilde{z} = z_0 + \xi_1 z_1 + \xi_2 z_2 \]
\[ \tilde{C}_F = C_{F_0} + \xi_1 C_{F_1} + \xi_2 C_{F_2} \]
\[ \tilde{G}_F = G_{F_0} + \xi_1 G_{F_1} + \xi_2 G_{F_2} \]
\[ \tilde{\Gamma}_F = \Gamma_{F_0} + \xi_1 \Gamma_{F_1} + \xi_2 \Gamma_{F_2} \]
\[ \tilde{Q}_{hF} = Q_{hF_0} + \xi_1 Q_{hF_1} + \xi_2 Q_{hF_2} \]
\[ \tilde{h}_{bF} = h_{bF_0} + \xi_1 h_{bF_1} + \xi_2 h_{bF_2} \]
\[ \tilde{u}_F = \tilde{Q}_{hF} \cdot \tilde{h}_{bF} \]
\[ \tilde{V} = V_0 + \xi_1 V_1 + \xi_2 V_2 \] (4.11)

In the next section, we discuss the solution process for the unknown coefficients (e.g., \( C_{F_0}, G_{F_0}, \Gamma_{F_0} \)) associated with basis of the polynomial chaos.

4.6 Full Order Coefficients

As an example, let us consider the full-order stochastic matrix \( \tilde{C}_F \) in (4.11)
\[ \tilde{C}_F = C_{F_0} + \xi_1 C_{F_1} + \xi_2 C_{F_2} \] (4.12)

For each random variable \( \xi_i \), we assume a Gaussian PDF
\[ \rho_i[x] = \frac{1}{\sigma_i \sqrt{2\pi}} e^{-(x-\mu_i)^2 / 2\sigma_i^2} \] (4.13)

where \( \mu_i \) is the mean, \( \sigma_i \) is the standard deviation, \( \forall i = 1, 2, \ldots, d \), and the dimensionality of random space \( d \) is the number of random variables.

Then, to compute the unknown coefficients \( C_{F_i}, i \in \{0, 1, 2\} \) we may integrate both sides of (4.12) over two-dimensional random space \( \Xi = [-1, 1]^2 \).

\[ \iint \tilde{C}_F \rho_1[\xi_1] \rho_2[\xi_2] d\xi_1 d\xi_2 = \iint (C_{F_0} + \xi_1 C_{F_1} + \xi_2 C_{F_2}) \rho_1[\xi_1] \rho_2[\xi_2] d\xi_1 d\xi_2 \] (4.14)

where \( \rho_1 \) and \( \rho_2 \) are the PDFs as a function of random variables \( \xi_1 \) and \( \xi_2 \), respectively.
Using the orthogonality property of polynomial chaos and (4.14), we obtain

\[ C_{F_i} = \sigma_i^2 \int \int \tilde{C}_{F_i} \rho_1 [\xi_1] \rho_2 [\xi_2] \xi_i d\xi_1 d\xi_2 \]  

(4.15)

where \( i \in \{0, 1, 2\} \), the standard deviation for the \( i^{th} \) random variable is given by \( \sigma_i \), and it is \( \sigma_0 \equiv 1 \), \( \xi_0 \equiv 1 \).

Let us designate the cubature (i.e., multi-dimensional numerical integration) operator \( I[\cdot] \) in (4.15) as follows:

\[ I[f] = \int \int f d\xi_1 d\xi_2 \]  

(4.16)

where the integrand \( f = \tilde{C}_{F_i} \rho_1 [\xi_1] \rho_2 [\xi_2] \xi_i \).

The efficient computation of accurate solutions for coefficients (4.15) is critically dependent on the efficiency and accuracy of the cubature technique used to approximate (4.16). The computational complexity of the stochastic collocation problem is \( M_{sc} \) times the deterministic problem, where \( M_{sc} \) is the number of collocation nodes on the Smoljak grid. For the sake of computational efficiency we need to find an optimal set of nodal points \( \Theta_d \) in \( d \)-dimensional random space that minimizes the number of collocation points while maintaining sufficient accuracy. In Section 4.10, we explore the chosen cubature technique in detail.

In the next section, we discuss the generation of the stochastic projection matrix.

### 4.7 Construction of the Stochastic Projection Matrix

We expand in terms of polynomial chaos basis to obtain the following truncated polynomial chaos expansion for the stochastic projection matrix:

\[ \tilde{V} = V_0 + V_1 \xi_1 + V_2 \xi_2 \]  

(4.17)

Integrating both sides gives

\[ \int \int \tilde{V} \rho_1 [\xi_1] \rho_2 [\xi_2] d\xi_1 d\xi_2 = \int \int (V_0 + \xi_1 V_1 + \xi_2 V_2) \rho_1 [\xi_1] \rho_2 [\xi_2] d\xi_1 d\xi_2 \]  

(4.18)
where $\rho_1$ and $\rho_2$ are the PDFs as a function of random variables $\xi_1$ and $\xi_2$, respectively.

Using orthogonality property of polynomial chaos, the coefficients are given by

$$V_i = \sigma_i^2 \iint \tilde{V} \rho_1[\xi_1] \rho_2[\xi_2] \xi_i d\xi_1 d\xi_2$$

(4.19)

where $i \in \{0, 1, 2\}$, the standard deviation for the $i^{th}$ random variable is given by $\sigma_i$, and it is $\sigma_0 \equiv 1$, $\xi_0 \equiv 1$.

The above requires computation of MOR for each node on the Smoljak grid, and the integration can be carried out using the cubature technique outlined in Section 4.10.

In the next section, we demonstrate usage of the stochastic projection matrix to obtain the coefficients in the polynomial chaos (PC) expansion of the reduced order system.

### 4.8 Coefficients in PC Expansion of Reduced Order System

Having obtained the stochastic projection matrix, we transform the full-order stochastic system (4.4) to the reduced order stochastic system (4.5). The process is demonstrated through the use of the full order stochastic loss matrix $\tilde{G}_F$ to obtain the reduced order stochastic loss matrix $\tilde{G}$, where $\tilde{G}_F = G_{F_0} + G_{F_1} \xi_1 + G_{F_2} \xi_2$ is comprised of full order coefficients $G_{F_0}, G_{F_1}, G_{F_2}$, and $\tilde{G} = G_0 + G_1 \xi_1 + G_2 \xi_2$ is comprised of reduced order coefficients $G_0, G_1, G_2$. The coefficients $G_0, G_1, G_2$ are associated with the orthogonal polynomial chaos basis $1, \xi_1, \xi_2$, respectively.
Using the orthogonality property of polynomial chaos, we may approximate the reduced order coefficients \( G_i \) by keeping only the first three terms on the Right Hand Side (RHS) of (4.20).

We obtain the reduced order coefficients \( Q_{h_i} \) below:

\[
Q_{h_0} + Q_{h_1} \xi_1 + Q_{h_2} \xi_2 = (V_0 + V_1 \xi_1 + V_2 \xi_2)^T \cdot (Q_{hF_0} + \xi_1 Q_{hF_1} + \xi_2 Q_{hF_2}) \quad (4.21)
\]

As before, we obtain the approximate reduced order coefficients \( Q_{h_i} \) by truncating all quadratic and higher powers of \( \xi_i \), as well all cross-terms (e.g., \( \xi_1 \xi_2 \)) on RHS of (4.21).

### 4.9 Computing the Exterior Stochastic Fields

In this section, we develop the methodology for computation of the stochastic fields exterior to the macro-model, followed by an algorithm for computing statistical data for the stochastic macro-modeling in FDTD.

The solution to the exterior problem of full-order stochastic field quantities outside the macro-model may be computed readily by cubature of orthogonal
expansion of $\tilde{e}_F = e_{F_0} + \xi_1 e_{F_1} + \xi_2 e_{F_2}$ on the Smoljak grid in simultaneity with the computation of the stochastic excitation $\tilde{h}_{b_F}$, as expressed below:

$$e_{F_i} = \sigma_i^2 \int \int \tilde{e}_F \rho_1[\xi_1]\rho_2[\xi_2]d\xi_1d\xi_2$$  \hspace{1cm} (4.22)$$

where $i \in \{0, 1, 2\}$, the standard deviation for the $i^{th}$ random variable is given by $\sigma_i$, and it is $\sigma_0 \equiv 1$, $\xi_0 \equiv 1$.

The fact that the total magnetic field excitation $\tilde{h}_{b_F} = \tilde{h}_{b_F}$ at the boundary of macro-model is a stochastic field quantity implies an important point worth highlighting. The solution to the exterior problem of full-order stochastic field quantities outside the macro-model may be computed readily by cubature of orthogonal expansion of $\tilde{e}_F = e_{F_0} + \xi_1 e_{F_1} + \xi_2 e_{F_2}$ in random space over the Smoljak grid, in simultaneity with the computation of the stochastic excitation $\tilde{h}_{b_F}$. One way to accomplish this with computational efficiency is to incorporate the stochastic collocation methodology in the time-update scheme of FDTD, such that in the FDTD simulations on each Smoljak node (from which the stochastic fields everywhere in the interior, boundary, and exterior are computed) we compute the coefficients of polynomial chaos basis as the FDTD time-update proceeds.

Using definition of expectation (4.23) and definition of variance (4.24), together with the expansion (4.25), we easily obtain the mean response $\mu_{\text{Response}} = e_{F_0}$ and the standard deviation response $\sigma_{\text{Response}} = \sqrt{\text{Var}} = \sqrt{\frac{\epsilon_1^2}{\sigma_1^2} + \frac{\epsilon_2^2}{\sigma_2^2}}$, for the exterior stochastic fields.

$$Exp[e] = \int \int e\rho_1\rho_2d\xi_1d\xi_2$$  \hspace{1cm} (4.23)$$

$$\text{Var} = \text{Exp}[e^2] - (\text{Exp}[e])^2$$  \hspace{1cm} (4.24)$$

$$\tilde{e}_F = e_{F_0} + e_{F_1}\xi_1 + e_{F_2}\xi_2$$  \hspace{1cm} (4.25)$$

The key advantage offered by the stochastic macro-model is twofold. First, it reduces computational cost by eliminating the need for repeated and unnecessary discretization of the deterministic domain of the boundary value problem for every possible random variation in fine-featured stochastic sub-domain. Second, it reduces the computational cost by carrying out the
stochastic field computations in the projected reduced order stochastic space through stochastic model order reduction.

4.10 Numerical Integration (Cubature)

At the heart of the stochastic macro-model is the accurate numerical integration of random variables over the pertinent orthogonal random space. Thus, we discuss this in further detail. We begin by defining the $d$-dimensional random space $\Xi \subset \mathbb{R}^d$ with $d \geq 1$. To preserve generality, we assume that the bounded support [80] for random variables $\xi_i$ is $\Xi^i = [-1, 1]$, for $i = 1, 2, \ldots, d$; which means that the bounded random space is a $d$-dimensional hypercube $\Xi = [-1, 1]^d$. We note that random variables with bounded support in $[a, b]$ can always be mapped to $[-1, 1]$.

4.10.1 The tensor product algorithm

Consider the multi-variate $d$-dimensional integral [100]

$$ I_d[f] = \int_{[-1,1]^d} f[x] dx \quad (4.26) $$

Define the sequence of quadrature (1-d numerical integration) formulas

$$ U^i[f] = \sum_{j=1}^{m_i} f[x^i_j] a^i_j \quad (4.27) $$

where $m_i \in \mathbb{N}$, and $\mathbb{N}$ denotes the set of natural numbers.

In the multi-variate case ($d > 1$), an intuitive choice would be to use tensor products, as follows:

$$ (U^{i_1} \otimes \ldots \otimes U^{i_d})[f] = \sum_{j_1=1}^{m_{i_1}} \ldots \sum_{j_d=1}^{m_{i_d}} f[x^{i_1}_{j_1}, \ldots, x^{i_d}_{j_d}] \cdot (a^{i_1}_{j_1} \cdot \ldots \cdot a^{i_d}_{j_d}) \quad (4.28) $$

The collocation nodes corresponding to $U^i$ are given by

$$ X^i = \{x^i_{m_i}, \ldots, x^i_{1}\} \subset [-1, 1] \quad (4.29) $$
The tensor product algorithm depends on the nodal grid, given by

\[ H[q, d] = (X^{i_1} \times \ldots \times X^{i_d}) \quad (4.30) \]

where the integer \( q \geq d \).

If the same number of nodes are chosen in each dimension (i.e. \( m_1 = m_2 = \ldots = m_d = m \)), then the total number of nodes \( M_{\text{tensor}} = m^d \); thus the above cubature, based on a tensor product realization, requires computation on a nodal set \( \Theta_d \) with \( m^d \) collocation nodes. Such a nodal set suffers from computational inefficiency via a slow convergence rate, especially for large dimensionality \( d \). We need to find computationally efficient approximations to the functional \( I_d[f] \) in the multivariate case based on good approximations of \( I_1[f] \) in the univariate case.

4.10.2 The Smoljak sparse grid algorithm

The algorithm of Smoljak [8] provides a computationally optimal nodal set, which is very sparse compared to the nodal set for the tensor product algorithm; as a result, the Smoljak algorithm provides an exponential rate of convergence under sufficient smoothness conditions.

Define \( U^0 = 0, \Delta^i = U^i - U^{i-1} \) for \( i \in \mathbb{N} \), and \( |i| = i_1 + \ldots + i_d \) with \( i \in \mathbb{N}^d \) [100]. Then, the Smoljak algorithm is given by

\[ A[q, d] = \sum_{i \leq q} ( \Delta^{i_1} \otimes \ldots \otimes \Delta^{i_d} ) \quad (4.31) \]

Alternatively, we may write (4.31) as the linear functional [89]

\[ A[q, d] = \sum_{q-d+1 \leq |i| \leq q} (-1)^{q-|i|} \cdot \binom{d-1}{q-|i|} \cdot (U^{i_1} \otimes \ldots \otimes U^{i_d}) \quad (4.32) \]

where \( \binom{d-1}{q-|i|} \) yields the binomial coefficient. This form is also referred to as the combination technique [104].

The Smoljak algorithm depends on values of \( f \) on the nodes at the union of grids.
Given that nested random variable sets $X^i \subset X^{i+1}$ give rise to nested nodal sets $H[q, d] \subset H[q + 1, d]$, we obtain the sparse grid

$$H[q, d] = \bigcup_{q-d+1 \leq |i| \leq q} (X^{i_1} \times \ldots \times X^{i_d}) \quad (4.33)$$

Hence, (4.27) need only be evaluated on the sparse grid nodes (4.34). For $q = k + d$, it can be shown [72] that the number of nodes in the Smoljak grid $M_{Smoljak} \approx \frac{2^k}{k!} d^k$, for fixed $k$ and $d \gg 1$; thus the dependence on dimensionality $d$ is much weaker in this case, compared to the tensor product case.

### 4.10.3 The Clenshaw-Curtis rule

To solve for the unknown coefficients of the polynomial chaos expansion, we employ the cubature with the Clenshaw-Curtis rule [100] on the Smoljak sparse grid [8].

Using the extrema of Chebyshev polynomials as coordinates of the collocation nodes for the random variables, the Clenshaw-Curtis formula is given by

$$U^i[f] = \sum_{j=1}^{m_i} f[x^i_j] a^i_j \quad (4.35)$$

where $m_i = 2^{i-1} + 1$ for $i > 1$, and $m_1 = 1$.

The random variable collocation nodes are given by

$$x^i_j = -\cos \left[ \frac{\pi(j - 1)}{m_i - 1} \right], \quad j = 1, \ldots, m_i \quad (4.36)$$

with $x^1_1 = 0$.

For $j = 2, \ldots, m_i - 1$ the weights are given by
\[ a_j^i = a_{m_i+1-j}^i = \frac{2}{m_i-1} \left( 1 - \frac{\cos(\pi(j-1))}{m_i(m_i-2)} \right)^{(m_i-3)/2} \]
\[ - 2 \sum_{k=1}^{(m_i-3)/2} \frac{1}{4k^2 - 1} \cos \left( \frac{2\pi k(j-1)}{m_i-1} \right) \] (4.37)

and for \( j = 1 \) and \( j = m_i \), the weights are given by
\[ a_1^i = a_{m_i}^i = \frac{1}{m_i(m_i-2)} \] (4.38)

Comparisons of the tensor product grid vs. the Smoljak grid are shown for two-dimensional random space with \( q = 7, d = 2 \) in Figure 4.2, and for three-dimensional random space with \( q = 8, d = 3 \) in Figure 4.3.

The weights corresponding to each collocation point are shown in Figure 4.4, where the radius of each disk in 2D and each sphere in 3D signifies the relative magnitude of the weight at that point, the color blue designates a negative weight and color red designates a positive weight. The collocation points and their associated weights may be conveniently precomputed once, before proceeding with the numerical integration.

4.11 Algorithm for Stochastic Macro-Modeling

For each macro-model with \( N \) random variables, we generate a Smoljak sparse grid (i.e., an \( N \)-dimensional hypercube in random space), using instructions outlined in Section 4.10.2. Using cubature of Section 4.10, we solve for all the coefficients of the polynomial chaos expanded parameters everywhere on this \( N \)-dimensional hypercube that constitutes the random space spanned by \( \{\xi_1, \ldots, \xi_N\} \). Assume we have \( M \) stochastic macro-models present in the FDTD grid, then each stochastic macro-model is placed at a fixed point inside the FDTD grid and simulations are performed over an \( M \times N \)-dimensional Smoljak grid. The polynomial chaos expansions of the random variables which constitute the system parameters provide a convenient interpolation mechanism for obtaining the values for all the random variables at any desired point within the \( M \times N \)-dimensional random space.

Finally, to obtain the stochastic field quantities, cubature is performed over
Figure 4.2: Collocation points in two-dimensional random space for (a) tensor product grid with 1089 nodes vs. (b) Smoljak grid with 145 nodes, where $q = 7, d = 2$. 

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Figure 4.3: Collocation points in three-dimensional random space for (a) tensor product grid with 35,937 nodes vs. (b) Smoljak grid with 441 nodes, where $q = 8, d = 3$. 
Figure 4.4: Collocation weights for each point in Smoljak grid. (a) For $d = 2, q = 7$ the negative values are depicted by dotted circles and the positive values are depicted by solid circles. (b) For $d = 3, q = 8$ the negative values are depicted by spheres and the positive values are depicted by ellipsoids. The minimum value is given by $r_{\text{min}}$, and the maximum value is given by $r_{\text{max}}$.
the $M \times N$-dimensional Smoljak grid to extract the statistical information. Algorithm 2 describes the generation of the stochastic macro-model, and Algorithm 3 describes the utilization of the stochastic macro-model inside an FDTD grid.

**Algorithm 2 Generation of the stochastic macro-model.**

1. Identify the system parameters which are expected to exhibit uncertainty and designate each parameter to an independent random variable $x_i, \forall i \in 1, 2, 3, \ldots$.

2. Choose an appropriate type and order of polynomial chaos basis for expansion of $x_i$, where the random variable $\xi_i$ in random space correspond to $x_i$ in physical space $\forall i \in 1, 2, 3, \ldots$ (e.g., (4.11)).

3. For each stochastic macro-model with $N$ random variables, generate a Smoljak sparse grid (i.e., an $N$-dimensional hypercube in random space), using instructions outlined in Section 4.10.2.

4. For each stochastic macro-model, use cubature of Section 4.10 to solve for the unknown coefficients of the expanded full-order random parameters everywhere on the $N$-dimensional Smoljak grid (e.g., (4.15) and (4.35)).

5. For each stochastic macro-model, construct the stochastic projection matrix $\tilde{V}$ (4.17), using (4.19) and (4.35). This step requires an MOR operation for each full order system on the Smoljak grid.

6. For each stochastic macro-model, determine the coefficients in the polynomial chaos expansion of the reduced order system (4.20), (4.21).

If needed, the interior fields inside each stochastic macro-model may be found simply by application of reverse projection on the reduced order field quantities, as discussed in step 4 of Algorithm 1.
Algorithm 3 Utilization of the stochastic macro-model.

1. Assume there are $M$ stochastic macro-models, each with $N$ random variables. Place each stochastic macro-model at a fixed location inside the FDTD grid.

2. Perform stochastic simulations over an $(M \times N)$-dimensional Smoljak grid. Use the interpolation mechanism, available through the polynomial chaos expansion of random variables found from Algorithm 2, to conveniently determine values for the random variables at any desired point within the $(M \times N)$-dimensional random space.

3. For each node on the $(M \times N)$-dimensional Smoljak grid, compute the stochastic fields everywhere (on boundary of the macro-models and the exterior region in the main FDTD grid).

4. In simultaneity with step 3 above, compute the coefficients of the polynomial chaos expansion for the stochastic field quantities (4.25) at each FDTD time-update as discussed in Section 4.9, by using cubature (4.35) to compute (4.22).

5. Use (4.23) and (4.24) to determine the statistical parameters of mean, variance, etc. at each time-update, for the stochastic field quantities.
5.1 Discussion

In this section, we present a series of numerical studies to illustrate the above ideas. In all the examples, we compare the stochastic collocation (SC) results against the base-line results provided by the standard Monte Carlo (MC) simulations. Since the standard Monte Carlo simulation converges as $1/\sqrt{K}$, we choose $K = 10,000$ sample points in random space, for each independent variable, to obtain a solution accuracy of within 1%, which is sufficient for illustrative purposes. The stochastic macro-models are generated using the MOR algorithm of ENOR with the expansion frequency $s_0 = f_{\text{max}}/2$, relative tolerance $tol_{\text{rel}} = 10^{-3}$, and maximum iteration $k_{\text{iter}} = 3$. The numerical examples are carried out with plane-wave excitation implemented with the TF/SF method described previously.

To perform the simulations in these numerical studies, we utilize the parallel computing resources of the Computational Science and Engineering program of the University of Illinois at Urbana-Champaign. Each stochastic FDTD simulation on the Smoljak grid, as well as on the Monte Carlo grid, is executed in parallel on the computing system, thereby significantly reducing the total execution time for performing these numerical experiments.

For the SC simulations, one stochastic macro-model with two random variables is generated per Algorithm 2. For each node on the Smoljak grid, we use numerical integration to obtain the coefficients of polynomial chaos expansion and perform MOR to obtain the stochastic projection matrix, and thus the stochastic reduced order system; this step is done prior to performing time-domain simulations and the model is stored for re-use as necessary. Then, simulations are performed using the stochastic macro-model and as the simulations run, the orthogonality of polynomial chaos is used to extract...
the expectation (mean) and variance of the stochastic field quantities at each time-step (or at each frequency after performing discrete Fourier transform (DFT) operation on time-domain data) through cubature on the Smoljak grid, as discussed in Algorithm 3.

Designate $M_{sc}$ to be the number of nodes on the Smoljak grid. The cost associated with the SC method is $C_{sc} = C_{gen_{sc}} + C_{sim_{sc}}$. The one-time cost of generating the stochastic macro-model is $C_{gen} = M_{sc} \times t_{gen}$, where $t_{gen}$ is comprised of cubature and MOR operations required to generate the reduced order model at each Smoljak node, and it is dominated by cost of MOR. The cost of simulation is $C_{sim_{sc}} = M_{sc} \times t_{sim}$, where $t_{sim}$ is the time required for simulation of an instance of the stochastic macro-model at one node of the Smoljak grid. Both $C_{gen_{sc}}$ and $C_{sim_{sc}}$ may be mitigated using parallel computing.

For the MC simulations, a macro-model is generated for each node in the Monte Carlo grid, where each node represents one combination of the random variable values mapped from physical space to normalized random space based on a truncated Gaussian distribution. For each node on the Monte Carlo grid, the MOR operation is performed once to obtain the corresponding reduced order system; this step is done prior to performing time-domain simulations and the model is stored for re-use as necessary. Then, simulations are performed using the reduced order system at each MC grid node. The results of simulations on each node, at each time-step (or at each frequency, after performing DFT operation on time-domain data), are submitted to statistical analysis to obtain the expectation (mean) and the variance of the response.

Designate $M_{mc}$ as the number of nodes in the MC grid. The cost associated with the MC method is $C_{mc} = C_{gen_{mc}} + C_{sim_{mc}}$. The cost of generating deterministic macro-models for the MC grid is $C_{gen_{mc}} = M_{mc} \times t_{gen}$, where $t_{gen}$ is dominated by the MOR time required to generate a reduced order model at one MC grid node. The cost of simulation is $C_{sim_{mc}} = M_{mc} \times t_{sim}$, where $t_{sim}$ is the time required for simulation at one node of the MC grid. Both $C_{gen_{mc}}$ and $C_{sim_{mc}}$ may be mitigated through parallel computing.

In the numerical examples of Section 5.3-5.5, for the stochastic collocation simulations, the stochastic macro-model is placed at a fixed location in the 2D/3D FDTD grid and the random movement of the cylinder (based on the Gaussian PDF) is modeled through the stochastic macro-model. For the
Monte Carlo simulations, the cylinder is fixed at the center of a deterministic macro-model (i.e., one instance of the stochastic macro-model where the random variables are at their mean value) and the deterministic macro-model itself is moved in the 2D/3D FDTD grid based on the Gaussian PDF. The stochastic field data from a single stochastic macro-model in the stochastic collocation simulations is then correlated against stochastic field data from multiple deterministic macro-models in the Monte Carlo simulations.

Other investigators have reported that under sufficiently smooth conditions in random space, the convergence rate of the SC solution may be almost exponential [81]; this significantly reduces the requirement on $M_{sc}$ compared to $M_{mc}$. In our examples, using Gaussian PDF to represent the uncertainty of the random variables, we find that indeed a relatively small number of sample points is sufficient for the SC solution to converge to the MC solution, for the mean of response. In all examples that follow, for random space of dimension $d = 2$, a Smoljak level $k = 5$ is used to generate the macro-models. The Smoljak level $k = 5, 6, 7$ (corresponding to 145, 321, 705 nodes, respectively) is sufficient to have the mean of response in the SC FDTD solution converge to the MC solution; however, for higher order moments (e.g., variance of the response) typically a more dense sampling of the Smoljak grid is required (e.g., Smoljak level $k = 8 - 9$, corresponding to 1537-3329 nodes). For random variables with relatively small variance (e.g., $\sigma^2 \leq 1$), the convergence rate of SC solution to the standard MC solution is indeed very fast; as demonstrated in Section 5.2 for random space of dimension $d = 2$, a Smoljak level $k = 5$ suffices to have the SC solution converge to the MC solution. However, as the physics of the problem (i.e., governing differential equations, and initial/boundary values) become more complex, the level of the Smoljak grid needs to be increased in accordance with complexity of the fields and in proportion to the degrees of freedom required to express their variations with sufficient accuracy; for example, in Section 5.3-5.4 it was necessary to increase the Smoljak level to $k = 9$ to have the variance of response for SC solution converge to the MC solution.

Although the higher order polynomial chaos is useful in capturing the impact of complex interactions of multiple random variables on the system response, increasing the polynomial order should be accompanied with a commensurate increase in the level of the Smoljak grid (i.e., more accurate cubature); otherwise, using higher order polynomials can lead to amplifica-
tion of errors and is ultimately harmful to the solution accuracy. In the numerical examples that follow, we use 1st order polynomial chaos to expand random variables.

While numerical integration based on the Clenshaw-Curtis rule is highly optimized to achieve accurate results for the mean of the response, it does not seem to be as well optimized for capturing higher order moments such as the variance of the response, as observed in the numerical experiments of Section 5.3-5.5. As one might expect, this mean-optimal behavior is related to the choice of node coordinates and weights for the Clenshaw-Curtis rule; that is, the heaviest weights are concentrated around the mean of the input random variables, as shown in Figure 4.4. The search for a variance-optimal choice of node coordinates and weights may be a topic of interest for further research.

In the numerical examples that follow, the perfectly matched layer (PML) is used as the absorbing boundary condition. The number of PML cells on each side is 20 cells, with a grading polynomial of order 3.0; details of this may be found in [10].

5.2 Numerical Example I

For the first numerical example, consider the aperture antenna depicted in Figure 5.1, through which we motivated the beginning of this chapter by allowing uncertainty in its structure. Let \( V_1 \) designate a certain portion of the fine-featured aperture region represented by a stochastic macro-model at the center of the grid, labeled as \( MM \). The macro-model is of dimension 9 x 9 grid cells, and it is placed at the center of the FDTD grid of size 200 x 200 cells, terminated at PML boundaries.

Assume that \( V_1 \) exhibits uncertainty in its relative permittivity according to the Gaussian (normal) probability density function

\[
\rho[x] = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}
\]  

(5.1)

where the mean is \( \mu \), and the standard deviation is \( \sigma \).

The random variable for relative permittivity has a mean \( \mu_p = 100 \) and exhibits a standard deviation according to the relation \( \pm 3\sigma_p = \pm \%10\mu_p \). We
ensure the FDTD grid resolution inside $V_1$ is fine enough to accurately resolve the fields. We plot the PDF of the random variable for relative permittivity as shown in Figure 5.2.

We run minimum-nominal-maximum relative permittivity FDTD simulations using the macro-model at three nodes: nominal, $\mu_{p_{\text{nom}}} = \mu_p$; minimum, $\mu_{p_{\text{min}}} = \mu_p - 3\sigma_p$; and maximum, $\mu_{p_{\text{max}}} = \mu_p + 3\sigma_p$. We compute the expected value (mean) and the standard deviation of the electric field (response). The results are shown in Figure 5.3 for 4000 time-steps where the temporal discretization $\Delta t \approx 2.78$ ps.

Next, let us designate $V_2$ as another portion of the fine-featured aperture region represented by the macro-model. Let us assume $V_2$ exhibits uncertainty in its conductivity according to the Gaussian PDF (5.1), while $V_1$ is held fixed at its nominal value. The conductivity has a mean $\mu_c = 10$ and a standard deviation $\sigma_c$ according to the relation $\pm 3\sigma_c = \pm 30\% \mu_c$. We plot the PDF of the random variable for conductivity as shown in Figure 5.4.

We run minimum-nominal-maximum conductivity FDTD simulations using the stochastic macro-model at three nodes: nominal, $\mu_{c_{\text{nom}}} = \mu_c$; mini-
Figure 5.2: (a) Probability density function $\rho$ for relative permittivity, in physical space. (b) Mapping (bounded support) of physical space to random space. (c) Probability density function $\rho$ for relative permittivity, in random space.
Figure 5.3: Electric field $E_z$ vs. time-step $\tau$, for minimum, nominal, and maximum relative permittivity variations inside macro-model. The mean at each time-point is depicted by a dot, and the standard deviation at each point is depicted by a vertical line.
Figure 5.4: (a) Probability density function $\rho$ for conductivity, in physical space. (b) Mapping (bounded support) of physical space to random space. (c) Probability density function $\rho$ for conductivity, in random space.
minimum, $\mu_{c_{\text{min}}} = \mu_c - 3\sigma_c$; and maximum, $\mu_{c_{\text{max}}} = \mu_c + 3\sigma_c$. The results are shown in Figure 5.5.

![Figure 5.5: Electric field $E_z$ vs. time-step $\tau$, for minimum, nominal, and maximum conductivity variations inside macro-model. The mean is depicted by a dot, and the standard deviation is depicted by a vertical line.](image)

Next, assuming both $V_1$ and $V_2$ exhibit uncertainty, we proceed to Monte Carlo simulations. For this, we run the standard Monte Carlo simulations using the pseudo-random distributions shown in Figure 5.6. The Monte Carlo simulation results are shown in Figure 5.7.

Again, assuming both $V_1$ and $V_2$ exhibit uncertainty, we proceed to stochastic collocation simulations. For this, we use Smoljak grid with level $k = 5$ containing 145 nodes, corresponding to Smoljak parameters $d = 2, q = 7$, shown in Figure 4.2. The stochastic collocation simulation results are shown in Figure 5.8. The exponential rate of convergence of the stochastic collocation method together with interpolation in random space makes it possible to obtain the stochastic response using a smaller number of sample points.
Figure 5.6: Histogram of pseudo-random numbers used in Monte Carlo simulations for (a) relative permittivity in $\mathbb{V}_1$, and (b) conductivity in $\mathbb{V}_2$. The overlapping black line shows the desired PDF.
Figure 5.7: Electric field $E_z$ vs. time-step $\tau$, from Monte Carlo simulations of relative permittivity and conductivity variations inside macro-model. The mean at each time-point is depicted by a dot, and the standard deviation at each point is depicted by a vertical line.
Figure 5.8: Electric field $E_z$ vs. time-step $\tau$, from stochastic collocation simulations of relative permittivity and conductivity variations in stochastic macro-model. The mean at each time-point is depicted by a dot, and the standard deviation at each point is depicted by a vertical line.
The detailed comparison of the electric field as a function of time-step, at a point inside the stochastic macro-model, computed through the stochastic collocation (SC) method vs. the Monte Carlo (MC) method, is shown in Figure 5.9.

The detailed comparison of the electric field as a function of time-step, at a point outside the stochastic macro-model, is shown in Figure 5.10.

As can be seen, the mean response from SC is an almost perfect match to the MC results, while the SC method requires a smaller set of simulations. The SC method improves in accuracy with increased accuracy of cubature; one way to accomplish this is to use higher level \( k = q - d \) for the Smoljak grid. Clearly, the smaller margins computed through the SC method are a marked improvement compared to margins computed through the corner (min-nom-max) simulations shown in Figures 5.3 and 5.5. It is clear that the match between the mean response in MC vs. SC is almost perfect, while the standard deviation is not always matched for all frequencies; this pattern is visible in all the proceeding numerical examples.

5.3 Numerical Example II

In this experiment, we compute the electromagnetic field scattering of an electromagnetic band-gap structure (EMBGS) [105–107]. Essentially, the EMBGS is a periodic structure which can be designed to trap certain electromagnetic modes, thereby allowing synthesis of material for various interesting and useful applications such as lasers [108], nano-tube based infrared sensors [109], waveguides [110–112], resonators, etc. For our 2D FDTD experiment, we assume invariance along the z-axis (i.e., \( \frac{\partial}{\partial z} = 0 \)), such that the EMBGS is comprised of infinitely long cylinders of radius \( r \) and separation \( a \), as shown in Figure 5.11. We design the EMBGS with ratio \( \frac{2r}{a} \approx \frac{38}{100} \) and set the relative permittivity of rods to that of alumina with \( \varepsilon_r = 8.9 \) [105].

We use a rectangular grid of dimension 5 × 5 rods and introduce a point defect into the perfect EMBGS by removing its center rod; this produces an EMBGS composed of a total of 24 rods. The EMBGS is placed inside the FDTD grid for simulation, such as shown in Figure 5.12.

Now, let us assume that one of the dielectric rods, specifically the cylinder labeled as MM in Figure 5.12 exhibits random variations in its position in
Figure 5.9: Comparison of Monte Carlo (MC) shown with circle or solid line vs. stochastic collocation (SC) shown with cross or dashed line, for a point inside the stochastic macro-model. (a) Mean, (b) standard deviation.
Figure 5.10: Comparison of Monte Carlo (MC) shown with circle or solid line vs. stochastic collocation (SC) shown with cross or dashed line, for a point outside the macro-model. Results of uncertainty in relative permittivity and conductivity. (a) Mean, (b) standard deviation.
Figure 5.11: Diagram of alumina rods in the EMBGS.

Figure 5.12: An example diagram of an EMBGS with center defect, where the center cylinder has been removed to produce a cavity resonator.
the $x - y$ plane. The simulations are run with a maximum grid frequency $f_{\text{max}} = 3.0 \text{ GHz}$, and a $-3 \text{ dB}$ source frequency $f_s = 1.0 \text{ GHz}$. We define the $-3 \text{ dB}$ source wavelength $\lambda_s = c/f_s$, where $c$ is the phase velocity of the wave. The computational domain is of size $3\lambda_s \times 3\lambda_s \times 3\lambda_s$, and all sides are terminated by PML. The radius of each dielectric rod $r \approx \frac{1}{16}\lambda_s$. The $x - y$ center position of the dielectric cylinder under uncertainty is assumed to follow a Gaussian distribution with mean $\mu_{\text{dis}} = 0$ and variance $\pm 3\sigma_{\text{dis}} = \pm \frac{1}{16}\lambda_s$. It is important to ensure that there is no overlap between the boundaries of adjacent macro-models; otherwise, macro-model fields will be overwritten and result in erroneous response. The displacement variation is assumed to be in the $x - y$ plane; thus, we have two random variables inside one stochastic macro-model. We would like to quantify the impact of such random variations on the resonant frequency $f_{\text{res}}$, and the quality factor $Q_f$.

For the SC simulations, we use $1^{st}$ order polynomial chaos as the expansion basis for variables in random space with dimension $d = 2$ and a Smoljak level $k = 9$ (i.e., 3329 nodes in Smoljak grid). We generate a single stochastic macro-model based on varying the position of the cylinder inside the macro-model according to the Smoljak grid distributions, then place the stochastic macro-model at a fixed position within the FDTD grid. We use MC simulations as the base-line solution for correlation of the SC solution. Given that the cylinders are variable only in position, and otherwise remain constant in material and geometry, for the MC simulations we generate only a single instance of the stochastic macro-model by placing the cylinder at the center of the macro-model region, then varying the position of the macro-model within the 2D FDTD grid according the the MC distributions.

The fields are then computed everywhere and we record the electric field $E_z$ at the center $\{i_c, j_c\}$ of the EMBGS where the resonant cavity is formed by the point defect. By applying DFT to the time-domain data we observe the resonance, as shown in Figure 5.13.

The peak of magnitude response is identified as the resonant frequency $f_{\text{res}}$, and the resonator’s quality factor $Q_f = \frac{f_{\text{res}}}{f_2 - f_1}$, where $f_1, f_2$ are the frequency values at $-3 \text{ dB}$ down from $f_{\text{res}}$. The values of $f_{\text{res}}$ and $Q$ for MC vs. SC are provided in Table 5.1. We observe excellent agreement between MC and SC results, while the MC method seems to provide the bounds of the standard deviation.
Figure 5.13: Monte Carlo vs. stochastic collocation, with one rod exhibiting uncertainty in its $x-y$ position. (a) Mean, (b) Standard deviation.
Table 5.1: Mean and standard deviation for resonant frequency $f_{res}$, and $Q_f$; Monte Carlo (MC) vs. stochastic collocation (SC), for two random variables.

<table>
<thead>
<tr>
<th></th>
<th>SC</th>
<th></th>
<th>MC</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean $f_{res}$ (GHz)</td>
<td>Standard deviation</td>
<td>Mean $f_{res}$ (GHz)</td>
<td>Standard deviation</td>
</tr>
<tr>
<td></td>
<td>1.11546</td>
<td>0.000501996</td>
<td>1.11534</td>
<td>0.000640625</td>
</tr>
<tr>
<td>$Q_f$</td>
<td>30.7226</td>
<td>2.42436</td>
<td>30.9179</td>
<td>2.57406</td>
</tr>
</tbody>
</table>

It is conceivable that an adaptive method based on optimization theory, which interactively evaluates the sensitivity of nodes on a sparse grid over random space, as the stochastic FDTD simulations are running, would further decrease the computational cost by eliminating the least significant nodes; investigation of such an adaptive method may be a topic for future research.

5.4 Numerical Example III

For the third numerical example, we utilize a 3D FDTD grid and simulate a EMBGS comprised of cylindrical dielectric scatterers, as shown in Figure 5.14. We design the EMBGS with ratio $\frac{2r_a}{a} \approx \frac{38}{100}$ and set the relative permittivity of rods to that of alumina with $\epsilon_r = 8.9$ [105]. The 3D structure is comprised of $5 \times 5$ dielectrics rods with their finite height parallel to the $z$-axis.

Each cylinder is represented by a 3D macro-model (see Appendix D). The simulations are run with a maximum grid frequency $f_{max} = 3.0$ GHz, and a $-3$ dB source frequency $f_s = 1.0$ GHz. We define the $-3$ dB source wavelength $\lambda_s = c/f_s$, where $c$ is the phase velocity of the wave. We induce a defect by removing the center rod; this produces an EMBGS composed of a total of 24 rods. The radius of each dielectric rod $r \approx \frac{1}{52} \lambda_s$. In addition, each dielectric cylinder now has a finite height of $\frac{1}{5} \lambda_s$. We place PMC boundaries on the top and bottom of the cylinders to mimic extension to infinity. The computational domain is of size $2\lambda_s \times 2\lambda_s \times 2\lambda_s$, and all sides are terminated by PML.

Let us assume that one of the dielectric rods, specifically the cylinder labeled as MM in Figure 5.14, exhibits random variations in its position in the $x-y$ plane. The $x-y$ center position of the dielectric cylinder under
uncertainty is assumed to follow a Gaussian distribution with mean $\mu_{\text{dis}} = 0$ and variance $\pm 3\sigma_{\text{dis}} = \pm \frac{1}{32}\lambda_s$. It is important to ensure that there is no overlap between the boundaries of adjacent macro-models; otherwise, macro-model fields will be overwritten and result in erroneous response. The 3D displacement variation is assumed to be only the $x - y$ plane; thus, we have two random variables inside a single stochastic macro-model. The electric field $E_z$ is recorded at the center of the EMBGS where the center cylinder has been removed to produce a cavity resonator.

For the SC simulations, we use 1st order polynomial chaos as the expansion basis for variables in random space with dimension $d = 2$ and a Smoljak level $k = 9$ (i.e., 3329 nodes in Smoljak grid). We generate a stochastic macro-model based on varying the position of the cylinder inside that macro-model according to the Smoljak grid distributions, then place the stochastic macro-model at a fixed position within the 3D FDTD grid. We use MC simulations as the base-line solution for correlation of the SC solution. Given that the cylinders are variable only in position, and otherwise remain constant in material and geometry, for the MC simulations we generate only a single
instance of the stochastic macro-model by placing a cylinder at the center of
the macro-model region, and varying its position within the 3D FDTD grid
according the the MC distributions.

The fields are then computed everywhere and we record the electric field
$E_z$ at center $\{i_c, j_c, k_c\}$ of the EMBGS where the resonant cavity is formed.
By applying DFT to the time-domain data we observe the resonance. The
results of SC vs. MC simulations for this numerical experiment are shown in
Figure 5.15 and Table 5.2.

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<td>2.03916</td>
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<td>0.00114263</td>
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<tr>
<td>$Q_f$</td>
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<td>56.0204</td>
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<tr>
<td>Standard deviation</td>
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It is evident that there is strong correlation between the MC and SC data.
The values of $f_{res}$ and $Q_f$ for MC vs. SC are provided in Table 5.2. We
observe that for all cases, the MC and SC results for the mean of response
are very well matched, while the standard deviation for MC seems to provide
the bounds of the standard deviation. This perfect match in the mean of
response is most likely due to the mean-optimal nature of the SC method, due
to the choice of node coordinates and weights in Clenshaw-Curtis cubature
rule.

5.5 Numerical Example IV

For the fourth and final numerical example, we simulate a 3D rectangular air-
filled waveguide with dielectric posts placed inside the waveguide, as shown
in Figure 5.16. The dimensions of the waveguide are $a = 75 \text{ mm}$, $b = 45$
mm. The computational domain is of size 75 mm $\times 615$ mm $\times 45$ mm, where
the ends of the waveguide are terminated by PML to mimic an infinitely long
waveguide.

First, we excite the empty waveguide with a short Gaussian pulse and
compute the wave impedance inside the waveguide for the $TE$ mode and
compare against the analytic expression of the wave impedance [58], as shown
Figure 5.15: Comparison of Monte Carlo (MC) shown with circle or solid line vs. stochastic collocation (SC) shown with cross or dashed line. Results of uncertainty in position of a cylindrical dielectric scatterer: (a) Mean, (b) standard deviation.
Figure 5.16: Diagram of the 3D waveguide, with array of dielectric posts placed inside.
in Figure 5.17. As can be observed, there is very good agreement between the FDTD computed result and the analytic solution.

![Figure 5.17: Real and imaginary part of the wave impedance in the rectangular waveguide, for the TE propagation mode. FDTD vs. Analytic.](image)

Let us place a single dielectric post inside the waveguide. The radius of the dielectric cylinder is $r \approx 5$ mm, its height is equal to the height of the waveguide $b$, and the relative permittivity of the dielectric cylinder is $\epsilon_r = 4.0$. Both open ends of the waveguide are terminated with matched loads by placing PML boundaries at either end. A Gaussian electric source modulated with a sine wave of frequency $f_s$ centered in the band-with spanning the frequencies of the dominant $TE_{10}$ mode is used to excite the waveguide, with negligible energy outside the cut-off limits of the $TE_{10}$ mode. The reflection coefficient $R$ is recorded at one source wavelength $\lambda_s = c/f_s$ along the $x$-axis down from the dielectric post, to ensure that only the $TE_{10}$ mode survives as the various scattered modes from the dielectric cylinders propagate back to the record point. The reflection coefficient is also computed using the approximate solution in [113]. The magnitude and phase of $R$ for 3D FDTD vs. approximate solution are plotted in the frequency range where the approximate solution holds valid, and shown in Figure 5.18.

Next, we place a $3 \times 3$ array of dielectric posts inside the waveguide as shown in Figure 5.16, where the center-to-center distance between posts in each row is $20$ mm, and the center-to-center distance between posts in each
Figure 5.18: Single post. Reflection coefficient $R$ for the $TE_{10}$ mode. (a) 
Magnitude and (b) phase.
column is 50 mm. The 3D FDTD solution of the response for this structure is shown in Figure 5.19.

Figure 5.19: The $3 \times 3$ array of posts. Reflection coefficient $R$ for the $TE_{10}$ mode.

We assume that the $x - y$ position of the center dielectric post exhibits uncertainty; thus, there are two independent random variables. The random variables of center position along $x$ and $y$ each experience uncertainty according to a Gaussian PDF with mean $\mu_{\text{dis}} = 0$ and variance $\pm 3\sigma_{\text{dis}} = \pm 5$ mm. We quantify the impact of this uncertainty on reflection coefficient $R$, using a stochastic macro-model with two random variables. The results are shown in Figure 5.20. We observe that the $Q_f$ and $f_{\text{res}}$ of the filter change as a function of the uncertainty in position of the post.

We note the rather large discrepancy between SC and MC for the variance of response. We use a $5^{th}$ order polynomial chaos, and observe an improvement in the variance of response near resonance, and degradation in variance of response away from resonance, as shown in Figure 5.21. We note that the mismatch in variance of response may be related to the choice of node coordinates and weights in the Clenshaw-Curtis integration rule, where the weights seem to be concentrated most heavily near the mean of the input random variables, as shown in Figure 4.4. The choice of node coordinates and weights that provide optimal convergence for the variance of response may be a topic for future research.
Figure 5.20: Monte Carlo vs. stochastic collocation of reflection coefficient for (a) frequency range 2.0 – 2.8 GHz, (b) zoomed-in near resonance.
Figure 5.21: Monte Carlo vs. stochastic collocation of reflection coefficient for (a) frequency range 2.0 – 2.8 GHz, (b) zoomed-in near resonance.
CHAPTER 6
CONCLUSION

In the current state of the art, and in absence of the stochastic macro-model, it is necessary to perform repeated discretization of the large deterministic domain for every random variation in the small fine-featured stochastic sub-domains. The development of the stochastic macro-model eliminates the need for repeated spatial discretization of the deterministic domain, for every random variation in its stochastic sub-domains. As such, only a single grid needs to be developed for the deterministic portion of the overall structure irrespective of the realization generated by a specific choice of the random parameters in the sub-domains exhibiting statistical variability; this results in significant computational savings!

The stochastic macro-model is developed by infusing the deterministic macro-model with the orthogonal polynomial chaos (PC), available through the machinery of homogeneous chaos, and the method of stochastic collocation (SC). By relying on the orthogonality property of PC, we expand the random variables and transform a deterministic electromagnetic system into a stochastic system which is an interpolated function of the random variables, thus providing a powerful and efficient way to compute the stochastic system parameters expediently at any desired point in random space.

The development of the stochastic macro-model begins with identification of the fine-featured region of the multi-scale structure which exhibits material/geometric uncertainty. We develop a full-order state-space realization of the discretized Maxwell’s equations for this region. The state-space representation provides a compact mathematical abstraction of the electromagnetic system which may be used to compute the electromagnetic fields of the structure.

The full-order system is expanded in the basis of the polynomial chaos, and by relying on the orthogonality property of PC, the unknown coefficients of this expansion are solved by cubature over random space in the sparse Smol-
The full-order parameters on each Smoljak node are also submitted to the model order reduction technique of ENOR, and a stochastic projection matrix \( \hat{V} \) is obtained, while ensuring system stability. The stochastic projection matrix \( \hat{V} \) is then expanded in basis of PC and once again the unknown coefficients are obtained through cubature over random space on the Smoljak grid. The expanded stochastic projection matrix \( \hat{V} \) is used with the expanded stochastic full-order parameters to obtain the approximate expanded stochastic reduced-order parameters through truncated polynomial projection.

The expanded stochastic reduced-order system is an interpolated function of the random variables which constitutes an extremely powerful and computationally efficient mechanism for computing the reduced-order stochastic system parameters at any point within the normalized truncated random space, and it is used in the stochastic collocation of FDTD solution over random space in a Smoljak grid of any desired resolution to obtain the solution of stochastic field quantities for the exterior region of the stochastic electromagnetic macro-models. A critical component of the stochastic macro-model is the highly accurate cubature over random space; for this, we rely on the method of stochastic collocation and the sparse Smoljak grid. In this work, we provide the algorithms for both the generation and utilization of the stochastic macro-model, as well as several numerical examples in 2D and 3D FDTD.

To enable the cost-effective and high-accuracy FDTD simulations involving design and manufacturing variations of multi-scale structure, the method of sub-gridding was utilized, with the stochastic macro-model implemented in the sub-gridded region. To enable the insertion of the high-fidelity stochastic macro-model inside the FDTD grid, a class of isotropic spatial filters was developed to suppress the spurious noise waves generated by the discrete wave-impedance mismatch at the boundary of the macro-model. To this end, we developed a class of spatial filter operators that: (a) are straightforward to design and implement within the existing Yee style FDTD explicit time-stepping scheme; (b) do not require complicated spatial/temporal interpolation in the field update equations; (c) are able to accommodate broadband electromagnetic sources; and (d) exhibit spatial isotropy in their suppression of the spurious numerical reflections while preserving the pertinent portions of the signal’s power spectral density. The isotropic spatial filter operator
was demonstrated through several examples in 2D and 3D FDTD.

A few of the key application areas for the stochastic electromagnetic macro-model are highlighted herein: (a) the development of robust computational electromagnetic field-solving software built with the intrinsic ability to model and simulate material, geometry, and electromagnetic sources, which exhibit uncertainty; (b) quantifying the impact of uncertainty on the response of circuits and systems, in the areas of microwaves, photonics, and nanostructures; and (c) various active/passive devices, such as lasers, sensors, waveguides, and antennas.

Several topics which may be of interest for further development are highlighted here. The stochastic macro-model developed in this work assumes the material properties contained within the macro-model are independent of frequency (i.e. non-dispersive); this was reflected by the assumption of frequency-independence in the system parameters $C, G, \Gamma$. The extension of the stochastic macro-model to the class of dispersive media may be the topic of future research.

The stochastic macro-model developed herein relies on an isotropic realization of the sparse grid, namely the Smoljak grid. It may be a topic of future research to consider the infusion of optimization techniques towards the development of an adaptive generation algorithm of the sparse grid, leading to an anisotropic sparse grid in random space which maximizes the number of nodes around those regions which exhibit slower convergence [73]. This could provide further computational efficiency in the cost of generation and utilization of the stochastic macro-model.

The stochastic macro-model developed herein utilizes the Clenshaw-Curtis rule of quadrature in one-dimensional space, for the realization of the numerical integration over multi-dimensional space. This cubature algorithm provides fast convergence for the mean of the response; however, the variance of response converges rather slowly. The choice of node coordinates and distribution of weights in the quadrature rule, which are most heavily concentrated about the mean of the input random variables, may contribute to this behavior. It may be a topic of future research to develop an alternative quadrature rule which is optimal for fast convergence of the variance of response.

Finally, the implementation of the stochastic macro-model in this work was based on central difference realization of the temporal discretization of system
equations, which is a conditionally stable explicit integration scheme based on the Courant stability criterion. The implementation of the stochastic macro-model based on an unconditionally stable temporal discretization (e.g. Newmark-\(\beta\)) may be a topic of future research.

In conclusion, we believe that the stochastic macro-model may be regarded as an important step towards addressing the challenges of computational electromagnetics for structures under uncertainty, by eliminating a major portion of computational cost, namely, the re-meshing of the deterministic domain for each random variation in the stochastic sub-domains.
APPENDIX A

A-PRIORI FILTER ORDER AND APPLICATION TIME INTERVAL

The spatial knee frequency for 1st through 5th order isotropic spatial filters are computed for $h/\lambda_{knee}$, where $|\Phi|_{h/\lambda_{knee}} = -3$ dB according to (2.43) and shown in Table A.1.

As the filter order increases, its spatial pass-band increases while at the same time its roll-off becomes steeper; this occurs while avoiding the well-known Gibbs phenomenon encountered in the traditional design procedure of FIR digital filters where it is resolved by multiplication of the frequency response with a smoothing function such as the Hamming or the Kaiser window.

Using this data together with the dispersion relation, and given the PSD of the source excitation, one can determine the appropriate filter order and application time interval to eliminate undesirable wavelengths, while preserving the signal of interest to within specification; for example, for applications involving digital signals, the specification is usually dictated by the receiver’s input voltage thresholds $V_{in}^{High}$ and $V_{in}^{Low}$ as well as sensitivity specifications.
Table A.1: $h/\lambda_{knee}$ vs. number of times filter is applied $p$, for 1st through 5th order spatial filters. (Source: Ata Zadehgol, Andreas C. Cangellaris, Isotropic Spatial Filters for Suppression of Spurious Noise Waves in Sub-Gridded FDTD Simulation. Copyright ©2011, IEEE Antennas Propagation Society. Reprinted by permission of IEEE.)

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APPENDIX B

3D 1ST ORDER SPATIAL FILTER OPERATION

The center of the cuboid (orange) shown in Figures B.1 and B.2 depicts the field $\phi$ in a 3D FDTD cell located at $\{i, j, k\}$ along the right-hand Cartesian unit vectors $\{\hat{x}, \hat{y}, \hat{z}\}$, where it is surrounded by its immediate neighbor (blue) cells. The space-shift operators are $\{z_i^{\pm \Delta x}, z_j^{\pm \Delta y}, z_k^{\pm \Delta z}\}$, where $\{z_i = e^{jk_i x}, z_j = e^{jk_j y}, z_k = e^{jk_k z}\}$ (with $j = \sqrt{-1}$) are the eigen-mode solutions of the Helmholtz wave equation. The space-shift operators act on the center (orange) cell to obtain the adjacent (blue) cell’s field value; these values are then used in the 1st order spatial filter operator to give a weighted spatial average, where the weighting is determined by the spatial convolution (Fourier) coefficients in (2.42). The coefficients are chosen to provide 2D circular or 3D spherical symmetry which yields the isotropic filter operators in 2D and 3D.

It is worth noting that increasing the filter order will decrease the signal’s spatial gradient, which helps to further reduce the energy of spurious reflections at the fine-coarse interface.
Figure B.1: The FDTD cells used in the weighted spatial averaging (time-convolution) in a 1st order spatial filter. Frames 1-8.
Figure B.2: The FDTD cells used in the weighted spatial averaging (time-convolution) in a 1\textsuperscript{st} order spatial filter. Frames 9-13.
C.1 Formulation for Full Order Model (ITF)

For the sake of completeness and to provide a means for comparison with the admittance transfer function, we provide the formulations for the impedance transfer function here.

In order to generate a macro-model for a portion of the FDTD grid, we start with the time-harmonic frequency phasor form of source-free Maxwell equations, where the time-harmonic term $e^{j\omega t}$ is suppressed.

\[ \nabla \times \mathbf{E} = -j\omega \mu \mathbf{H} \quad \text{(C.1)} \]

\[ \nabla \times \mathbf{H} = j\omega \epsilon \mathbf{E} + \sigma \mathbf{E} \quad \text{(C.2)} \]

where $j = \sqrt{-1}$, $\omega$ is the angular frequency, $\mathbf{E}$ is the electric field intensity vector, $\mathbf{H}$ is the magnetic field intensity vector, $\sigma$ is the material conductivity tensor, $\mu$ is the material permeability tensor, and $\epsilon$ is the material permittivity tensor.

For the macro-model implemented as an impedance transfer function (ITF), equations (C.1)-(C.2) can be written as a finite-difference based semi-discretized system in the Laplace (s-domain) in matrix form as follows:

\[ D_E \mathbf{e} + Q_\epsilon \mathbf{e}_b = -sP_\mu \mathbf{h} \quad \text{(C.3)} \]

\[ D_H \mathbf{h} = sP_\epsilon \mathbf{e} + P_\sigma \mathbf{e} \quad \text{(C.4)} \]

where the Laplace variable $s$ is the complex frequency $s = \alpha + j\omega$, $\alpha$ is the real part of frequency, $\omega$ is the imaginary part of frequency, $D_E$ is the
spatial Curl-$\mathbf{E}$ operator matrix, $D_H$ is the spatial Curl-$\mathbf{H}$ operator matrix, $\mathbf{e}$ is the electric field vector inside the macro-model, $\mathbf{e}_b$ is the electric field vector containing boundary conditions on the perimeter of the macro-model, $Q_e$ is the selector matrix for electric field at boundary, $\mathbf{h}$ is the magnetic field vector inside and on the perimeter of the macro-model, and the diagonal matrices $P_\epsilon, P_\mu,$ and $P_\sigma$ relate to material permittivity, permeability, and conductivity, respectively, as functions of position inside the macro-model.

With the above formulation, we have

$$D E = D_H^T$$

(C.5)

where the symbol $T$ denotes the matrix transpose operator.

And in state-space form it is

$$\begin{bmatrix} D_E & 0 \\ P_\sigma & -D_H \end{bmatrix} \begin{bmatrix} \mathbf{e} \\ \mathbf{h} \end{bmatrix} + \begin{bmatrix} Q_e \\ 0 \end{bmatrix} \mathbf{e}_b + s \begin{bmatrix} 0 & P_\mu \\ P_\epsilon & 0 \end{bmatrix} \begin{bmatrix} \mathbf{e} \\ \mathbf{h} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

(C.6)

The dimensions for each tensor are as follows:

- $\mathbf{e}$ : $N \times 1$
- $\mathbf{e}_b$ : $n \times 1$
- $Q_e$ : $M \times n$
- $\mathbf{h}$ : $M \times 1$
- $D_E$ : $M \times N$
- $D_H$ : $N \times M$
- $P_\epsilon$ : $N \times N$
- $P_\sigma$ : $N \times N$
- $P_\mu$ : $M \times M$

where $M, N, n$ are integers, determined by the size of the macro-model.

Solving (C.4) for $\mathbf{e}$, we obtain

$$\mathbf{e} = (s P_\epsilon + P_\sigma)^{-1} D_H \mathbf{h}$$

(C.7)

where $I$ is the identity matrix.

Substitution of (C.7) in (C.3) gives the relation

$$Z \mathbf{h} = -Q_e \mathbf{e}_b$$

(C.8)
where the impedance transfer function matrix $Z$ is

$$Z = D_E (sP_\epsilon + P_\sigma)^{-1} D_H + sP_\mu$$  \hspace{1cm} (C.9)

From (C.8) $h$ is simply obtained by

$$h = -Z^{-1} Q_e e_b$$  \hspace{1cm} (C.10)

For a lossless system, $P_\sigma = 0$, and (C.9) becomes

$$Z = \frac{1}{s} D_E P_\epsilon^{-1} D_H + sP_\mu$$  \hspace{1cm} (C.11)

The Laplace operator $s$ can be written in time domain as

$$s \leftrightarrow \frac{d}{dt}$$  \hspace{1cm} (C.12)

Similarly, the Laplace operator $s^2$ can be written in time domain as

$$s^2 \leftrightarrow \frac{d^2}{dt^2}$$  \hspace{1cm} (C.13)

We assume that the only time-dependent quantities are $h$ and $e_b$. Then, using (C.12),(C.13) we may transform (C.8) (with (C.11)) to its time-domain equivalent

$$D_E P_\epsilon^{-1} D_H h + P_\mu \frac{d}{dt^2} h = -Q_e \frac{d}{dt} e_b$$  \hspace{1cm} (C.14)

With a central-difference based time-derivative operator, operating on a generic function of time $f[t]$, we have

$$\frac{d}{dt} f[t] = \frac{f[t + \Delta t] - f[t - \Delta t]}{2\Delta t}$$  \hspace{1cm} (C.15)

$$\frac{d^2}{dt^2} f[t] = \frac{f[t + \Delta t] - 2f[t] + f[t - \Delta t]}{(\Delta t)^2}$$  \hspace{1cm} (C.16)

where $\Delta t$ is the temporal discretization.

Using (C.15),(C.16), we expand the time-derivatives in (C.14) to obtain the discrete time-domain relation

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\[ D_E P_{\epsilon}^{-1} D_H h[n + 1] - 2h[n] + h[n - 1] = \]
\[ -Q_e \frac{e_b[n + 1/2] - e_b[n - 1/2]}{\Delta t} \]
\[ (\Delta t)^2 \]  

(C.17)

where \( n \) is the discrete time variable

Solving for the magnetic field in the future time-step at \( n + 1 \), we obtain the following time-stepping formulation:

\[ h[n + 1] = 2h[n] - h[n - 1] - (\Delta t)^2 P_{\mu}^{-1} D_E P_{\epsilon}^{-1} D_H h[n] \]
\[ -\Delta t P_{\mu}^{-1} Q_e (e_b[n + 1/2] - e_b[n - 1/2]) \]  

(C.18)

It is important to note that \( D_E \) in the impedance transfer function matrix (C.9) is a non-square matrix; therefore, (C.9) does not easily lend itself to derivation of a time-stepping relation where lossy material is present. Thus, this fact motivates the development of the admittance transfer function (ATF) in Chapter 3.

This completes the derivation of the full-order impedance transfer function. Next, we discuss an appropriate model order reduction scheme, to be applied to the above full-order system.

C.2 Model Order Reduction (ITF)

Following the procedure outlined in [5], we define the matrix quantities \( C \in \mathbb{R}^{M \times M} \), \( B \in \mathbb{R}^{M \times n} \), \( J \in \mathbb{R}^{n \times n} \), \( X \in \mathbb{R}^{M \times n} \), and \( \Gamma \in \mathbb{R}^{M \times M} \), where \( M, n \) are integers, as follows:

\[ C = P_{\mu} \]  

(C.19)

\[ \Gamma = D_E P_{\epsilon}^{-1} D_H \]  

(C.20)

\[ B = -Q_e \]  

(C.21)
Using (C.19) - (C.20), we may re-write the impedance transfer function matrix (C.11) as

\[ Z = \left( Cs + \frac{1}{s} \Gamma \right) \]  

(C.22)

The total system in Laplace (s-domain) is given by

\[ \left( Cs + \frac{1}{s} \Gamma \right) X[s] = BJ[s] \]  

(C.23)

We set \( s = s_0(1 - z) \), where the complex variable \( z = \frac{-1}{s_0}(s - s_0) \). Also, we define the auxiliary variable

\[ Y[z] = \frac{X[z]}{1 - z} \]  

(C.24)

Next, we expand \( X[z], Y[z], J[z] \) in powers of \( z \) about the frequency \( s_0 \), substitute these expansions into (C.23) and (C.24), equate coefficients of the same powers of \( z \), and after some algebraic manipulations obtain the following recurrence relation:

\[ \left( Cs_0 + \frac{1}{s_0} \Gamma \right) X_k = Cs_0X_{k-1} - \frac{1}{s_0} \Gamma Y_{k-1} - Q_eJ_k \]  

(C.25)

where the desired number of iterations \( k \) is an integer and decided by choice of the relative tolerance \( tol_{rel} \), and

\[ Y_k = X_k + Y_{k-1} \]
\[ X_{-1} = Y_{-1} = 0 \]

The yet unknown \( X_k \) are proportional to the (block) moments of the magnetic field (i.e. system response) when expanded about the frequency \( s_0 \).

We set the \( e \)-field source (i.e. system excitation) as follows:

\[ J_k = \begin{cases} 
I^{n \times n} & \text{if } k = 0, \\
0 & \text{if } k \neq 0,
\end{cases} \]  

(C.26)

and solve (C.25) for as many \( k \)-terms as desired.

The choice of setting \( J_{(k=0)} = I^{n \times n} \), where \( I^{n \times n} \) is the \( n \times n \) identity matrix, is equivalent to having a discrete impulse (electric) source at each node in
and the resulting system response is that of an impulse response.

Once the solutions to $X_k$ are obtained, we form $V = [X_0, X_1, ..., X_q]$, where the projection matrix $V \in \mathbb{R}^{M \times m}$ is comprised of the first $q$ block moments, and the integer $m \ll M$ is the order of reduction.

Next, we apply the above MOR technique to project the full-order system to obtain a reduced order system.

### C.3 Formulation for Reduced Order Model (ITF)

In order to apply the MOR technique on the full-order system, we proceed as follows.

Using the projection matrix $V$, we obtain the following projected quantities:

$$C_p = V^T CV$$  \hspace{1cm} (C.27)

$$\Gamma_p = V^T \Gamma V$$  \hspace{1cm} (C.28)

$$Q_{ep} = V^T Q_e$$  \hspace{1cm} (C.29)

To obtain the reduced order impedance transfer function (about $s_0$), we simply replace $C$ by $C_p$ and replace $\Gamma$ by $\Gamma_p$ in (C.22), to obtain

$$Z_p = \left( C_p s + \frac{1}{s} \Gamma_p \right)$$  \hspace{1cm} (C.30)

Then, to obtain the reduced order $h$-field, we replace $Z$ with $Z_p$ and replace $Q_e$ with $Q_{ep}$ in (C.10) to obtain

$$h_p = -Z_p^{-1} Q_{ep} e_0$$  \hspace{1cm} (C.31)

Finally, the reduced order time-stepping formula is given by

$$h_p[n + 1] = 2h_p[n] - h_p[n - 1] - (\Delta t)^2 C_p^{-1} \Gamma_p h_p[n]$$

$$- \Delta t C_p^{-1} Q_{ep} (e_0[n + 1/2] - e_0[n - 1/2])$$  \hspace{1cm} (C.32)
Having obtained the time-stepping formulation, we modify the standard Yee time-stepping algorithm as shown in Algorithm 4.

**Algorithm 4** Modified Yee time-update algorithm (ITF).

1. Initialize the FDTD grid with boundary and initial conditions.
2. At time-step $n$, update the $H$-field in the coarse grid using the usual FDTD update scheme.
3. Update the magnetic field (response) $h_p$ using the electric field (excitation) $e_b$ and (C.32).
4. Obtain $h = V.h_p$, to be used in next update of $E$-field in the coarse-grid.
5. At time-step $n + 1/2$, update the $E$-field in the coarse grid, including $e_b$ on boundary of the macro-model.
6. Update the source, located in the coarse grid.
7. Iterate to $n + 1/2$ and goto 2.

C.4 Use of the (ITF) Macro Model Inside an FDTD Grid

The diagram in Figure C.1 shows the relative locations of electric and magnetic field vector components with respect to each other and the computational grid.

The fields are used in the time-stepping routine, as follows:

- The $e$-fields at disks and meshed disks are the macro-model input (excitation). These are the boundary electric field state variables $e_b$. The $e$-fields at disks and meshed disks are updated using $H$-fields at solid arrows, $h$-fields at double arrows, and $h$-fields at triple arrows.

- The $h$-fields at the triple arrows are the macro-model output (response) at the perimeter of macro-model immediately inside the electric field boundary layer. These are updated by the macro-model system matrix equations. The vector $h$ contains the state variables of $h$-field inside the macro-model and at the perimeter of the macro-model.
Figure C.1: Diagram of field arrangement for the macro-model implemented as an impedance transfer function.
• The $h$-fields at double arrows, as well as the $e$-field at the disks, are updated through finite difference instead of using interpolation. If finite-difference is chosen, the advantages are: (1) Better accuracy with finite difference vs. linear interpolation. (2) Ability to use 3:1 sub-gridding which minimizes spurious reflections at the fine-coarse interface [48]. The downside is that the macro-model now lies a few cells inside the sub-grid region; therefore, updating the sub-grid nodes outside of macro-model adds to computational cost.

• The dotted circles (inside the macro-model) are the place-holders for the $e$-field that are never updated, since they fall into the macro-model region. When MOR is applied, it reduces the degrees of freedom of the original model, as dictated by the dotted circles domain, to a desired level as specified by the relative tolerance $tol_{rel}$ and maximum iteration factor $k_{iter}$ during computation of the projection vector.
D.1 Formulation for 3D Macro-Model

Discretization of the Maxwell equations in three-dimensional space yields the 3D macro-model. We use the Yee algorithm with the convention of H-field on edge and E-field on center of each face as shown in Figure D.1, to provide the admittance transfer function for structures in 3D FDTD. From the discretized fields we obtain the state-space form discussed in Section 3.2, and time-stepping formulation derived in Section 3.5. An example 3D macro-model of cell size $2 \times 2 \times 2$ is shown in Figure D.1-d, where the number of elements in each state vector $h, h_b, e$ is provided.
Figure D.1: Diagram of the 3D macro-model depicting field components used in derivation of curl operator matrices. (a) Curl of $E_z$ operator. (b) Curl of $E_x$ operator. (c) Curl of $E_y$ operator. (d) An example 3D macro-model, where the number of elements in each state vector $h$, $h_b$, $e$ is provided.
REFERENCES


[31] A. Zadehgol and A. C. Cangellaris, “Isotropic spatial filters for suppression of spurious waves in finite difference time domain simulations with sub-gridding,” in IEEE International Symposium on Antennas


